Location and Causality in Quantum Theory

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Contents

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Abstract

An operational development of quantum theory is presented, from general correlations through single-particle theories to elementary quantum field theory, with a focus throughout on causal relations. The objective is to establish the extent to which quantum theories are consistent with the principle of relativistic causality (that no two events separated by a distance greater than their separation in time multiplied by the speed of light may have a causal influence on each other) and to examine the assumptions that this analysis requires. It is necessary to pay particular attention to the notions of spatial location and measurement.

It is found that in a relativistically causal theory, any measurement made in a finite spatial region must have the capacity for particle creation.

A number of derivations are presented, including some relativistic single-particle propagators and a Hamiltonian based on the square root of the Klein Gordon equation.

Declaration

No portion of the work referred to in this dissertation has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.

Copyright Statement

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1 Introduction

1.1 Causality

The notion that some phenomena arise in dependence upon others is basic to any attempt to understand the world we find ourselves in. The relationship between the dependent events ('effects') and the sets of events that they depend upon ('causes') is known as *causality*. The purpose of this work is to investigate this relationship in the context of quantum theory.

Perhaps the most striking quality of causality is that we intuitively associate its direction – from cause to effect – with the direction of *time*. Causes appear to precede effects. Quantum theory is not known for its respect of what we might intuitively think, but in this case we will find our intuitions to be correct. Before I introduce the content and scope of this work, let us take a moment to narrow down what we mean by cause and effect.

The philosophy of causal relations has deep roots and many subtleties [1, 2], but from the outset I wish to adopt a simplification that I suggest preserves the essential characteristics of causality without exposing us to crippling ambiguities. Consider the following causal relation: stepping outside in the rain causes you to get wet. Two characteristics contribute the majority of what is meaningful about this relation:

- the effect (getting wet) is something we could detect and respond to in some way, and
- the causes (stepping outside, rain) include some that are at least partly responsive to something we could do.[1]

Following this example, our simplification will be to focus only on **effects that can be responded to**, either by a device that can detect the event and is programmed to respond in a certain way or by a human being who can observe the effect and choose to act on what he or she finds, and to **causes that are responsive** to such a device or to something a human being could choose to do. There need be no limit on how quickly a response can take place.

[1] For example, if we chose to stay indoors, one of the causes would cease in response to our choice. We might object to the restriction that causes should be responsive to something we could do, as it is not hard to imagine causal relations that might interest us in which this does not apply: the events in the first fraction of a second of the universe are an extreme example. But if that interest stems from a curiosity regarding the fundamental laws of nature, and if that curiosity tends to manifest in terms of 'thought experiments', then even this example is not so distant from the conditions above.

With these restrictions, if an effect could *precede* its cause for the same subject (human or device), the causal relation becomes nonsensical. For example, if you were to get wet today in dependence on stepping outside in the rain tomorrow, then you could respond to getting wet by choosing to stay indoors tomorrow, which contradicts the cause. We need not rely on free will to make this argument: consider instead a robot programmed to respond by staying indoors if and only if it got wet on the previous day.[2] Even if the robot could only alter the *probability* with which it stayed indoors by a minuscule amount in response to an assessment of wetness on the previous day, the logical contradiction remains.[3] More generally, if the laws of nature allowed events to precede causes, a device could be programmed to signal backwards in time to itself if and only if it does not receive its own signal. Because this contradicts itself, it follows that there is a *simple law of causality*:

- **An effect cannot precede a cause for the same subject**.

It is worth noting that, in adopting these restrictions, we are implicitly defining an effect to be something that can be made to give rise to a lasting and discernible trace of its having happened. This caveat will have some bearing on how we might interpret anything that follows from these assumptions.

1.2 Relativistic causality

The laws of special relativity add an extra dimension or three to this situation, in that it can be proven (see the box in Section 6.1.3) that if a subject could send a signal to another subject faster than light, then it is also possible to pre-arrange a scenario by which it could signal backwards in time to itself. With this in mind, we should strengthen our law to the *law of relativistic causality*:[4]

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[2]We could propose a law that constrains free will and programmable devices, but it is unclear how such a law could co-exist with other physical laws without introducing 'conspiratorial' elements. In relation to a closely-related problem (time loops rather than causal loops): *"It seems there is a chronology protection agency, which prevents the appearance of closed timelike curves and so makes the universe safe for historians."* – S. Hawking [3].

[3]If the relative frequency that the robot stays indoors if it didn't get wet is p_1 and the relative frequency that it stays indoors if it did get wet is $p_2 \neq p_1$, then the relative frequency that it stays indoors at all ceases to have a value. We could respond by challenging our understanding of probability [4], for example by introducing laws that restrict the repeatability of experiments. That route won't be considered here.

[4]For an influential account of relativistic causality, see [5].

- **An effect cannot occur outside the future light cone[5] of any cause**.

One of the implications of this is that any immediate effect of a cause must be *local*. If it is possible for the conditions at a point $\mathbf{x_A}$ in space to act as a cause at a time t_A, then any future effect at time t is confined to a ball of radius $c(t-t_A)$ centred on $\mathbf{x_A}$. Causality is bound together not only with the direction of time, but with *spatial location* as well. To make sense of this, we will need to investigate how and to what extent an event can be considered to be spatially located at all.

1.3 The structure of this document

To explore causality in the context of quantum theory, we will retrace the logical development of the theory from its operational foundations through single-particle theory to field theory, with especially close attention being paid to the notions of **measurement** and **position** at each stage.

In **Section 2**, largely following a paper by Bub [6], we see how the Hilbert space formulation of quantum theory emerges from a much larger landscape of imaginable ways in which a world *could* provide information. A 'measurement' in this context is anything that can generate information and could influence other measurements. It is significant for our discussion because it encompasses any 'cause' or 'effect' that meets our requirements, at least in information-theoretic terms. No explicit reference is made to space or time. The most important development in this Section is the concept of **signalling** – the ability of one observer to infer from their own measurements information generated by another.

Having identified quantum theory in this context, three postulates are presented, in as simple a form as possible, to characterise it more generally. We could instead have sought quantum postulates that are suitable as a basis for a mathematically rigorous, even axiomatic theory (see for example [7, 8, 9]), but we will find that these three brief conceptual statements are sufficient to cover a remarkable amount of ground.

The first two postulates (which include the Born rule and the projection postulate) are presented in **Section 3**, along with some immediate consequences including their implications for signalling. In preparation for the

[5] Assuming that the cause takes place entirely within a region of spacetime $\mathcal{R}_A$, the future light cone of the cause is the set of spacetime points that can be reached from any point within $\mathcal{R}_A$ without exceeding the speed of light.

need to locate events in continuous space, in Section 3.4 we focus on how these postulates are applied to continuous information.

Time and space formally enter the picture in **Section 4**. The third quantum postulate (the time evolution postulate) is introduced here, and guarantees a correspondence between quantum theory and the Hamiltonian formulation of classical mechanics. This leads us to consider the **single-particle** system, not only for its simplicity but for the fact that it is the only system for which the set of generalised Hamiltonian coordinates represents a position in space.

We are then ready to consider signalling and causality in the context of space and time. In **Section 5** we establish the connection between the **propagator** and causality, and present ways in which propagators may be calculated. In **Section 6** this is developed further for *relativistic* single-particle theories.

A novel representation for the Hamiltonian of a relativistic single particle is presented in Section 6.2. Two other representations – the Feshbach–Villars Hamiltonian and the Dirac Hamiltonian – are also explored. We find that the notion of the position of a single particle in space is necessarily ambiguous and, if taken literally, gives rise to irreconcilable causality violations. By pushing onwards with the single-particle theory in spite of these problems, we find we can shed a little light onto some of the properties that a more successful theory should have.

These difficulties are resolved in **Section 7** by applying our three postulates to a covariant field theory instead of a single particle. We see that measurements corresponding to locations in spacetime can be defined for a quantum field, and that two such measurements can never be used to signal faster than light. The emergence of particles in this theory is described, and we find that *any measurement capable of locating a single particle in a finite region of space must also have the capacity for particle creation.*

In Section 7.5, the spectre of causality violation re-emerges for cases involving more than two measurements; we conclude by considering whether this should be taken to imply that the limits of the Hilbert space formulation have finally been found.

2 Correlations

2.1 Operational descriptions

Any piece of observational science can be described in the following way: on a number of occasions, a number of observers each make one of a number of possible measurements and each obtain one of a number of feasible results, and the results are analysed mathematically. This bare-bones approach to science is known as operationalism [10].

Consider a situation in which a system S receives a disturbance D and a measurement M is subsequently taken in order to determine the effect of D on S. In an operational description *each* of S, D and M must represent a set of measurement choices *and* measured outcomes. By S we mean the measurements we select and the outcomes of those measurements that we believe are sufficient to identify the system; D is what we do and see in order to specify what kind of disturbance was carried out; M is to identify some potential effect.

The most basic condition necessary before any kind of dynamics or other causal process can be proposed is for M to be correlated in some way with D and S when sets of observations are taken.

If the correlations are perfect, the process is *deterministic*. If we trust our measuring devices to be perfectly reliable, it would be natural to wish to interpret this in terms of deterministic *dynamics*, in the sense of a physical law or mechanism for its evolution. If, in contrast, the results are entirely uncorrelated – *i.e.* if M is statistically independent of D and S – then there can be no predictability, and no evidence of any dynamics at all.

Anything between these extremes is a *stochastic process*, and we may wish to explain it using some stochastic dynamical theory and/or a stochastic model of measurements. The aim of a model is to supply a consistent set of physical reasons as to why the *probabilities* of a particular set of measured outcomes for M are affected by the choices and outcomes in D and S.

2.2 Restrictions on non-local correlations in a classical theory

In any theory based on classical mechanics, the types of correlations between any measurements at different places are restricted. These restrictions follow from what once might have seemed self-evident assumptions about the nature of reality – now known as the principle of local realism:

1. The results of measurements performed on an individual object at a given

place are (at least stochastically) determined by real properties of the object, the nature of the measuring process and other causal influences at that place;

2. Actions at one place cannot *immediately* influence what is measurable at a different place. More specifically, causal influences must be limited by the speed of light.[6]

These assumptions may be used to derive a number of conditions that must be satisfied by the correlations between measurable quantities in any theory that accords with local realism. These conditions are collectively known as 'Bell inequalities' after the first such derivation by John Bell [11], and they enable the assumptions of local realism to be directly tested by experiment.

An important example is the Clauser Horne Shimony Holt (CHSH) inequality [12]. Consider an experiment consisting of two observers, Alice and Bob, who are *spacelike separated*: that is, **their experiments take place within well-defined regions of space and over well-defined periods of time, separated by sufficient distance that no signal propagating at the speed of light could carry information from one to the other while they are taking place.** Each makes one choice, A and B respectively, from a set of two possible choices of measurement $A \in \{A_1, A_2\}$ and $B \in \{B_1, B_2\}$ and each then obtains one of two possible measured outcomes $a \in \{+1, -1\}$ and $b \in \{+1, -1\}$.

The CHSH inequality[7] can be stated as follows [13]: local realism requires

$$| \langle ab \rangle_{A_1 B_1} - \langle ab \rangle_{A_1 B_2} | + | \langle ab \rangle_{A_2 B_1} + \langle ab \rangle_{A_2 B_2} | \leq 2, \tag{2.1}$$

[6]The significance of the speed of light for causality is outlined in Section 6.1.3.

[7]Proof of the CHSH inequality: given any complete set $(\boldsymbol{\lambda}_A, \boldsymbol{\lambda}_B)$ of properties or random variables pertaining to the measurement of each object, $\langle ab \rangle_{A_i B_j \boldsymbol{\lambda}_A \boldsymbol{\lambda}_B}$ is simply a product of two definite values, $a_{A_i \boldsymbol{\lambda}_A}$ and $b_{B_j \boldsymbol{\lambda}_B}$, each of which must be ± 1. It follows that $\langle ab \rangle_{A_1 B_1 \boldsymbol{\lambda}_A \boldsymbol{\lambda}_B} - \langle ab \rangle_{A_1 B_2 \boldsymbol{\lambda}_A \boldsymbol{\lambda}_B}$ can only be 0 or ± 2. The ± 2 value arises only if $b_{B_1 \boldsymbol{\lambda}_B} = -b_{B_2 \boldsymbol{\lambda}_B}$, whereupon $\langle ab \rangle_{A_2 B_1 \boldsymbol{\lambda}_A \boldsymbol{\lambda}_B} + \langle ab \rangle_{A_2 B_2 \boldsymbol{\lambda}_A \boldsymbol{\lambda}_B}$ must be 0. Evaluating the expectation values over any probability distribution of $(\boldsymbol{\lambda}_A, \boldsymbol{\lambda}_B)$, the LHS of equation (2.1) cannot exceed 2.

where $\langle ab \rangle_{A_i B_i}$ is the expectation value of the product of measured outcomes a and b when the measurement choices of A_i and B_i are made.[8] The left hand side of this inequality, or any variant of it under interchange of $A \leftrightarrow B$ or $1 \leftrightarrow 2$, is known as a CHSH coefficient.

The experimental sensitivity required to test these kinds of inequalities was not available until many decades after the overturning of classical physics by quantum theory. In the meantime it remained conceivable that an explicitly locally real formulation of quantum physics could be found. Several experiments in the 1970s suggested very strongly that the Bell inequalities may not hold [14], but the conclusive experiments were performed by Aspect *et al.* in 1982 [15, 16], measuring the linear polarisation of pairs of photons from coherently excited calcium atoms. The CHSH inequality was indeed violated, proving[9] that correlations can be found in nature that cannot be accounted for by classical stochastic dynamics or any other forms of local realism.

2.3 Parameter spaces of general correlations

The Bell inequalities were originally formulated in the context of quantum mechanics; but the most comprehensive response to the violation of the Bell inequalities requires us to drop the context altogether, allow all imaginable correlations, and attempt to isolate the essential characteristics of the ones that occur in nature.

The minimum requirements for correlations between a set of outcomes and a set of measurements is that there be at least two choices of measurements and at least two possible outcomes for each measurement choice.

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[8] The quantity $\langle ab \rangle$ in this case is equal to the statistical covariance $\langle ab \rangle - \langle a \rangle \langle b \rangle$ of the measured outcomes. A non-zero covariance is equivalent to *linear* correlation between the variables – a sufficient but not strictly necessary condition for two variables to be correlated in general. (A counterexample is (x, y) such that $x \in \{-1, 0, +1\}$ with a symmetric probability distribution and $y = x^2$. Correlated variables with zero covariance like this rely on fine-tuning or a symmetry in the distribution of the 'independent' variable, and will not be relevant here.)

[9] Notwithstanding one or two logically possible but rather contrived loopholes [17, §35.4]. *"Most of the dozens of experiments performed so far have favoured Quantum Mechanics, but not decisively because of the 'detection loophole' or the 'communication loophole.' The latter has been nearly decisively blocked by a recent experiment and there is a good prospect for blocking the former."* [14]

2.3.1 Imaginable parameter spaces for one binary observer

We start by considering an experiment consisting of $n=1$ observers choosing from a set of $m=2$ possible choices of measurement, abbreviated to $A \in \{1,2\}$, and obtaining one of $v=2$ possible measured outcomes $a \in \{+1,-1\}$. I will refer to an observer of this type as a 'binary observer'.

The set of conditional probabilities $p(a|A)$ can be expressed as follows:

$$\begin{aligned} p(+|1) &= \alpha; \quad p(-|1) = 1-\alpha; \\ p(+|2) &= \beta; \quad p(-|2) = 1-\beta. \end{aligned} \tag{2.2}$$

There are two free parameters, α and β, and the parameter space $\{0 \leq \alpha \leq 1\} \otimes \{0 \leq \beta \leq 1\}$ has the form of a square. Any choice of α or β in this square corresponds to a system that can be described classically in accordance with assumption 1 above, and assumption 2 is trivially satisfied.

If we were to increase the number m of possible measurements or the number of possible outcomes v of each measurement, the parameter space would be more complicated, but it would remain unambiguously compatible with the classical assumptions of local realism.

2.3.2 One-way signalling between two observers

Consider now an experiment consisting of $n=2$ observers, who we can again call Alice and Bob. Alice has a choice of $m_A=2$ measurements $A \in \{1,2\}$, each of which can give only a single possible outcome $a=+1$. Bob is restricted to $m_B=1$ measurements $B=1$, which can give $v_B=2$ possible outcomes $b \in \{+1,-1\}$. The set of conditional probabilities $p(ab|AB)$ can be expressed as follows:

$$\begin{aligned} p(++|11) &= \alpha; \quad p(+-|11) = 1-\alpha; \\ p(++|21) &= \gamma; \quad p(+-|21) = 1-\gamma; \\ p(-b|A1) &= 0 \quad \forall\, b, A. \end{aligned} \tag{2.3}$$

If $\alpha=1$ and $\gamma=0$, then the correlation is deterministic. Should Alice choose to perform measurement $A=1$, Bob will measure $b=+1$ with 100% reliability; should she choose measurement $A=2$, Bob will measure $b=-1$. A single bit of information can be reliably transmitted from Alice to Bob each time the experiment is performed.

More generally, if $\alpha \neq \gamma$, then by repeating the experiment a sufficiently large number of times, Bob could receive information from Alice with an arbitrary level of confidence. Unlike the deterministic example, there is noise; but there is also a signal, and any amount of noise can in principle be overcome

in an exactly repeatable experiment.

The necessary and sufficient condition for this experiment to be incapable of signalling is

$$\alpha = \gamma. \tag{2.4}$$

We may apply the CHSH inequality (2.1) to this experiment to find the conditions under which the first assumption of local realism will be true. To do this, we require the expectation values $\langle ab \rangle_{AB}$. The first one is

$$\begin{aligned} \langle ab \rangle_{11} &\equiv + + p(++|11) + - p(+-|11) - + p(-+|11) - - p(--|11) \\ &= 2\alpha - 1. \end{aligned}$$

Similarly, $\langle ab \rangle_{21} = 2\gamma - 1$. The remaining two quantities $\langle ab \rangle_{A2}$ don't apply to this situation – but let us imagine instead that Bob *could* choose a second measurement $B = 2$, which has an entirely predictable outcome $b = +1$, but that he never does so. (Adding this dummy measurement into the experiment cannot in any case increase the amount of information he can receive, nor can it allow Alice to receive any information from Bob.) In this equivalent case, $\langle ab \rangle_{12} = \langle ab \rangle_{22} = 1$.

There are two independent CHSH coefficients – as defined by the RHS of (2.1) – obtainable from permutations of the measurements:

$$\begin{aligned} K_1 &\equiv |\langle ab \rangle_{11} - \langle ab \rangle_{12}| + |\langle ab \rangle_{21} + \langle ab \rangle_{22}| \\ &= 2(\gamma + 1 - \alpha) \qquad \therefore K_1 \leq 2 \;\Rightarrow\; \gamma \leq \alpha \\ K_2 &\equiv |\langle ab \rangle_{22} - \langle ab \rangle_{21}| + |\langle ab \rangle_{12} + \langle ab \rangle_{11}| \\ &= 2(\alpha + 1 - \gamma) \qquad \therefore K_1 \leq 2 \;\Rightarrow\; \alpha \leq \gamma \end{aligned} \tag{2.5}$$

The CHSH inequality is satisfied if and only if $\alpha = \gamma$. It is identical to the no-signalling condition (2.4).

An experiment of this kind could therefore be used to challenge the *second* assumption of local realism of Section 2.2. If the experiments of Alice and Bob are spacelike separated (as defined above) and indicated that $\alpha \neq \gamma$, then we would have direct evidence that causal influences are *not* limited by the speed of light. It cannot be used to test the first assumption, however, because the CHSH inequality is indistinguishable from the no-signalling condition.

No experiment to date has confirmed any violation of the no-signalling condition for spacelike separated observers (the second assumption), and we know, at least for the kinds of events described in the Introduction, that there are very strong reasons for expecting this condition to hold. To observe

departures from the *first* assumption of local realism, we need a parameter space with more structure. It is sufficient, as we see in the next section, to make both observers 'binary observers' in the sense described in Section 2.3.1.

2.3.3 Imaginable parameter spaces for two spacelike-separated binary observers

Let us now consider an experiment carried out by Alice and Bob, in which each makes one choice A and B from a set of $m=2$ possible acts of measurement $A \in \{1,2\}$ and $B \in \{1,2\}$ and each obtains one of $v=2$ possible measured outcomes $a \in \{+1,-1\}$ and $b \in \{+1,-1\}$. The parts of the experiment carried out by the two observers are assumed to be strictly spacelike separated from each other.

The set of conditional probabilities $p(ab|AB)$ is now

$$\begin{array}{llll} p(++|11)=\alpha_1; & p(+-|11)=\alpha_2; & p(-+|11)=\alpha_3; & p(--|11)=1-\alpha_1-\alpha_2-\alpha_3; \\ p(++|12)=\beta_1; & p(+-|12)=\beta_2; & p(-+|12)=\beta_3; & p(--|12)=1-\beta_1-\beta_2-\beta_3; \\ p(++|21)=\gamma_1; & p(+-|21)=\gamma_2; & p(-+|21)=\gamma_3; & p(--|21)=1-\gamma_1-\gamma_2-\gamma_3; \\ p(++|22)=\delta_1; & p(+-|22)=\delta_2; & p(-+|22)=\delta_3; & p(--|22)=1-\delta_1-\delta_2-\delta_3. \end{array} \tag{2.6}$$

There are 12 free parameters. The full parameter space is $\{0 \le \alpha_1 \le 1\} \otimes \{0 \le \alpha_2 \le 1-\alpha_1\} \otimes \{0 \le \alpha_3 \le 1-\alpha_1-\alpha_2\}$, and similarly for β_i, γ_i and δ_i.

The set of α_i parameters has the form of a trapezium, with three of its edges along the three α_i axes from 0 to 1; likewise for β_i, γ_i and δ_i. The overall parameter space is therefore the 12-dimensional polytope formed by the cartesian product of four trapezia.[10]

We may identify regions of the parameter space with very different characteristics. A general point, which we may label

$$(\alpha_1,\alpha_2,\alpha_3\,;\ \beta_1,\beta_2,\beta_3\,;\ \gamma_1,\gamma_2,\gamma_3\,;\ \delta_1,\delta_2,\delta_3),$$

represents the statistics for a set of experimental results that Alice and Bob might obtain.

[10] Generalising this result is fairly straightforward: the trapezium encountered in the case of $n=2$ observers is the $p=4$ case of an p-vertex simplex. A simplex is a polytope in $(p-1)$ dimensions having edges between every pair of vertices. For the $n=1$ observer case above, the line $\{0 \le \alpha \le 1\}$ is also a $(p=2)$-vertex simplex. The general parameter space for correlations between n observers making m measurements, each with v possible outcomes, is the cartesian product of m^n (v^n)-vertex simplexes, which is a polytope in $m^n(v^n-1)$ dimensions. Each dimension represents a degree of freedom in the full set of conditional probabilities for the system.

Deterministic correlations: The parameter space has $4^4 = 256$ vertices: each one is a vertex of a trapezium in all four subspaces. At these points, all conditional probabilities are either 0 or 1, so they represent deterministic experimental situations. $(0,1,0\,;\ 0,1,0\,;\ 0,0,0\,;\ 0,0,0)$ is an example: here, every run of the experiment gives $b = +1$ for Bob, but Alice finds $a = +1$ if she chooses $A = 1$ and $a = -1$ if she chooses $A = 2$. Both experiments are deterministic and independent of each other.

$(1,0,0\,;\ 1,0,0\,;\ 1,0,0\,;\ 0,1,0)$ is another example, but one with a quite different character, and belongs to a class of points that cannot appear in any relativistic causal theory. Here, if Bob sets $B = 2$, he will always obtain $b = +1$ if Alice has set $A = 1$ and $b = -1$ if Alice has set $A = 2$. This means Bob can immediately detect Alice's choice of measurement setting, despite their spacelike separation. This is termed a **signalling** correlation, because if such a scenario existed it would enable Alice to send messages to Bob.

No-signalling correlations: Formally, a no-signalling correlation is one for which Alice's result a gives her *no statistical information* about Bob's choice of measurement B, and likewise b gives him no statistical information about A. That is,[11]

$$\begin{aligned} p(a|AB) &= p(a|A) \qquad \forall a, A, B \\ \Rightarrow \sum_b p(ab|A1) &= \sum_b p(ab|A2) \quad \forall a, A \end{aligned} \tag{2.7}$$

and

$$\begin{aligned} p(b|AB) &= p(b|B) \qquad \forall b, B, A \\ \Rightarrow \sum_a p(ab|1B) &= \sum_a p(ab|2B) \quad \forall b, B \end{aligned} \tag{2.8}$$

Defining

$$S_A^{(B\to A)} \equiv \left| \sum_b \left(p(ab|A1) - p(ab|A2) \right) \right|$$

and

$$S_B^{(A\to B)} \equiv \left| \sum_a \left(p(ab|1B) - p(ab|2B) \right) \right|,$$

[11] There appear to be eight conditions here, but only four are independent. For example $p(+|AB) = p(+|A) \Leftrightarrow p(-|AB) = p(-|A)$ because $\sum_a p(a|AB) = \sum_a p(a|A) = 1$.

the no-signalling condition is

$$\begin{array}{rcccl} S_1^{(B\to A)} & = & |(\alpha_1+\alpha_2)-(\beta_1+\beta_2)| & = & 0 \\ S_2^{(B\to A)} & = & |(\gamma_1+\gamma_2)-(\delta_1+\delta_2)| & = & 0 \\ S_1^{(A\to B)} & = & |(\alpha_1+\alpha_3)-(\gamma_1+\gamma_3)| & = & 0 \\ S_2^{(A\to B)} & = & |(\beta_1+\beta_3)-(\delta_1+\delta_3)| & = & 0. \end{array} \tag{2.9}$$

Our signalling example has $S_1^{(B\to A)} = 0$, $S_2^{(B\to A)} = 0$, $S_1^{(A\to B)} = 0$ and $S_2^{(A\to B)} = 1$, indicating that Alice will be able to signal to Bob with 100% efficiency if Bob chooses measurement 2.

Of the 256 deterministic correlations, 16 satisfy the no-signalling condition.

The full **set of no-signalling correlations** for $n=2$, $m=2$ and $v=2$ is an 8-dimensional cross-section of the full 12-dimensional parameter space. No inequalities are involved, therefore its boundaries are located at the boundaries of the full parameter space. It is a polytope with 24 vertices [6]. The 16 no-signalling deterministic correlations must be vertices of this subset because they are vertices of the full parameter space itself; the other 8 vertices are correlation extremes known as 'Popescu-Rohrlich boxes' (PR boxes) [18], about which more later. An example of a PR box correlation is $(\frac{1}{2},0,0\,;\ \frac{1}{2},0,0\,;\ \frac{1}{2},0,0\,;\ 0,\frac{1}{2},\frac{1}{2})$.

The no-signalling polytopes for $n=2$ observers making $m=2$ measurements each with an *arbitrary* number of measured outcomes are derived in [19]. Those for $n=2$ observers making an arbitrary number of measurements each with $v=2$ measured outcomes are derived in [20]. Arbitrary n involves a considerably greater increase in complexity: the $n=3$ case [21] will be briefly discussed in Section 2.3.6.

Locally real correlations: For a correlation to accord with the assumptions of local realism, it must (a) satisfy the no-signalling condition above and (b) satisfy the CHSH inequality (2.1) in both of the independent CHSH correlation coefficients. This requires $K_i \le 2$, where

$$\begin{array}{rcl} K_1 & \equiv & |\,\langle ab\rangle_{11} - \langle ab\rangle_{12}\,| + |\,\langle ab\rangle_{21} + \langle ab\rangle_{22}\,| \\ & = & 2\,|\alpha_2+\alpha_3-\beta_2-\beta_3| + 2\,|\gamma_2+\gamma_3+\delta_2+\delta_3-1| \\ K_2 & \equiv & |\,\langle ab\rangle_{22} - \langle ab\rangle_{21}\,| + |\,\langle ab\rangle_{12} + \langle ab\rangle_{11}\,| \\ & = & 2\,|\gamma_2+\gamma_3-\delta_2-\delta_3| + 2\,|\alpha_2+\alpha_3+\beta_2+\beta_3-1|\,. \end{array} \tag{2.10}$$

The 16 no-signalling deterministic correlations all have $K_1 = K_2 = 2$, so are limiting cases of locally real correlations. The PR boxes, on the other hand, have $K_1 = 0$ and $K_2 = 4$ or vice versa, violating the CHSH inequality.

The **full set of locally real correlations** is the subset of the no-signalling polytope consisting of all points that satisfy the CHSH inequality.[12] It remains 8-dimensional as there are no constraints in the form of equations. New boundaries are created by the linear inequalities given above (all of which are Bell inequalities). As they remain limiting cases, all of the no-signalling deterministic correlations must also be vertices of the locally real polytope. No new vertices are formed by the inequalities, but the PR boxes are excluded, leaving 16 vertices.

Factorisable correlations: Some locally real correlations are factorisable, *i.e.* the set of conditional probabilities can be expressed in the form $p(ab|AB) = p_A(a|A)p_B(b|B)$.[13] This tells us that the observations of Alice and Bob are statistically independent of each other. Signalling is therefore not possible, and local realism is not challenged. The set of factorisable correlations is the cartesian product of two copies of the parameter space for a single observer as described above, which makes the polytope of factorisable correlations a four-dimensional hypercube.

The rest of the set of locally real correlations (which is almost all of it) are non-factorisable, but with the introduction of a set of 'hidden variables' $\boldsymbol{\lambda}$

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[12]The case of two binary observers described in this Section is not the simplest case in which CHSH-violating regions of parameter space exist within the no-signalling set. There are intermediate cases between this and the much simpler one described in Section 2.3.2 that may be investigated:

Case 1. Restrict Alice to one outcome per measurement – equivalent to the constraint $\alpha_3 = \beta_3 = \gamma_3 = \delta_3 = 0$ and $\alpha_4 = \beta_4 = \gamma_4 = \delta_4 = 0$ (where $\alpha_4 \equiv 1 - \alpha_1 - \alpha_2 - \alpha_3$ *etc.*).

Case 2. Restrict Bob to a single measurement – equivalent to $\beta_2 = \delta_2 = 0$ and $\beta_4 = \delta_4 = 0$.

Case 3. Restrict Bob to a single measurement *and* restrict Alice to one outcome on measurement 1 – equivalent to $\alpha_2 = \beta_2 = \delta_2 = 0$ and $\alpha_3 = \beta_3 = \beta_4 = \delta_4 = 0$.

The two sets of conditions (2.9) and (2.10) can be applied in each case. Of these three cases, **only Case 2** has a no-signalling subset that is partly CHSH-violating and partly CHSH-compliant. The no-signalling constraints can be expressed as $\beta_1 = \alpha_1 + \alpha_2$, $\delta_1 = \gamma_1 + \gamma_2$ and $\alpha_1 + \alpha_3 = \gamma_1 + \gamma_3$, which defines a 5-dimensional region bounded by the boundaries of the original 12-parameter set (2.6). Retaining the parameters $\gamma_1, \gamma_2, \gamma_3, \alpha_2$ and $\chi \equiv \alpha_1 - \alpha_3$, we find there are three non-trivial CHSH inequalities: $\gamma_1 + \alpha_2 \leq 1$, $\gamma_3 + \alpha_2 \leq 1$ and $\gamma_1 + 2\gamma_2 + \gamma_3 + |\chi| \leq 2$.

[13]An example is $(\frac{1}{12}, \frac{3}{12}, \frac{2}{12}\,;\ \frac{3}{12}, \frac{1}{12}, \frac{6}{12}\,;\ \frac{2}{12}, \frac{6}{12}, \frac{1}{12}\,;\ \frac{6}{12}, \frac{2}{12}, \frac{3}{12})$, which corresponds to $p_A(0|0) = \frac{1}{3}$, $p_A(0|1) = \frac{2}{3}$, $p_B(0|0) = \frac{1}{4}$, $p_B(1|0) = \frac{3}{4}$.

they can be expressed as a sum of factorisable terms:[14]

$$p(ab|AB) = \sum_{\lambda} p(\lambda) p_A(a|A\lambda) p_B(b|B\lambda).$$

If λ is some shared information that is part of the make-up of the systems that Alice and Bob are investigating, then this type of correlation could straightforwardly be generated by a classical theory in accordance with local realism. For any given λ, all of the conditional probabilities factorise. The measurements are therefore fully independent of each other given a set of variables that are already known to be shared, so signalling is not possible.

2.3.4 The parameter space in nature for two spacelike-separated binary observers

We have seen that the parameter space for $n = 2$, $m = 2$, $v = 2$ can be resolved into nested subsets:

Local determinism	$\subset$	No hidden variables	$\subset$	Local realism	$\subset$	No-signalling	$\subset$	Full parameter space
(0D: 16 points)		(4D hypercube)		(8D polytope)		(8D polytope)		(12D polytope)

(2.11)

All correlations in any *causal theory* must be restricted to the no-signalling set. It is well established that Nature does not restrict herself to local realism – however, it is also apparent that she does not make use of the full set of no-signalling correlations [18], but supplies her own constraints intermediate between the two:

$$\text{Local Realism} \subset \text{Nature} \subset \text{No-signalling} \tag{2.12}$$

The full subset of conditional probabilities that are available to general systems in nature is something that can, in principle, be explored experimentally. The shape of the polytopes that such experiments reveal is the shape of the operational laws of physics at their most basic level.

[14] For example, $(\frac{13}{24}, \frac{3}{24}, \frac{2}{24}\,;\ \frac{3}{24}, \frac{13}{24}, \frac{6}{24}\,;\ \frac{2}{24}, \frac{6}{24}, \frac{13}{24}\,;\ \frac{6}{24}, \frac{2}{24}, \frac{3}{24})$ is not factorisable as it stands, but it could be generated using $\lambda \in \{0, 1\}$ and $p(\lambda = 0) = \frac{1}{2}$ such that if $\lambda = 0$ the probabilities are those given in the factorisable example in Footnote[13] above, whereas if $\lambda = 1$ there is a deterministic correlation with $a = A$ and $b = B$.

Our ability to carry out experiments on the kinds of systems that would allow us to explore nature beyond the locally real polytope is still in its infancy. In addition, the problem of using Bell inequalities to define the boundaries of that polytope for an arbitrary system is known to be NP-complete,[15] even for $n = 2$ and $v = 2$ (two observers choosing from an arbitrary number of binary-valued measurements) [23, §6], so solutions with any kind of generality are unlikely to be forthcoming. But progress has been and continues to be made; some of this is outlined below.

2.3.5 The parameter space in quantum theory for two spacelike-separated binary observers

Thus far, nothing has been assumed about what is being measured in our two-observer experiment, or how it could be modelled. Having dispensed with local realism, it is clear that we should consider our 'input' as a whole, rather than as two individual objects.

In classical physics, systems are considered to be made of parts, each of which has a set of properties that define its *state*. When we make a measurement, the conditional probabilities for the results we obtain are determined by the properties of those parts and the nature of the measurement process.

In quantum mechanics, a physical state is represented by a vector in a vector space such that the probabilities for the outcomes of any measurement are given by the square of the norm of a projection of this vector onto some subspace that is characteristic of the measurement being made.[16]

Some of the familiar implications of this postulate will be reviewed in Section 3.1. Of relevance here is the result that any measurement may be

[15]The class of NP-complete problems is the 'hardest' class of NP problems, which are problems whose known solutions can be *verified* algorithmically in 'polynomial time' (a computing time scale that is a polynomial function of the size n of the problem). Problem A is said to be 'harder' than problem B if and only if there cannot exist a polynomial-time algorithm transforming A into B.

If a proof is found that all problems verifiable in polynomial time are also *solvable* in polynomial time ('NP=P'), then no NP problems could be harder than any other, and the concept of NP-complete would cease to be meaningful. This is considered improbable by the majority of computer scientists [22].

Having made that disclaimer, the implication of an NP-complete problem in practice is that there can be no algorithmic method of solution for general n: each instance of the problem must be solved individually, and the process of finding each solution, if it exists at all, increases rapidly in complexity as n increases.

[16]As the notion of a vector space is such a straightforward one, one could argue that this is no more strange than the equivalent classical proposition: that the laws of nature are somehow responsible for assigning and maintaining the objective properties of subsets of the Universe, and that this is what our measurements reflect.

represented by a self-adjoint operator, and that two measurements permit signalling if and only if the corresponding self-adjoint operators do not commute.[17] What follows are some results that are significant in the discussion of correlations.

In 1980, Tsirelson [24] showed that a CHSH correlation coefficient (2.1) cannot exceed $2\sqrt{2}$. The proof is as follows:

If $\hat{K} \equiv \hat{A}_1\hat{B}_1 + \hat{A}_1\hat{B}_2 + \hat{A}_2\hat{B}_1 - \hat{A}_2\hat{B}_2$, where $\hat{A}_i$ and $\hat{B}_j$ are self-adjoint operators with eigenvalues of ± 1 and satisfying $[\hat{A}_i, \hat{B}_j] = 0$, then

$$\begin{aligned} 4 \pm \sqrt{2}\hat{K} &= \left(\hat{A}_1^2 + \hat{A}_2^2 + \hat{B}_1^2 + \hat{B}_2^2\right) \pm \sqrt{2}\left(\hat{A}_1\hat{B}_1 + \hat{A}_1\hat{B}_2 + \hat{A}_2\hat{B}_1 - \hat{A}_2\hat{B}_2\right) \\ &= \left(\hat{A}_1 \pm \tfrac{1}{\sqrt{2}}\left(\hat{B}_1 + \hat{B}_2\right)\right)^2 + \left(\hat{A}_2 \pm \tfrac{1}{\sqrt{2}}\left(\hat{B}_1 + \hat{B}_2\right)\right)^2. \end{aligned}$$

The right hand side is a sum of squares of self-adjoint operators, and its expectation value is therefore necessarily positive. Hence $\langle 4 \pm \sqrt{2}\hat{K}\rangle \geq 0$, and

$$\left|\langle \hat{K} \rangle\right| \leq 2\sqrt{2}. \tag{2.13}$$

Since the proof applies under the interchange of $\hat{A} \leftrightarrow \hat{B}$ or $1 \leftrightarrow 2$, the **Tsirelson bound** of $2\sqrt{2}$ for any CHSH coefficient follows. As we have seen, the magnitude of the CHSH coefficient reaches 4 in the case of the PR box, so this bound immediately excludes significant regions of the no-signalling polytope. The correlations excluded in this way are known as 'superquantum' correlations. The remaining 8-dimensional set has curved boundaries lying between the boundaries of the locally real and the no-signalling polytopes.

However, not all correlations within the Tsirelson bound can be generated by quantum states. **Necessary and sufficient conditions** are [25]

$$\left|\sin^{-1}(\langle ab\rangle_{A_1B_1}) + \sin^{-1}(\langle ab\rangle_{A_1B_2}) + \sin^{-1}(\langle ab\rangle_{A_2B_1}) - \sin^{-1}(\langle ab\rangle_{A_2B_2})\right| \leq \pi. \tag{2.14}$$

This (and the corresponding inequalities after notation interchange) defines a convex set with curved boundaries lying between those of the Tsirelson bound and the locally real polytope, definitively separating those correlations that can be attained in a quantum theory from those that cannot.

Thus:

$$\begin{matrix} \text{Local} \\ \text{Realism} \end{matrix} \subset \begin{matrix} \text{Quantum} \\ \text{theory} \end{matrix} \subset \begin{matrix} \text{Tsirelson} \\ \text{bound} \end{matrix} \subset \begin{matrix} \text{No-} \\ \text{signalling} \end{matrix} \tag{2.15}$$

[17] The equivalence between commuting operators and no-signalling will be discussed in Section 3.3.1.

The boundaries of all four of these nested subsets meet at the 16 locally deterministic correlations.

In 2004, Cabello [26] expressed the boundaries of this quantum set for $n=2$, $m=2$ and $v=2$ in terms of directly measurable parameters, and proposed an experiment to test those boundaries. The experiment was carried out in the same year [27] and the results traced the boundaries as predicted.[18]

Quantum theory has been tested rigorously in many other ways over the past eight decades, and some of its predictions – particularly in the measurements of bound states and the results of scattering experiments – have been verified with far greater precision than any exploration of correlation parameter spaces of the type mentioned here. But what is so significant about these correlation experiments, for whatever systems they can be carried out on, and to the extent that the statistical power of the tests allow, is that by mapping out the quantum set itself they reveal *directly* that there is a Hilbert space formulation, as defined above, encompassing the conditional probabilities of every observation that can be made on those systems. To that extent, the Hilbert space formulation of quantum mechanics ceases to be a postulate, and becomes directly observable as a recognisable shape in the space of imaginable experimental outcomes.

2.3.6 Parameter spaces for three or more spacelike-separated binary observers

The no-signalling polytope for $n=3$ observers choosing from $m=2$ measurements each with $v=2$ possible outcomes is a 26-dimensional subset of the full 56-dimensional parameter space, with 53856 vertices [21].

The vertices fall into 46 distinct classes, of which only one represents correlations that could be generated by a local realist theory. A further 11 could be generated by a two-party no-signalling theory, involving any kind of correlation from the $n=2$ no-signalling set discussed above.[19] The remaining 34 classes of vertices are 'fully tripartite': they require **correlations between**

[18] Note that violations of the Tsirelson bound are predicted under quantum theory [28] and have been observed [29] for cases in which the outcomes of measurements are conditional on the values of a third system ('post-selection').

[19] The requirement is that all conditional probabilities $P(abc|ABC)$ may be expressed in the form

$$q_1 \sum_{i=1}^{3} q_i P_i(ab|AB) P_i(c|C) + q_2 \sum_{i=1}^{3} q_i P_i(ca|CA) P_i(b|B) + q_3 \sum_{i=1}^{3} q_i P_i(bc|BC) P_i(a|A),$$

with each $P_i(xy|XY)$ being a conditional probability from the $n=2$ no-signalling set.

all three measurements that cannot be generated by correlations between pairs.

The nature of the quantum subset of this no-signalling set has yet to be ascertained, but quantum theory cannot generate fully tripartite correlations [30]. Probabilities in quantum theory arise from inner products involving linear combinations of vectors, so there is no scope for pure three-way correlations without departing from the Hilbert space formalism.

Searches for fully tripartite correlations in quantum systems have been undertaken using triple-slit diffraction [31] and three-path interference in nuclear magnetic resonance [32], both involving photons. They have set modest upper limits on the ratio of three-path to two-path amplitudes.

A framework for these experiments is provided by Sorkin's 'generalized measure theory'[20] [30]. A hierarchy of sum rules is set out, each of which effectively disallows pure multipartite correlations above a given order. Classical physics satisfies the lowest non-trivial order of sum rule; quantum theory and superquantum correlations such as PR boxes satisfy the next, the 34 fully tripartite vertex classes described above would satisfy the next beyond that, and so on. A discussion of how the CHSH inequalities and Tsirelson's bound might be generalised in such theories can be found in [33].

[20]Measure theory is the natural mathematical framework for probability. A probability space is a special case of a measure space in which the measure of the whole space is 1. See also Section 3.4.

3 Hilbert Space

3.1 The Postulates and their implications

The arguments of Section 2 are not necessary to justify the use of Hilbert space in quantum mechanics – it has been used as a means to perform calculations of astonishing reliability and precision since the 1930s, long before any Bell correlation experiments were possible – but the correlation picture motivates and verifies it in a way that is arguably simpler and more direct than anything that predates it.

We have seen that, at the most basic operational level, the correlations in nature appear to fill causal regions of parameter space whose boundaries are determined by a Hilbert space model of quantum mechanics. The foundations for this model can be expressed in three postulates. Two are given below, the third in Section 4.1.

Postulate 1 *Any physical state can be represented by a vector in a vector space such that the probabilities for the outcomes of any measurement are given by the square of the norm of a projection of this vector onto some subspace that is characteristic of the measurement being made.*

We represent a vector as $|\psi\rangle$ and the vector space as $\mathcal{H}$. Immediate implications include:

1. As the set of outcomes for any measurement can be specified so that it is both mutually exclusive and exhaustive, it follows that any measurement must have associated with it a set of mutually orthogonal projection operators spanning the space $\mathcal{H}$, each one corresponding to a possible outcome;

2. $\mathcal{H}$ must be a Hilbert space;[21]

3. For any discrete set of mutually orthogonal projection operators $\{\hat{P}_i^{(A)}\}$ representing a measurement A with real-valued outcomes, there exists a self-adjoint operator $\hat{A} = \sum_i a_i \hat{P}_i^{(A)}$ whose eigenspaces are precisely

[21]Strictly, it only necessarily follows that $\mathcal{H}$ is a *pre-Hilbert space*: this is the requirement that a positive norm is defined for every non-zero vector, and an inner product is defined between every pair of vectors that is no more than the product of the norms of the two vectors (which is required in order that orthogonal projection operators can be employed). For a Hilbert space, we also require it to be *complete* – meaning that for every Cauchy sequence of vectors in $\mathcal{H}$, the limit is also in $\mathcal{H}$ – which enables the use of calculus in quantum theory. Quantum mechanics is almost universally formulated in a *complex* Hilbert space, as it must be for the postulate in this form, though it need not be in general [34].

the target spaces of each projection operator, and whose corresponding eigenvalues $\{a_i\}$ are the values of each distinct possible outcome of the measurement. The Spectral Theorem[35, §3], [7, §III.6] extends this principle to continuous measurements. Thus every observable can be represented by a self-adjoint operator.

4. **The Born rule:** Given a state $|\psi_s\rangle \in \mathcal{H}$, we can write the probability of obtaining outcome a_i from measurement A in the form

$$p(a_i|A,s) = |\hat{P}_i^{(A)}|\psi_s\rangle|^2. \tag{3.1}$$

5. Since all conditional probabilities must sum to 1, any vector representing the state of a system must be normalised[22] to $||\psi\rangle|^2 = 1$;

6. **Unitarity:** as the state of a system evolves over time, the sum of all conditional probabilities cannot deviate from 1 for any measurement. This implies that an operator $\hat{U}_{21}$ mapping from any initial state $|\psi_1\rangle$ of the system at time t_1 to the state of the same system at a later time t_2 must satisfy $\langle\psi_1|\hat{U}_{21}^\dagger\hat{U}_{21}|\psi_1\rangle = \langle\psi_1|\psi_1\rangle$. If, in addition, this operator is a *linear* operator, then it follows that $\hat{U}_{21}$ is unitary.[23]

7. Compound systems: given two systems in which states are represented by vectors in $\mathcal{H}_a$ and $\mathcal{H}_b$ respectively, vectors in the direct product space $\mathcal{H}_{ab} = \mathcal{H}_a \times \mathcal{H}_b$ will represent the space of states for the compound system in precisely the same way with respect to the probabilities of joint outcomes from pairs of measurements. This extends to any number of such systems.

None of these points need be separately postulated: they all follow directly from Postulate 1, subject to a few caveats (some of the most significant of which are footnoted). A second postulate is, however, required in order to

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[22] $||\psi_s\rangle|^2 = \langle\psi_s|\hat{1}\hat{1}|\psi_s\rangle = \langle\psi_s|\sum_i \hat{P}_i^{(A)}\sum_j \hat{P}_j^{(A)}|\psi_s\rangle = \sum_i\langle\psi_s|\hat{P}_i^{(A)}|\psi_s\rangle = \sum_i p(a_i|A,s) = 1.$

[23] Non-linear approaches to quantum evolution have been proposed, but have not met with experimental success [17, §28.2]. Linearity $\Rightarrow$ $\hat{U}(\alpha|\chi\rangle + \beta|\phi\rangle) = \alpha\hat{U}|\chi\rangle + \beta\hat{U}|\phi\rangle$. If $\langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle = \langle\psi|\psi\rangle\ \forall\ |\psi\rangle \in \mathcal{H}$, then

$$\begin{aligned}
(\alpha^*\langle\chi| + \beta^*\langle\phi|)\hat{U}^\dagger\hat{U}(\alpha|\chi\rangle + \beta|\phi\rangle) &= (\alpha^*\langle\chi| + \beta^*\langle\phi|)(\alpha|\chi\rangle + \beta|\phi\rangle) \\
\Rightarrow\ (\alpha^*\beta\langle\chi|\hat{U}^\dagger\hat{U}|\phi\rangle) + (\beta^*\alpha\langle\phi|\hat{U}^\dagger\hat{U}|\chi\rangle) &= (\alpha^*\beta\langle\chi|\phi\rangle) + (\beta^*\alpha\langle\phi|\chi\rangle) \\
\Rightarrow\ \mathrm{Re}((\alpha^*\beta\langle\chi|(\hat{U}^\dagger\hat{U} - \hat{1})|\phi\rangle) &= 0\ \ \forall\alpha,\beta \in \mathbb{C} \\
\Rightarrow\ \hat{U}^\dagger\hat{U} &= \hat{1}.
\end{aligned}$$

specify the effect on $|\psi\rangle$ of making a measurement. This is known as the 'projection postulate'.

Postulate 2 *Every measurement updates the state by projecting it onto the subspace associated with the outcome of the measurement.*

As this new state must be normalised, this means:

$$|\psi\rangle \to |\psi'\rangle = \frac{\hat{P}_i^{(A)}|\psi\rangle}{|\hat{P}_i^{(A)}|\psi\rangle|}. \tag{3.2}$$

This transformation is clearly not unitary: $\langle\psi_1'|\psi_2'\rangle$ will not be the same as $\langle\psi_1|\psi_2\rangle$ in general.

While arguments over the physical interpretation of postulates and their implications have proliferated, and more recent developments have begun to unify them by expressing the measurement process in terms of unitary evolution of a system along with a complex environment [36],[24] experimental quantum physics has consistently and reliably employed this same formalism since it was outlined in the treatments of Dirac in 1930 [38] and von Neumann in 1932 [39].

A theory that makes no claim about reality aside from these postulates is known as an *operational quantum theory* [40], and could be considered as the bare minimum for any quantum theory.[25] I will adopt here a working definition of quantum theory as being any theory that reproduces the results of operational quantum theory.

3.2 Operational stochastic quantum theory

For a quantum theory to give realistic probabilities, we require a means of taking into account unknowns regarding the initial state and the measurements themselves. These unknowns may be **internal** to the Hilbert space of the system itself – we may not know precisely which of the vectors in the Hilbert space of the system describes its current state, and we may not know precisely which of the operators in the Hilbert space of the system describes the measurement we are taking. Or they may be **external** to the system – the Hilbert

[24]The forebear of these developments, whether or not it is subscribed to by modern theorists in its original form, is the relative state interpretation of Everett [37].

[25]For example: *"It's a minimal interpretation of quantum theory. Even if you might at heart be a realist, you can still follow the operational approach to get clear on what the theory tells us, without any extra baggage. It's a useful way of presenting the basic formalism of quantum mechanics in a neutral way."* – R. Spekkens [41]

space we are considering for our system may not be the full picture, because the system may have some interaction with a larger environment.

The four permutations of these are introduced below (largely following Spekkens [41]), along with their implications for the evolution of a system over time, and some basic results and definitions. These are used to derive a general no-signalling theorem in Section 3.3.1.

3.2.1 Internal unknowns regarding the initial state

If we believed our system would be better modelled by a probability distribution over states in $\mathcal{H}$ than by a single state, and we wanted a way to treat this distribution stochastically, the Born rule equation (3.1) would be problematic because it is non-linear in the state vector. In 1932, von Neumann [39] showed that this could be remedied by using *density operators* instead of state vectors.

For any state $|\psi_s\rangle \in \mathcal{H}$, there exists a projection operator $|\psi_s\rangle\langle\psi_s|$ mapping $\mathcal{H}$ onto the one-dimensional subspace containing $|\psi_s\rangle$. The density operator for a system known to be in this state is exactly this projection operator: $\hat{\rho}_s = |\psi_s\rangle\langle\psi_s|$. The Born rule for all conditional probabilities relating to this state is then:[26]

$$p(a_i|A, s) = \mathrm{Tr}(\hat{P}_i^{(A)}\hat{\rho}_s). \tag{3.3}$$

If we have an initial state which has a probability of $\frac{1}{3}$ of being $|\psi_{s_1}\rangle$ and a probability of $\frac{2}{3}$ of being $|\psi_{s_2}\rangle$, then the sum $\hat{\rho} = \frac{1}{3}|\psi_{s_1}\rangle\langle\psi_{s_1}| + \frac{2}{3}|\psi_{s_2}\rangle\langle\psi_{s_2}|$ will also generate the correct set of probabilities in (3.3). Such a mixture is referred to as a 'mixed state', and a state represented by a projection operator onto a single one-dimensional subspace is called a 'pure state'.

The density operator can be used to represent any probability distribution over any set of vectors in $\mathcal{H}$. It is a positive-definite self-adjoint operator with unit trace.[27]

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[26] The trace is defined by $\mathrm{Tr}(\hat{P}_i^{(A)}\hat{\rho}_s) \equiv \sum_j \langle\phi_j|(\hat{P}_i^{(A)}\hat{\rho}_s)|\phi_j\rangle$, and is independent of the choice of orthonormal basis $\{\phi_j\}$. With $\hat{\rho}_s = |\psi_s\rangle\langle\psi_s|$, we have

$$\mathrm{Tr}(\hat{P}_i^{(A)}\hat{\rho}_s) = \sum_j \langle\psi_s|\phi_j\rangle\langle\phi_j|\hat{P}_i^{(A)}|\psi_s\rangle = \langle\psi_s|\hat{P}_i^{(A)}|\psi_s\rangle = p(a_i|A, s).$$

[27] It is self-adjoint because all projection operators are self-adjoint, positive-definite because for every state $|\psi\rangle \in \mathcal{H}$, the value of $\langle\psi|\hat{\rho}|\psi\rangle$ is the probability of finding the system in that state using some suitable ideal measurement; and it is unit trace because orthogonal projection operators in a spanning set sum to the identity operator $\sum_i \hat{P}_i^{(A)} = \hat{1}$ and conditional probabilities sum to one: $\mathrm{Tr}(\hat{\rho}) = \mathrm{Tr}(\sum_i \hat{P}_i^{(A)}\hat{\rho}) = \sum_i p(a_i|A) = 1$.

3.2.2 External unknowns regarding the initial state

All systems are influenced by their environment to some extent. If we wish to take this into account, the classical stochastic procedure described above will not be sufficient. In this situation, we are faced with a probability distribution over the vastly larger joint Hilbert space of the system and its environment. Fortunately, any state coupled to its environment in this way can still be represented in the form of a density operator acting in the Hilbert space of the system alone.

Given a pure state $\hat{\rho}^{ab} = |\psi^{ab}\rangle\langle\psi^{ab}|$ in a Hilbert space $\mathcal{H}_{ab} = \mathcal{H}_a \times \mathcal{H}_b$, the mixed state $\hat{\rho}^a = \mathrm{Tr}_b(\hat{\rho}^{ab})$ defined[28] in $\mathcal{H}_a$ satisfies the same Born rule as the pure state:

$$\begin{aligned} p(a_i|A) &= \mathrm{Tr}\big((\hat{P}_i^{(A)} \otimes \hat{1}^{(B)})\,\hat{\rho}^{ab}\big) \\ &= \mathrm{Tr}_a\big(\hat{P}_i^{(A)}\mathrm{Tr}_b(\hat{1}^{(B)}\,|\psi^{ab}\rangle\langle\psi^{ab}|)\big) \\ &= \mathrm{Tr}(\hat{P}_i^{(A)}\hat{\rho}^a) \end{aligned} \tag{3.4}$$

This shows that a complete description of any state of knowledge about any quantum system, no matter how entangled it may be with other systems, can therefore be provided by a positive-definite, unit-trace self-adjoint operator $\hat{\rho}_a$ acting in $\mathcal{H}_a$.

3.2.3 Internal unknowns regarding the measurement

We may also wish to generalise from a 'pure' measurement (with a set of orthogonal subspaces) to a probability distribution over a set $A = \{A_j\}$ of such measurements, each with probability p_j.

There still must exist a set of possible outcomes for this 'mixed' measurement, but they need not conform to Postulate 1. Each outcome a_i is now associated with a *probability distribution over projection operators* of the form

$$\hat{E}_i^{(A)} = \sum_j p_j \hat{P}_i^{(A_j)}. \tag{3.5}$$

The set $\{\hat{E}_i^{(A)}\}$ is referred to as a *positive operator valued measure* (POVM),

[28] Tr_b refers to the 'partial trace', which is performed in $\mathcal{H}_{ab}$ by summing over a set of basis vectors spanning $\mathcal{H}_b$ to yield an operator acting in $\mathcal{H}_a$.

and it also satisfies a Born rule:

$$p(a_i|A,s) = \mathrm{Tr}(\hat{E}_i^{(A)}\hat{\rho}_s), \tag{3.6}$$

which implies

$$\begin{aligned} \sum_i \hat{E}_i^{(A)} &= \hat{1} \\ \langle\psi|\hat{E}_i^{(A)}|\psi\rangle &\geq 0 \quad |\psi\rangle \in \mathcal{H}. \end{aligned} \tag{3.7}$$

3.2.4 External unknowns regarding the measurement

A real measurement process is also subject to influence from the larger Hilbert space of its environment. It can be shown [17, §18.5] that a POVM satisfying equations (3.7) exists that encapsulates the whole of the measurement process with regard to the Hilbert space of the system, including the Born rule (3.6).

Further, for *any* set of operators $\{\hat{E}_i^{(A)}\}$ in $\mathcal{H}_a$ satisfying equations (3.7) that are not themselves projection operators, there exists a mutually orthogonal set of projection operators $\{\hat{P}_i^{(A)}\}$ in a larger Hilbert space $\mathcal{H}_{ab} = \mathcal{H}_a \times \mathcal{H}_b$ for which the set $\{\hat{E}_i\}$ would correctly represent the measurement made on a state in $\mathcal{H}_a$.[29] That is,

$$\hat{E}_i^{(A)} = \hat{P}_{\mathcal{H}_a}\hat{P}_i^{(A)}\hat{P}_{\mathcal{H}_a}, \tag{3.8}$$

where $\hat{P}_{\mathcal{H}_a}$ is the projection operator from $\mathcal{H}_{ab}$ onto the original space $\mathcal{H}_a$, and

$$p(a_i|A,s) = \mathrm{Tr}(\hat{E}_i^{(A)}\hat{\rho}_s^a) = \mathrm{Tr}(\hat{P}_i^{(A)}\hat{\rho}_s^{ab}). \tag{3.9}$$

Here, $\hat{\rho}_s^{ab}$ is the density operator for a state in the larger Hilbert space $\mathcal{H}_{ab}$. This can be taken to have the form $\hat{\rho}_s^a \otimes \hat{\rho}^b$, where $\hat{\rho}^b$ is a one-dimensional projection operator (a pure state) in $\mathcal{H}_b$.

The set $\{\hat{P}_i^{(A)}\}$ could of course be represented (non-uniquely) by a self-adjoint operator in $\mathcal{H}_{ab}$.

3.2.5 The generalised update rule

Equation (3.2) describes the effect of a measurement A on a state $|\psi\rangle$, as prescribed by Postulate 2. For a *pure* measurement A, the effect on $\hat{\rho}$ is given

[29] This is the Naimark extension theorem [40, §II.2]. The same cannot be said for mixed measurements. While any probability distribution over sets of pure measurements can be represented by a POVM, not every POVM can be expressed as a probability distribution over sets of pure measurements.

by:

$$\hat{\rho} \to \hat{\rho}' = \frac{\hat{P}_i^{(A)} \hat{\rho} \hat{P}_i^{(A)}}{\mathrm{Tr}(\hat{P}_i^{(A)} \hat{\rho})}. \tag{3.10}$$

The numerator is an example of a linear *superoperator* – a linear map $\mathcal{T}$ from operators on $\mathcal{H}$ to operators on $\mathcal{H}$. This one yields an operator $\hat{P}_i^{(A)} \hat{\rho} \hat{P}_i^{(A)}$ which has a trace less than or equal to the original $\hat{\rho}$; and it is 'positive', *i.e.* it preserves the positive-definiteness of an operator. Further, it is 'completely positive', *i.e.* $\mathcal{T} \otimes 1$ will preserve the positive-definiteness of any $\hat{\rho}^{ab}$ in $\mathcal{H}_a \times \mathcal{H}_b$.

For a *general* measurement $\{\hat{E}_i\}$, the effect on $\hat{\rho}$ is as follows. For a given outcome $\hat{E}_i$, a trace-non-increasing, completely positive linear superoperator $\mathcal{T}_i$ can be defined for every operator $\hat{R}$ acting in $\mathcal{H}$ by

$$\mathrm{Tr}(\mathcal{T}_i(\hat{R})) = \mathrm{Tr}(\hat{E}_i^{(A)} \hat{R}) \qquad \forall\ \hat{R} : \mathcal{H} \to \mathcal{H} \tag{3.11}$$

The updated state following the measurement is then given, somewhat implicitly, by

$$\hat{\rho} \to \hat{\rho}' = \frac{\mathcal{T}_i(\hat{\rho})}{\mathrm{Tr}(\hat{E}_i^{(A)} \hat{\rho})} \tag{3.12}$$

For a given superoperator $\mathcal{T}_i$, the operator $\hat{E}_i$ defined by equation (3.11) is called the *effect* of that superoperator [17, §18.1].[30]

It can be seen from these two equations that $\mathrm{Tr}(\hat{\rho}') = 1$ is ensured and, with reference to (3.6), that the action of $\mathcal{T}_i$ on $\hat{\rho}$ is indeed trace-non-increasing for any $\hat{E}_i$.

Any trace-*preserving*, completely positive, linear superoperator $\mathcal{T}_{21}$ acting on a density operator $\hat{\rho}_1$ yields an operator $\hat{\rho}_2$ that immediately satisfies all the requirements of a density operator itself.

The Stinespring dilation theorem states that the action of *any* such superoperator on any state $\hat{\rho}^a$ in $\mathcal{H}_a$ can be reproduced by a *unitary* operator $\hat{U}$ acting on state vectors in a larger Hilbert space $\mathcal{H}_{ab}$ [41].

Thus, any unitary evolution of states in a larger Hilbert space of the system plus its environment can be represented stochastically in the Hilbert space of the system by a trace-preserving, completely positive, linear superoperator; and vice versa. This gives a general formalism for the evolution of any stochastic or entangled system in accordance with the postulates.

[30] Superoperators are referred to as 'operations' by some authors, including the one cited.

3.3 Causality in quantum mechanics

Now that we have a general formalism for quantum mechanics, we can apply it to the matter of causality.

3.3.1 The no-signalling condition

The outcome b_j of a measurement B cannot be said to have been even partly 'caused' by an event A_k unless some statistical correlation exists between the set of possible outcomes $\{b_j\}$ and the set of possible events $\{A_k\}$. This sufficient condition for the absence of causal influence is equivalent to the no-signalling condition defined (from Alice to Bob) by equation (2.8):

$$\begin{aligned} p(b_j|A_kB) &= p(b_j|B) \qquad \forall j,k \\ \Rightarrow \sum_i p(a_ib_j|A_{k_1}B) &= \sum_i p(a_ib_j|A_{k_2}B) \quad \forall j,k_1,k_2 \end{aligned} \tag{3.13}$$

where a_i refers to whatever local effect the event A_k may have, as distinct from the remote outcome b_j.

In operational stochastic quantum theory, in the most general case, our knowledge of the event A_k together with the measurement B is treated as a single joint measurement A_kB. The value of $p(b_j|A_kB)$ is given by (3.6):

$$\sum_i p(a_ib_j|A_kB) = \sum_i \mathrm{Tr}(\hat{E}_{ij}^{(A_kB)}\hat{\rho}^{ab}) \tag{3.14}$$

where $\{\hat{E}_{ij}^{(A_kB)}\}$ is the POVM for the joint measurement on the joint system $\hat{\rho}^{ab}$ in the joint Hilbert space $\mathcal{H}_{ab} = \mathcal{H}_a \times \mathcal{H}_b$.

To investigate causality, we need to split the joint measurement into A_k and B and use the formalism to establish what the statistical independence of b_j on A_k implies about the system.

Because of the nature of the update rule for each measurement outcome, it is necessary to specify an order in which the measurements take place. We will consider A to have taken place first: then we can consider the separate POVMs $\{\hat{E}_i^{(A_k)}\}$ and $\{\hat{E}_j^{(B)}\}$, both of which act in the joint space $\mathcal{H}_{ab}$.

The probability of each outcome of A and the resulting state update are given as follows:

$$p(a_i|A_k) = \mathrm{Tr}(\hat{E}_i^{(A_k)}\hat{\rho}^{ab}) \tag{3.15}$$

$$\hat{\rho} \to \hat{\rho}_i = \frac{\mathcal{T}_i^k(\hat{\rho}^{ab})}{\mathrm{Tr}(\hat{E}_i^{(A_k)}\hat{\rho}^{ab})}. \tag{3.16}$$

The probability of the outcome b_j is then given by (3.14):

$$\begin{aligned} p(b_j|A_kB) &= \sum_i p(b_j|a_iA_kB)p(a_i|A_k) \\ &= \sum_i \mathrm{Tr}\left[\hat{E}_j^{(B)} \frac{\mathcal{T}_i^k(\hat{\rho}^{ab})}{\mathrm{Tr}(\hat{E}_i^{(A_k)}\hat{\rho}^{ab})}\right] \mathrm{Tr}(\hat{E}_i^{(A_k)}\hat{\rho}^{ab}) \\ &= \sum_i \mathrm{Tr}\left[\hat{E}_j^{(B)}\mathcal{T}_i^k(\hat{\rho}^{ab})\right]. \end{aligned} \tag{3.17}$$

If, and only if, this expression has any dependence on k, can we say that there is some statistical causal connection from A_k to b_j.[31]

We know from (3.8) that a Hilbert space $\mathcal{H}_{abc} = \mathcal{H}_{ab} \times \mathcal{H}_c$ exists in which both the measurements $\{\hat{E}_i^{(A_k)}\}$ and $\{\hat{E}_j^{(B)}\}$ can be expressed as projection operators $\{\hat{P}_i^{(A_k)}\}$ and $\{\hat{P}_j^{(B)}\}$; therefore we can write

$$\begin{aligned} p(b_j|A_kB) &= \sum_i \mathrm{Tr}\left[\hat{P}_j^{(B)}\left(\hat{P}_i^{(A_k)}\hat{\rho}^{abc}\hat{P}_i^{(A_k)}\right)\right] \\ &= \mathrm{Tr}\left[\left(\sum_i \hat{P}_i^{(A_k)}\hat{P}_j^{(B)}\hat{P}_i^{(A_k)}\right)\hat{\rho}^{abc}\right]. \end{aligned} \tag{3.18}$$

Since this must apply to any feasible quantum state $\hat{\rho}^{abc}$, there will be a potential for a causal link if and only if $\sum_i \hat{P}_i^{(A_k)}\hat{P}_j^{(B)}\hat{P}_i^{(A_k)}$ depends on k.

Choosing a basis in which the $\hat{P}_i^{(A_k)}$ are diagonal for all i, and representing $\hat{P}_j^{(B)}$ in block form according to the subspaces of each i, a typical element within this sum has the form

$$\begin{aligned} \hat{P}_i^{(A_k)}\hat{P}_j^{(B)}\hat{P}_i^{(A_k)} &= \begin{pmatrix} \hat{0} & & & \\ & \hat{1} & & \\ & & \hat{0} & \\ & & & \ddots \end{pmatrix} \begin{pmatrix} \hat{u} & \hat{v} & \hat{w} & \cdots \\ \hat{v}^\dagger & \hat{x} & \hat{y} & \cdots \\ \hat{w}^\dagger & \hat{y}^\dagger & \hat{z} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \hat{0} & & & \\ & \hat{1} & & \\ & & \hat{0} & \\ & & & \ddots \end{pmatrix} \\ &= \begin{pmatrix} \hat{0} & & & \\ & \hat{x} & & \\ & & \hat{0} & \\ & & & \ddots \end{pmatrix}. \end{aligned}$$

[31] Assuming the choice of measurement A_k could be made with free will – that is, assuming k is not constrained by some factors that also affect the outcome b_j – then there can be no sense in which fundamental quantum statistical expressions such as these could be dependent on k without there being some causal connection from A_k to b_j.

Thus

$$\sum_i \hat{P}_i^{(A_k)} \hat{P}_j^{(B)} \hat{P}_i^{(A_k)} = \begin{pmatrix} \hat{u} & & & \\ & \hat{x} & & \\ & & \hat{z} & \\ & & & \ddots \end{pmatrix} = \hat{P}_j^{(B)} - \hat{\Delta}_j^{(B,A_k)}, \tag{3.19}$$

where $\hat{\Delta}_j^{(B,A_k)}$ contains all the off-diagonal blocks of $\hat{P}_j^{(B)}$.

If $\hat{\Delta}_j^{(B,A_k)} = 0$ for all available measurements A_k, then it is clear that there is no k-dependence and therefore no potential for a causal link. This requires $\hat{P}_j^{(B)}$ to be of block-diagonal form for any basis in which any of the $\hat{P}_i^{(A_k)}$ is diagonal, which implies $\hat{P}_j^{(B)}$ is simultaneously diagonalisable with every $\hat{P}_i^{(A_k)}$.

In terms of the self-adjoint operators that represent these measurements,[32] this implies

$$\left[\hat{A}_k, \hat{B}\right] = 0 \quad \forall k. \tag{3.20}$$

To prove that this is *necessary* as well as sufficient as a no-signalling condition, we need only consider the fact that Alice is free to choose to take no measurement at all. In this case, $\hat{A}_k = \hat{1}$ and $\hat{\Delta}_j^{(B,A_k)} = 0$. Therefore, if *any* measurements have $\hat{\Delta}_j^{(B,A_k)} \neq 0$, then signalling would be possible.

Hence, in a general operational stochastic quantum system, there is no potential for a causal link between Alice and Bob if and only if the self-adjoint extension of every possible measurement available to Alice commutes with that of every possible measurement available to Bob.

3.3.2 Special cases

If measurements A_k and B were already projective measurements – that is, if no internal unknowns or external influences are involved in the measurement process – then (3.20) is a straightforward relationship between the self-adjoint operators representing the measurements in $\mathcal{H}_{ab}$. If they can be considered to

[32] Note that these are operators in $\mathcal{H}_{abc}$, some larger Hilbert space in which both measurements can be represented by self-adjoint operators. Physically, this could be thought of as the space of states for the system plus its entire environment; but an equally suitable Hilbert space can be constructed by enlarging $\mathcal{H}_{ab}$ in accordance with the Naimark extension theorem (3.8) using the measurement $\{\hat{E}_i^{(A_k)}\}$ itself.

act on separate subspaces $\mathcal{H}_a$ and $\mathcal{H}_b$, then the commutation relation holds trivially.

The derivation of the Tsirelson bound (2.13) employs self-adjoint operators and relies on this commutation relation. With no restrictions on the commutators, the relation[33] is insufficient to prevent $\langle \hat{K} \rangle$ from taking its algebraic maximum value of 4. The Tsirelson bound of $\langle \hat{K} \rangle \leq 2\sqrt{2}$ is therefore strictly a *no-signalling* bound.

For POVMs representing *mixtures* of measurements of the form (3.5), no extension of $\mathcal{H}_{ab}$ is required: the no-signalling condition is simply that all the self-adjoint operators $\{\hat{A}_i\}$ and $\{\hat{B}_j\}$ over which all of the probability distributions are taken must satisfy $[\hat{A}_i, \hat{B}_j] = 0$.

For POVMs that are neither projective nor mixtures of projective measurements, but nevertheless operate in separate spaces $\mathcal{H}_a$ and $\mathcal{H}_b$ so that the partial traces follow equation (3.11) – specifically, $\mathrm{Tr}_a[\mathcal{T}_i^k(\hat{\rho}^{ab})] = \mathrm{Tr}_a[\hat{E}_i^{(A_k)}\hat{\rho}^{ab}]$ – then the no-signalling condition can also be shown to hold automatically:

$$\begin{aligned} p(b_j|A_k B) &= \sum_i \mathrm{Tr}\left[\hat{E}_j^{(B)}\mathcal{T}_i^k(\hat{\rho}^{ab})\right] \\ &= \sum_i \mathrm{Tr}_b\left\{\hat{E}_j^{(B)}\mathrm{Tr}_a\left[\mathcal{T}_i^k(\hat{\rho}^{ab})\right]\right\} \\ &= \mathrm{Tr}_b\left\{\hat{E}_j^{(B)}\mathrm{Tr}_a\left[\sum_i \hat{E}_i^{(A_k)}\hat{\rho}^{ab}\right]\right\} \\ &= \mathrm{Tr}\left[(\hat{1}\otimes\hat{E}_j^{(B)})\hat{\rho}^{ab}\right], \end{aligned} \tag{3.21}$$

which is independent of the choice of measurement A_k.

3.4 From discrete to continuous sets of outcomes

3.4.1 Partitions of discrete sets

Postulate 1 tells us that – at least for ideal measurement on a pure state – all probabilities have the form $|\hat{P}_i|\psi\rangle|^2$, where $\hat{P}_i$ is a projection operator for outcome i. Since any complete set of possible outcomes is, by definition, mutually exclusive and exhaustive for any given measurement, a set of projection

[33] It becomes $|\ \langle \hat{K} \rangle - \frac{1}{2}\sum_{i,j}\langle [\hat{A}_i, \hat{B}_j]\rangle\ |\ \leq\ 2\sqrt{2}$.

operators is a very natural way to represent them because, by definition,

$$\hat{P}_i\hat{P}_j = \delta_{ij}\hat{P}_i \tag{3.22}$$

$$\sum_i \hat{P}_i = \hat{1} \tag{3.23}$$

$$\langle\psi|\hat{P}_i|\psi\rangle \geq 0 \quad \forall|\psi\rangle \in \mathcal{H}. \tag{3.24}$$

The third equation here reflects the fact that probabilities can never be negative.

These three equations not only hold for a discrete set $\mathcal{S} = \{a_i\}$ of individual outcomes, they also hold for any *partition* of that set.

A partition is a mutually exclusive and exhaustive set $\{S_i\}$ of sets of outcomes $S_i \subset \mathcal{S}$ (with $S_i \cap S_j = \emptyset$ and $\bigcup_i S_i = \mathcal{S}$). For each set of outcomes S_i, we can define a projection operator as simply the sum of the projection operators for each individual outcome $\hat{P}_{S_i} = \sum_{a_k \in S_i} \hat{P}_k$, and equations equivalent to (3.22) to (3.24) remain true no matter how the set $\mathcal{S}$ is partitioned.

Postulate 2 tells us that, if an ideal measurement gives an outcome a_i, the state vector is updated to a projection onto the subspace of that outcome (which is one of the eigenvectors of the self-adjoint operator for the measurement). If the measurement cannot distinguish between the individual outcomes within a set S_i, the updated state will have the general form $\hat{\rho} = \sum_{a_k \in S_i} p_k|\psi_k\rangle\langle\psi_k|$.

3.4.2 Partitions of continuous sets

For a measurement with **continuous** set $\mathcal{S}$ of outcomes, we can arbitrarily partition the set in precisely the same way, so the same principles should apply. To achieve this requires the mathematics of measure theory [35, §A.1].

The possible outcomes of a measurement are represented using a *measure space* $(\mathcal{S}, \Sigma, \mu)$ which consists of three objects: a set $\mathcal{S}$, which here is the sample space (the set of possible values that an outcome could be considered to take); the set Σ of all measurable subsets of $\mathcal{S}$, which is a σ-algebra[34] over $\mathcal{S}$; and the measure, which is a function $\mu : \Sigma \to \mathbb{R}$ giving a real value[35] $\mu(S_i)$

[34] A σ-algebra over $\mathcal{S}$ is a set of subsets, including $\mathcal{S}$ and $\emptyset$, that is closed under countable applications of the binary operations of union and intersection. The set of all 'measurable' subsets includes every imaginable subset of the sample space, provided the imagination is not inclined to go to a great deal of trouble to seek mathematically pathological counterexamples.

[35] A measure is required to be non-negative for all subsets, and to satisfy the condition that the measure of the union of any two non-overlapping subsets of $\mathcal{S}$ must be equal to the sum of the measures of each subset.

to each subset $S_i \in \Sigma$.

If the outcomes are discrete, a value of $\mu_k = 1$ for every individual outcome a_k would be a simple example. If the outcomes may take a continuous value a, then $\mu(S_i) = \int_{a \in S_i} da$ would be the simplest example of a measure: this can be expressed unambiguously as $d\mu(a) = da$. The extension to any number of parameters is straightforward.

The question now is: given a continuous sample space $\mathcal{S}$ and *any* chosen partition $\{S_i\}$, does a set of projection operators $\{\hat{P}_i\}$ exist that satisfy equations (3.22) to (3.24)? The answer [35, §3.1], for any Hilbert space of countably infinite dimensionality, is yes.

This result enables us to apply Postulates 1 and 2 to measurements with continuous outcomes without modification.

A function $\hat{P}(S)$ that gives us a projection operator for any measurable subset S of the sample space is called a *projection-valued measure* (PVM). Its only difference from a real-valued measure as defined above is that it assigns a projection operator rather than a numerical value to each subset of the sample space.

If $\mathcal{S}_\alpha$ is the set of all outcomes with $a < \alpha$, we can define a projection-valued function called the *resolution of the identity*: $\hat{P}(\alpha) = \hat{P}(\mathcal{S}_\alpha)$, for which $\lim_{\alpha \to \infty} \hat{P}(\alpha) = \hat{1}$. This allows the definition of an 'infinitesimal projection operator'

$$\frac{d}{d\alpha}\hat{P}(\alpha) = \lim_{\delta\alpha \to 0} \frac{\hat{P}(\alpha + \delta\alpha) - \hat{P}(\alpha)}{\delta\alpha}. \tag{3.25}$$

This is not itself an operator in $\mathcal{H}$, but it can be used to construct *operator-valued integrals* that do act in $\mathcal{H}$:

$$\hat{P}(S_i) = \int_{S_i} da \, \frac{d}{da}\hat{P}(a). \tag{3.26}$$

The definition of a PVM tells us that $\hat{P}(S_i)\hat{P}(S_j) = \hat{P}(S_i \cap S_j)$, whereupon

$$\begin{aligned} \int_{S_i} da \int_{S_j} da' \;\; \frac{d}{da}\hat{P}(a) \, \frac{d}{da'}\hat{P}(a') &= \int_{S_i \cap S_j} da \, \frac{d}{da}\hat{P}(a) \\ \Rightarrow \quad \frac{d}{da}\hat{P}(a)\frac{d}{da'}\hat{P}(a') &= \delta(a - a')\frac{d}{da}\hat{P}(a). \end{aligned} \tag{3.27}$$

These 'infinitesimal projection operators' are sometimes expressed in Dirac's

Probability, $p : \Sigma \to \mathbb{R}$, is an example of a measure, with the additional requirement that $p(\mathcal{S}) = 1$.

'continuous basis' form:

$$\frac{d}{da}\hat{P}(a) = |a\rangle\langle a|. \tag{3.28}$$

More generally, we could consider there to be a ν-dimensional subspace that is preserved by each projection:[36]

$$\frac{d}{da}\hat{P}(a) = \sum_{\alpha=1}^{\nu} |a^\alpha\rangle\langle a^\alpha|. \tag{3.29}$$

Superficially, the objects $|a\rangle$ in (3.28) appear to satisfy an eigenvalue equation $\hat{A}|a\rangle = a|a\rangle$ and an orthonormalisation condition $\langle a|a'\rangle = \delta(a-a')$,[37] and they may be referred to as eigenvectors of the measurement $\hat{A}$. However, they are not members of the Hilbert space in which $\hat{A}$ acts, and they do not represent possible states of the system in quantum theory. An operator of this type has no eigenstates or eigenvalues.

3.4.3 Unbounded operators

If the set of outcomes of an operator doesn't have any explicit limit, the operator is said to be *unbounded*. More precisely, an operator $\hat{A}$ is unbounded if there is no maximum value of $\big|\hat{A}|\psi\rangle\big|/\big||\psi\rangle\big|$ over $|\psi\rangle \in \mathcal{H}$. An operator in $\mathcal{H}$, by definition, must map a vector $|\psi\rangle$ to another vector $|\phi\rangle$, both of which must have finite norm: this immediately implies that no such operator can act on all states in $\mathcal{H}$, which raises a suite of technical difficulties that are beyond the scope of this work.[38] However, if an operator is self-adjoint, then it must have a domain that is *dense* in $\mathcal{H}$ [8, §4], meaning that for any vector that is not in its domain, there is a vector arbitrarily close to it that is.[39]

The existence of a 'continuous basis' $\{|a\rangle\}$ for self-adjoint operators is guaranteed by the spectral theorem [35, §3], as is the real-valued set of outcomes a if the operator is used to represent a measurement.

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[36] This could be seen as ascribing a ν-fold degeneracy to $\hat{A}$. More formally, we are admitting a ν-dimensional quotient space on which the $\hat{A}$ acts as the identity operator. The dimensionality ν may be anything from 1 to countably infinite.

[37] More generally, $\hat{A}|a^\alpha\rangle = a|a^\alpha\rangle$ and $\langle a^\alpha|a'^\beta\rangle = \delta(a-a')\delta^{\alpha\beta}$.

[38] See *e.g.* [7, 8, 35].

[39] The domain of $\hat{A}$ is dense in $\mathcal{H}$ if, for all $|\psi\rangle \in \mathcal{H}$ and all $\epsilon > 0$, there exists a state $|\psi'\rangle \equiv |\psi\rangle + |\delta\psi\rangle$ such that $\hat{A}|\psi'\rangle \in \mathcal{H}$ and $\langle\delta\psi|\delta\psi\rangle < \epsilon$.

3.4.4 Continuous observables

Given a pure state $|\psi\rangle$, the probability of obtaining an outcome in S_i, from (3.1), is

$$p(a_i \in S_i|A) = \langle\psi|\,\hat{P}(S_i)\,|\psi\rangle = \int da\langle\psi|a\rangle\langle a|\,\hat{P}(S_i)\,|\psi\rangle. \tag{3.30}$$

It can be seen that the trace form (3.3) remains valid if we adopt the definition $\mathrm{Tr}(\hat{P}\hat{\rho}) \equiv \int da\langle a|\hat{P}\hat{\rho}|a\rangle$.

If an idealised measurement determines that the outcome a lies within the range $a_1 < a < a_2$ but can give no further information regarding its location, then the updated state in the continuous basis can be given using (3.10):

$$\begin{aligned}\hat{\rho} \to \hat{\rho}' &= \frac{\left(\int_{a_1}^{a_2} da|a\rangle\langle a|\right)\hat{\rho}\left(\int_{a_1}^{a_2} da'|a'\rangle\langle a'|\right)}{\int da\langle a|\left(\int_{a_1}^{a_2} da''|a''\rangle\langle a''|\right)\hat{\rho}|a\rangle} \\ &= \frac{\int_{a_1}^{a_2} da\int_{a_1}^{a_2} da'\ |a\rangle\langle a|\hat{\rho}|a'\rangle\langle a'|}{\int_{a_1}^{a_2} da''\langle a''|\hat{\rho}|a''\rangle}.\end{aligned} \tag{3.31}$$

Uncertainty can be represented by replacing the projective measurement operator $\hat{A}$ with a continuous distribution of possible measurements $\hat{A}(r)$, each of which has the same set $\mathcal{S}$ of outcomes, distributed with probability distribution function $f(r)$. This is an example of an *unsharp measurement*, which could for example yield an outcome $a_1 < a < a_2$ representing a value of a to a certain number of significant figures, for example, but without the observer being entirely sure of precisely what measurement took place.

For a given outcome S_i, this defines a POVM $\{\hat{E}_i\}$ of the form[40]

$$\frac{d}{da}\hat{E}(a) = \int dr\ f(r)\ \frac{d}{da}\hat{P}(a_r), \tag{3.32}$$

where $a_r = a + \Delta a(a, r)$ is a stochastic adjustment to every $a \in \mathcal{S}$. The change $\Delta a(a, r)$ is the mismatch between the measurement that is taking place (for a given value of the random variable r) and an idealised projective measurement $\hat{A}$ that would give the outcome a. We may parametrise r so that $\Delta a(a, 0) = 0$.

Provided $\int da\frac{d}{da}\hat{P}(a_r) = \hat{1}$ for all r, the POVM satisfies equations corresponding to (3.23) and (3.24) in common with a projective measure; in general

[40] As noted in Section 3.2.4, this is not the most general form of a POVM. Measurements that may involve coupling to other quantum systems don't necessarily fit this kind of distribution over projection-valued measures in $\mathcal{H}$.

it will not satisfy (3.22).

If a measurement now determines that the outcome a lies in the range $a_1 < a < a_2$, the probability of that outcome and the resulting updated state would then be

$$p(a_1 < a < a_2) = \int dr\ f(r) \int_{a_1}^{a_2} da\ \langle a_r|\ \hat{\rho}\ |a_r\rangle \tag{3.33}$$

$$\hat{\rho} \to \hat{\rho}' = \int dr\ f(r)\ \frac{\int_{a_1}^{a_2} da \int_{a_1}^{a_2} da'\ |a_r\rangle\langle a_r|\hat{\rho}|a'_r\rangle\langle a'_r|}{\int_{a_1}^{a_2} da''\langle a''_r|\hat{\rho}|a''_r\rangle}. \tag{3.34}$$

Equation (3.31) can be seen to be a limiting case with $f(r) = \delta(r)$.

We may note that while a discrete, ideal measurement $\{\hat{P}_i\}$ can be repeated on any otherwise undisturbed state and yield a consistent single outcome a_i every time, this can never be the case for a continuous measurement. This is irrespective of any limitations on the accuracy of a measurement: it is a consequence of the fact that such an outcome would require a projection onto a 'state' $|a\rangle$ that does not exist in the Hilbert space of the system.

An outcome of a_i from a mixture of discrete measurements such as (3.5) could be interpreted as having objectively projected the state into *one* of a set of known subspaces, with it merely being unknown to us which one. In the continuous case, however, such an interpretation is not available to us. If it were suggested that an unsharp measurement objectively projects a state onto one of a range of states $|a\rangle$ with it merely being unknown to us which one, then that suggestion is meaningless if none of those states exist in the space of states of the system.[41]

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[41] One way around this is by imagining an expansion of the Hilbert space to include the eigenstates of continuous operators. This was the approach taken in 1930 by Dirac: *"The bra and ket vectors we now use form a more general space than a Hilbert space."* [38, §10]. This has been followed implicitly or explicitly by many since – for example Shankar [42, §1.10] refers to *"the physical Hilbert space, which is of interest in quantum mechanics... we use the quantifier 'physical' to distinguish it from the Hilbert space as defined by mathematicians."*

Such a space was not defined rigorously until the 1960s [43] and is now known as a 'rigged Hilbert space'. Allowing the elements of the continuous basis expansion to have some ontological status is appealing – it enables a more thorough mathematical discussion of the use of plane waves as approximations, for example [44]. It also permits an interpretation of a physical state in terms of a mixture of eigenstates, as discussed. The cost is a substantial loss of simplicity in the formalism in order to accommodate what would remain states of zero probability in any case. Treating $|a\rangle$ as a physical state on which repeatable measurements could take place would also entail physical infinities for any observable that does not commute with $\hat{A}$, via an uncertainty relation. Although rarely mentioned explicitly in standard textbooks, it could be argued [45] that rigged Hilbert spaces are now ubiquitous in forming part of the formalism of quantum theory in use. The question of whether or not we should consider them to be part of the formalism in this way remains a matter of taste.

If we wish quantum theory to describe quantities that are continuous without imposing physical limits on them, we need to work with self-adjoint unbounded operators with continuous outcomes. It may ultimately be the case that the quantities we think of as continuous are in fact discrete at some level of detail that we do not yet have access to,[42] but in the absence of knowledge of such a scale, we require operators that are not limited by this. On the other hand, no real measurement has an infinite set of outcomes – a measurement can only give a finite amount of information. Operators of the kind described in this section illustrate one way such measurements can be represented.

[42]The search for a theory of quantum gravity has motivated many theories in which spacetime is fundamentally discrete, *e.g.* [46], [47].

4 The relationship between Hilbert space and spaces of generalised coordinates

Thus far, quantum theory has been introduced in a way that is abstracted from space and time. The notion of spacelike separated observers (used for establishing the failure of local realism in Section 2.2), and the unitary evolution of states over time (noted in Section 3.1) have been touched upon; but in order to discuss causality, it will be necessary to examine the relationship between space, time and the quantum state. This relationship will be introduced in this Section.

To begin with, however, we will consider Hamiltonian systems in which the generalised coordinates $\mathbf{x} \equiv \{x_i\}$ *need not* represent positions in space.

4.1 Relationship to classical mechanics

Assuming a linear theory of quantum mechanics, as discussed under the implications of Postulate 1, any evolution of a state[43] from a time t_1 to a time t_2 must take place via a unitary operator $\hat{U}_{21} = \hat{U}(t_2, t_1)$, so that $|\psi_2\rangle = \hat{U}_{21}|\psi_1\rangle$ and $\hat{\rho}_2 = \hat{U}_{21}\hat{\rho}_1\hat{U}_{21}^\dagger$. With time as a continuous parameter, and with the assumptions $\lim_{t_2 \to t_1} \hat{U}_{21} \to \hat{1}$ and $\hat{U}_{31} = \hat{U}_{32}\hat{U}_{21}$, we can always write $\hat{U}_{21} = e^{i\hat{X}_{21}}$ where $\hat{X}_{21}$ is self-adjoint.[44] In the limit $\delta t \to 0$ this gives

$$\hat{U}(t + \delta t, t) = \hat{1} + i\frac{\partial \hat{X}}{\partial t}\delta t. \tag{4.1}$$

The operator $\frac{\partial \hat{X}}{\partial t}$ is referred to as the generator of time evolution.

The expectation value $\langle \hat{A} \rangle \equiv \int p(a|A)da = \mathrm{Tr}(\hat{A}\hat{\rho})$ of any continuous observable $\hat{A}$ then evolves as follows:

$$\begin{aligned}
\frac{d}{dt}\langle \hat{A} \rangle &= \lim_{\delta t \to 0} \frac{1}{\delta t} \left\{ \mathrm{Tr}\left[\hat{A}(t+\delta t)\hat{\rho}(t+\delta t)\right] - \mathrm{Tr}\left[\hat{A}(t)\hat{\rho}(t)\right] \right\} \\
&= \lim_{\delta t \to 0} \frac{1}{\delta t} \left\{ \mathrm{Tr}\left[\hat{A}\hat{\rho}(-i\frac{\partial \hat{X}}{\partial t}\delta t) + \hat{A}(i\frac{\partial \hat{X}}{\partial t}\delta t)\hat{\rho} + \frac{\partial \hat{A}}{\partial t}\hat{\rho}(t)\delta t \right] \right\} \\
&= i\,\langle\, [\hat{A}, \frac{\partial \hat{X}}{\partial t}]\,\rangle + \langle \frac{\partial \hat{A}}{\partial t} \rangle.
\end{aligned} \tag{4.2}$$

In a classical system, we know that any quantity $A(x_i, p_i, t)$ that can be ex-

[43] The convention that the state is considered to evolve, rather than the operators defining observables, is referred to as the Schrödinger picture. I will be employing this convention throughout Sections 3 to 5.

[44] Stone's theorem [35, §5], [7, §IV.6].

pressed in terms of generalised coordinates $\{x_i\}$ and generalised momenta $\{p_i\}$ obeying Hamilton's equations[45] satisfies

$$\frac{dA}{dt} = \{A, H\}_P + \frac{\partial A}{\partial t}. \tag{4.3}$$

This tells us that any operator proportional to the generator of time evolution, $\hat{H} = -\kappa\frac{\partial \hat{X}}{\partial t}$ with some constant κ, can act as a Hamiltonian operator. Given any self-adjoint operators $\hat{A}_i$ for which $i\langle\,[\hat{A}_i, \hat{H}]\,\rangle = -\kappa\{A_i, H\}_P$, the outcomes a_i of the measurements of those observables will, on average, reproduce the values of the classical quantities A_i as they change through time.

This requires only the following:

Postulate 3 *The generator of time evolution can be expressed as a function of a set of continuous operators that commute with each other, a set of operators canonically conjugate*[46] *to them, and a set of discrete operators that commute with them.*

For the purposes of this Section, we will suppose that these operators are *observables*, *i.e.* that they are self-adjoint operators that can represent measurements, at least in an unsharp form such as (3.32). (They need not be in general: we will encounter counterexamples in Section 7.)

We may therefore write the generator of time evolution as a function $\hat{H}(t) = H(\hat{x}_i, \hat{p}_i, \hat{\tau}_\alpha; t)$ of a set of continuous operators $\{\hat{x}_i\}$, a set of conjugate operators $\{\hat{p}_i\}$ satisfying $[\hat{x}_i, \hat{p}_j] = i\kappa\delta_{ij}$, and a set of discrete operators $\{\hat{\tau}_\alpha\}$. Discrete operators in this context give rise to non-classical degrees of freedom, as we will see in Section 4.2. For now, let us consider the case where there are no $\hat{\tau}_\alpha$.

If we have an observable of the form $\hat{A}(t) = A(\hat{x}_i, \hat{p}_i; t)$, then it follows that

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[45] I am taking Hamilton's equations, $\frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i}$ and $\frac{dx_i}{dt} = \frac{\partial H}{\partial p_i}$, to be the defining characteristic of a classical mechanical system. The Poisson bracket of two functions $f(x_i, p_i, t)$ and $g(x_i, p_i, t)$ is defined by $\{f, g\}_P \equiv \sum_i \left(\frac{\partial f}{\partial x_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial x_i}\right)$ [48, §12], [49, §10].

[46] Two self-adjoint operators $\hat{A}$ and $\hat{B}$ are canonically conjugate to one another if their commutator $[\hat{A}, \hat{B}]$ is a multiple of the unit operator. If a linearly independent set of continuous observables $\{\hat{x}_i\}$ exists such that $[\hat{x}_i, \hat{x}_j] = 0$, it is straightforward to find operators $\hat{k}_i$ for which $[\hat{x}_i, \hat{k}_j] = Z\delta_{ij}$. These may be self-adjoint provided Z is imaginary, in which case they are called conjugate observables. In the continuous basis defined by $\hat{\mathbf{x}}$, $\hat{k}_i = \int d\mathbf{x}\,|x\rangle i\frac{\partial}{\partial x_i}\langle x|$ is sufficient.

It can be proven that canonically conjugate operators are necessarily unbounded [50, §7.3]. An alternative form of canonical commutation relation that does not involve unbounded operators was also developed in 1927 by Weyl, and is in widespread use where rigorous mathematical formulations of quantum theory are required. See *e.g.* [7, §IV.6], [51].

the time evolution of its expectation value $\langle A \rangle$ will be identical[47] to the time evolution of a classical variable $A(x_i, p_i, t)$ in a system with classical Hamiltonian $H(x_i, p_i, t)$. The Hamiltonian we observe that describes this classical behaviour is *the same function* of x_i and p_i as the operator $\hat{H}(t) = H(\hat{x}_i, \hat{p}_i; t)$ is of $\hat{x}_i$ and $\hat{p}_i$.

By appropriating known classical Hamiltonians, for example that of a non-relativistic particle of mass m, $H(\mathbf{x}, \mathbf{p}) = \mathbf{p}^2/2m + V(\mathbf{x})$, it is therefore possible to describe quantum systems capable of giving rise to known classical behaviour; and correspondences of this type allow us to evaluate the constant κ as $\hbar$, the reduced Planck's constant.

Conceptually, however, all we need postulate is the existence of continuous observables and their conjugates, and a generator of time evolution that is determined by them. The classical behaviour of expectation values then emerges automatically. The expectation values of the continuous observables and their conjugates then corresponds to canonical pairs of generalised coordinates.

From the fact that we recognise classical Hamiltonian systems in which the coordinates $\mathbf{x}$ correspond directly to one or more positions in space, we can assert that **our quantitative experience of space is an emergent property of these three postulates.**

We have arrived at Ehrenfest's theorem:

$$\frac{d}{dt}\langle \hat{A} \rangle = \frac{1}{i\hbar} \langle\, [\hat{A}, \hat{H}] \,\rangle + \langle \frac{\partial \hat{A}}{\partial t} \rangle. \tag{4.4}$$

If $\hat{H}$ is not explicitly time-dependent, the time evolution operator can therefore be written $\hat{U}(t_2, t_1) = \exp\,[\frac{\hat{H}}{i\hbar}(t_2 - t_1)]$.

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[47] We can verify this for any Hamiltonian operator that can be expressed as a series $\hat{H} = \sum_n (\hat{p}_k)^n f_n(\hat{x}_i, \hat{p}_{i\neq k}, t)$. (For any sum of products of operators it is always possible to re-order using commutators to obtain this form.) This automatically satisfies $\langle [\hat{x}_\alpha, \hat{H}] \rangle = i\hbar \langle \frac{\partial \hat{H}}{\partial \hat{p}_k} \rangle = i\hbar \frac{dx_k}{dt} = i\hbar \{x_k, H\}_P$. For functions $\hat{A}(t) = A(\hat{x}_i, \hat{p}_i, t)$ and $A(x_i, p_i, t)$, the equivalence of commutators with Poisson brackets follows similarly.

In the general case,[48]

$$\hat{U}(t+\delta t,t) = \hat{1} + \frac{1}{i\hbar}\hat{H}(t)\delta t \tag{4.5}$$

$$\hat{U}(t_2,t_1) = T\exp\int_{t_1}^{t_2}\frac{1}{i\hbar}\hat{H}(t)dt \tag{4.6}$$

$$\equiv \sum_{k=0}^{\infty}\frac{1}{k!}\frac{1}{(i\hbar)^k}\int_{t_1}^{t_2}dt'\int_{t_1}^{t_2}dt''\ldots\int_{t_1}^{t_2}dt^{(k)}\ T\Big\{\hat{H}(t')\hat{H}(t'')\ldots\hat{H}(t^{(k)})\Big\}.$$

The Schrödinger equation follows from (4.5):

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle &= i\hbar\lim_{\delta t\to 0}\frac{1}{\delta t}\left(\hat{U}(t+\delta t,t)-\hat{1}\right)|\psi(t)\rangle \\ &= \hat{H}(t)|\psi(t)\rangle, \end{aligned} \tag{4.7}$$

or, more generally,[49]

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}(t) = -[\hat{\rho}(t),\hat{H}]. \tag{4.8}$$

A canonical operator or set of operators such as $\hat{\mathbf{x}} \equiv \{\hat{x}_i\}$ can, like any self-adjoint operator with a measure space of outcomes $(\mathcal{S},\Sigma,d\mathbf{x})$, be used to generate projection operators of the form $\hat{P}(S) = \int_S d\mathbf{x}\ |x\rangle\langle x|$ for any subset of outcomes $S \in \Sigma$. We may take the dimensionality of the measure space to be the number n of canonical pairs $(\hat{x}_i,\hat{p}_i)$ for the system, so that $d\mathbf{x} \equiv \prod_{i=1}^{n} dx_i$. Using this continuous basis $\{|x\rangle\}$, a *wavefunction* can be defined:

$$\psi(\mathbf{x},t) \equiv \langle x|\psi(t)\rangle. \tag{4.9}$$

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[48]The notation 'T exp' refers to the time-ordered exponential, defined by the sum of time-ordered products as shown in (4.6).

The time-ordered product $T\{\hat{A}_1(t_1)\hat{A}_2(t_2)\ldots\hat{A}_k(t_k)\}$ of a set of operators $\{\hat{A}_i(t_i)\}$ evaluated at different times (or at equal times provided the operators commute) is defined to be the product of those operators when arranged from left to right in order of increasing time. That is,

$$T\{\hat{A}_1(t_1)\hat{A}_2(t_2)\ldots\hat{A}_k(t_k)\} \equiv \hat{A}_{i_1}(t_{i_1})\hat{A}_{i_2}(t_{i_2})\ldots\hat{A}_{i_k}(t_{i_k}),$$

where $\{i_1,i_2,...,i_k\}$ is the permutation of $\{1,2,...,k\}$ for which $t_{i_1} \le t_{i_2} \le \ldots \le t_{i_k}$.

[49]This equation is, using (4.4), equivalent to $\frac{d}{dt}\langle\hat{\rho}\rangle = 0$. For *open* systems, in which unitary evolution effectively takes place in a larger Hilbert space as described in Section 3.2.5, equation (4.8) can be generalised further to

$$i\hbar\frac{\partial\hat{\rho}}{\partial t} = -[\hat{\rho},\hat{H}] + i\hbar\mathcal{L}_d(\hat{\rho}),$$

where $\mathcal{L}_d(\hat{\rho}) = \frac{1}{2}\sum_j\left([\hat{V}_j\hat{\rho},\hat{V}_j^\dagger]+[\hat{V}_j,\hat{\rho}\hat{V}_j^\dagger]\right)$ is the Lindblad dissipation term, constructed from a set of operators $\{\hat{V}_j\}$ on $\mathcal{H}$ representing the effect of the environment on the system. This equation may be employed to investigate the nature of decoherence in quantum mechanics, including the measurement process itself [17, §21].

The absolute square of the wavefunction, from (3.30), is a probability distribution function for the measure space of outcomes:

$$p(\mathbf{x} \in S) = \int_S d\mathbf{x}\, |\psi(\mathbf{x}, t)|^2 \qquad \forall S \in \Sigma. \tag{4.10}$$

The nature of the conjugate operators $\hat{p}_i$ in this basis can be deduced from the commutation relation $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}\hat{1}$. We are looking for a linear operator $\hat{p}_i^{(x)}$ to satisfy the equivalence $\hat{p}_i|\psi\rangle = |\phi\rangle \;\Leftrightarrow\; \hat{p}_i^{(x)}\psi(\mathbf{x}) = \phi(\mathbf{x})$. The most general form in n coordinate dimensions is

$$\hat{p}_i^{(x)}\psi(\mathbf{x}) = \sum_{r_1=0}^{\infty} \cdots \sum_{r_n=0}^{\infty} a_i^{(\mathbf{r})}(\mathbf{x}) \frac{\partial^{r_1+\ldots+r_n}\psi(\mathbf{x})}{\partial x_1^{r_1} \ldots \partial x_n^{r_n}}.$$

Using the commutation relation as a constraint, all but two of the terms vanish and we're left with

$$\hat{p}_i^{(x)}\psi(\mathbf{x}, t) = \left[a_i^{(\mathbf{0})}(\mathbf{x}) - i\hbar \frac{\partial}{\partial x_i} \right] \psi(\mathbf{x}, t), \tag{4.11}$$

with an arbitrary function $a_i^{(\mathbf{0})}(\mathbf{x})$. If we propose a momentum basis $\{|p\rangle\}$ such that $\hat{p}_i|p\rangle = p_i|p\rangle$, then by definition we have $\hat{p}_i^{(x)}\langle x|p\rangle = p_i\langle x|p\rangle$. This can be solved using (4.11), provided $a_i^{(\mathbf{0})}(\mathbf{x})$ can be written in the form $\hbar\frac{\partial\phi}{\partial x_i}$,[50] giving

$$\langle x|p\rangle = A\, e^{i\phi(\mathbf{x})} e^{i\mathbf{x}.\mathbf{p}/\hbar}, \tag{4.12}$$

where A is a real constant and $\phi(\mathbf{x})$ an arbitrary differentiable scalar field. The completeness requirement $\int d\mathbf{p}\, |p\rangle\langle p| = \hat{1}$ together with $\langle x'|x\rangle = \delta(\mathbf{x}-\mathbf{x}')$ then implies $A = (2\pi\hbar)^{-n/2}$.

The function $\phi(\mathbf{x})$ may be eliminated by a change of basis of the form $|x\rangle \to |x'\rangle = e^{i\phi(\mathbf{x})}|x\rangle$, which preserves all relevant relations; we will adopt this simpler basis here.

$$\begin{aligned} \hat{p}_i^{(x)} &= -i\hbar \frac{\partial}{\partial x_i} \\ \langle x|p\rangle &= (2\pi\hbar)^{-n/2}\, e^{i\mathbf{x}.\mathbf{p}/\hbar}\,. \end{aligned} \tag{4.13}$$

In the case where our system is a non-relativistic single particle with Hamiltonian $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}})$, the quantum mechanics of that system is reduced by the Schrödinger equation to a differential equation in $\psi(\mathbf{x}, t)$ with respect to

[50] *i.e.* provided $\mathbf{a}^{(\mathbf{0})}(\mathbf{x})$ is a curl-free field.

spatial coordinates and time that has the characteristics of a wave equation. Using this equation, observations of the wave-like properties of particles allow the evaluation of $\hbar$.[51]

4.2 Non-classical degrees of freedom

In Section 4.1, we employed a generalised coordinate basis $\{|x\rangle\}$ generated from n pairs of classical canonical variables (x_i, p_i). This basis satisfies the n-dimensional equivalent of equation (3.28):

$$\frac{d}{d\mathbf{x}}\hat{P}(\mathbf{x}) \equiv \frac{d^n}{dx_1 \dots dx_n}\hat{P}(\mathbf{x}) = |x\rangle\langle x|, \tag{4.14}$$

from which the components of the continuous operator $\hat{\mathbf{x}}$ could be expressed as

$$\hat{x}_i = \int d\mathbf{x}\; x_i\; |x\rangle\langle x|. \tag{4.15}$$

A more general formulation would involve equation (3.29), in which a ν-dimensional subspace of $\mathcal{H}$ is preserved by each projection:

$$\frac{d}{d\mathbf{x}}\hat{P}(\mathbf{x}) = \sum_{\alpha=1}^{\nu} |x^\alpha\rangle\langle x^\alpha|. \tag{4.16}$$

and

$$\hat{x}_i = \sum_{\alpha=1}^{\nu} \int d\mathbf{x}\; x_i\; |x^\alpha\rangle\langle x^\alpha|. \tag{4.17}$$

We can introduce a ν-component wavefunction

$$\psi^\alpha(\mathbf{x}) \equiv \langle x^\alpha|\psi\rangle. \tag{4.18}$$

If the Hamiltonian operator $\hat{H}(t)$ takes the same functional form as the classical Hamiltonian, then the resulting dynamics would be identical to the dynamics generated in Section 4.1. We can generalise by introducing discrete observables $\hat{\tau}_i$ into the Hamiltonian:

$$\hat{H}(t) = H(\hat{\mathbf{x}}, \hat{\mathbf{p}}, \hat{\tau}_i; t). \tag{4.19}$$

[51] $\hbar = 1.054571726 \times 10^{-34}$Js, with a standard error of one part in 22 million [52].

We can express any local[52] operator in a coordinate representation:

$$\hat{A} = \sum_{\alpha\beta} \int d\mathbf{x}\, |x^\alpha\rangle \hat{A}^{(x)\alpha\beta}(\mathbf{x}) \langle x^\beta| \tag{4.20}$$

where $\hat{A}^{(x)\alpha\beta}(\mathbf{x}) \equiv \langle x^\alpha|\, \hat{A}\, |x^\beta\rangle$. From (4.17), $\hat{x}_i^{(x)\alpha\beta}(\mathbf{x}) = x_i \delta^{\alpha\beta}$. The commutation relations $[\hat{x}_i, \hat{p}_j] = i\hbar\, \delta_{ij}$ then imply the following general form for the momentum operator:

$$\hat{p}_i^{(x)\alpha\beta} \psi(\mathbf{x}, t) = \left[a_i^{(\mathbf{0})\alpha\beta}(\mathbf{x}) - i\hbar\, \delta^{\alpha\beta} \frac{\partial}{\partial x_i} \right] \psi(\mathbf{x}, t). \tag{4.21}$$

with an arbitrary set of matrix functions $a_i^{(\mathbf{0})\alpha\beta}(\mathbf{x})$.

As these are matrices, an exponential equation for $\langle x^\alpha | p^\beta \rangle$ of the form (4.12) only follows if a function $\phi^{\alpha\beta}(\mathbf{x})$ exists which satisfies $a_i^{(\mathbf{0})\alpha\beta}(\mathbf{x}) = \hbar\, \partial\phi^{\alpha\beta}/\partial x_i$ for all i **and** which commutes with the $a_i^{(\mathbf{0})\alpha\beta}(\mathbf{x})$ for all $\mathbf{x}$.

These are significant restrictions, so we cannot give a general form for $\langle x^\alpha | p^\beta \rangle$. They are, of course, trivially satisfied by $\phi^{\alpha\beta}(\mathbf{x}) = 0$, which is sufficient for the non-relativistic theory. In that case, we may use

$$\begin{aligned} \hat{p}_i^{(x)\alpha\beta} &= -i\hbar\, \delta^{\alpha\beta} \frac{\partial}{\partial x_i} \\ \langle x^\alpha | p^\beta \rangle &= (2\pi\hbar)^{-n/2}\, \delta^{\alpha\beta}\, e^{i\mathbf{x}.\mathbf{p}/\hbar}\, . \end{aligned} \tag{4.22}$$

Given any $\nu \times \nu$ self-adjoint matrix with fixed components $\tau_i^{\alpha\beta}$, the operator

$$\hat{\tau}_i = \sum_{\alpha\beta} \int d\mathbf{x}\, |x^\alpha\rangle \tau_i^{\alpha\beta} \langle x^\beta|$$

is a coordinate-independent operator acting on $\mathcal{H}$. It clearly commutes with the operators $\hat{x}_i$ and $\hat{p}_i$. Any operator of this type represents an inherently quantum degree of freedom.

Each of these quantum variables may have a scalar, vector or general tensor character with respect to the labels i of the canonical operators. An example

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[52] The completeness of the coordinate basis implies that any operator, local or otherwise, is expressible as follows:

$$\hat{A} = \sum_{\alpha\beta} \int d\mathbf{x}'\, d\mathbf{x}\, |x'^\alpha\rangle \hat{A}^{(x,x')\alpha\beta}(\mathbf{x}, \mathbf{x}') \langle x^\beta|$$

where $\hat{A}^{(x,x')\alpha\beta}(\mathbf{x}, \mathbf{x}') \equiv \langle x'^\alpha|\, \hat{A}\, |x^\beta\rangle$. A local operator, by definition, is one whose coordinate representation has the form $\hat{A}^{(x,x')\alpha\beta}(\mathbf{x}, \mathbf{x}') = \hat{A}^{(x)\alpha\beta}(\mathbf{x})\, \delta(\mathbf{x} - \mathbf{x}')$.

of a vector operator for a particle in n=3 dimensions with a ν=2-dimensional quotient space is the spin variable $\hat{\boldsymbol{\sigma}}$ (see below). While the functional form no longer duplicates that of the classical Hamiltonian $H(x_i, p_i, t)$, it should reproduce the behaviour of the classical system given the appropriate conditions.

The **Pauli–Schrödinger Hamiltonian** for a spin-$\frac{1}{2}$ particle in an electromagnetic field (in three-dimensional Cartesian coordinates) is an example of a Hamiltonian containing discrete observables. The classical Hamiltonian for a particle with charge q in an electromagnetic field is

$$H(\mathbf{x}, \mathbf{p}, t) = \frac{(\mathbf{p} - q\mathbf{A}(\mathbf{x}, t))^2}{2m} + q\phi(\mathbf{x}, t), \tag{4.23}$$

from which we can obtain the Lorentz force law (here using Cartesian coordinates):

$$\begin{aligned} \dot{x}_i &= \frac{\partial H}{\partial p_i} &&= \frac{p_i - qA_i}{m} \\ \dot{p}_i &= -\frac{\partial H}{\partial x_i} &&= q\left[\dot{x}_j \frac{\partial A_j}{\partial x_i} - \frac{\partial \phi}{\partial x_i}\right] && (4.24) \\ \Rightarrow \quad m\ddot{\mathbf{x}} &&&= q\left[(\dot{\mathbf{x}} \times (\nabla \times \mathbf{A})) - \nabla\phi - \frac{\partial \mathbf{A}}{\partial t}\right]. && (4.25) \end{aligned}$$

Creating a Hamltonian operator by direct replacement of $\mathbf{x} \to \hat{\mathbf{x}}$ and $\mathbf{p} \to \hat{\mathbf{p}}$ gives rise to equivalent expressions for the expectation values $\frac{d}{dt}\langle \hat{x}_i \rangle$, $\frac{d}{dt}\langle \hat{p}_i \rangle$ and $m\frac{d^2}{dt^2}\langle \hat{\mathbf{x}} \rangle$, per Ehrenfest's theorem. For electrons, however, this treatment as a classical particle fails to account for its intrinsic magnetic moment. This is remedied by introducing an inherently quantum degree of freedom $\hat{\boldsymbol{\sigma}}$ with three components $\hat{\sigma}_i = \sum_{\alpha\beta} \int d\mathbf{x}\, |x^\alpha\rangle \sigma_i^{\alpha\beta} \langle x^\beta|$, where $\sigma_i^{\alpha\beta}$ are the Pauli matrices, into the Hamiltonian:

$$\hat{H}(t) = \frac{[\hat{\boldsymbol{\sigma}}.(\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{x}}, t))]^2}{2m} + q\phi(\hat{\mathbf{x}}, t). \tag{4.26}$$

The expectation values now satisfy

$$\begin{aligned} \frac{d}{dt}\langle \hat{x}_i \rangle &= \frac{1}{i\hbar}\,[\hat{x}_i, \hat{H}] &&= \left\langle\, \frac{\hat{p}_i - qA_i}{m} \,\right\rangle \\ \frac{d}{dt}\langle \hat{p}_i \rangle &= \frac{1}{i\hbar}\,[\hat{p}_i, \hat{H}] &&= q\left\langle\, \frac{\hat{p}_j - qA_j}{2m}\frac{\partial A_j}{\partial \hat{x}_i} + \frac{\partial A_j}{\partial \hat{x}_i}\frac{\hat{p}_j - qA_j}{2m} - \frac{\partial \phi}{\partial \hat{x}_i} \,\right\rangle \\ & && \quad + \frac{\hbar q}{2m}\left\langle\, \epsilon_{jkl}\hat{\sigma}_j \frac{\partial^2 A_l}{\partial \hat{x}_i \partial \hat{x}_k} \,\right\rangle \qquad (4.27) \end{aligned}$$

$$\Rightarrow \quad m\frac{d^2}{dt^2}\langle\hat{\mathbf{x}}\rangle \;=\; q\,\langle\,\frac{\hat{\mathbf{p}}-q\mathbf{A}}{2m}\times(\nabla\times\mathbf{A})-(\nabla\times\mathbf{A})\times\frac{\hat{\mathbf{p}}-q\mathbf{A}}{2m}\,\rangle+q\,\langle -\nabla\phi-\frac{\partial\mathbf{A}}{\partial t}\rangle$$
$$+\frac{\hbar q}{2m}\,\langle\,\nabla(\hat{\boldsymbol{\sigma}}.\nabla\times\mathbf{A})\,\rangle. \qquad (4.28)$$

The first terms in (4.27) and (4.28) can be seen to be equivalent to those of (4.24) and (4.25), with a symmetrisation of the operator products. The final term in each of (4.27) and (4.28) is the expectation value of the force on a magnetic moment of $(\hbar q/2m)\hat{\boldsymbol{\sigma}}$ in a magnetic field $\nabla\times\mathbf{A}(\hat{\mathbf{x}})$.

The introduction of extra degrees of freedom directly into the Hamiltonian operator in this way is consistent with Postulate 3. The new operators may alter the dynamics, but the position operator $\hat{\mathbf{x}}$ and momentum operator $\hat{\mathbf{p}}$ remain well-defined, and they retain a consistent and straightforward interpretation in relation to the canonical variables of the original classical Hamiltonian.

We will find in Section 6 that this consistency is not retained when we begin to consider relativistic Hamiltonians.

4.3 The single particle

The motivation for setting out the correspondence between Hamiltonian systems and quantum theories in this Section was to establish a connection between the postulates of quantum theory and our quantitative experience of spatial location.

Hamiltonian mechanics would not normally be said to *define* spatial coordinates.[53] Rather, it is a well-established description of the classical world in terms of any parametrisation of its degrees of freedom. The key is that some parametrisations can be arranged *by definition* to correspond to spatial locations. The simplest such system – and the only one for which the set of generalised coordinates *is* a set of coordinates for a location in space – is the **single particle**.

In effect, we have a 'test-particle' definition for quantifying a spatial location: *a set of numbers* $\mathbf{x}$ *that would be valid as Hamiltonian coordinates for a classical single particle system if such a particle were to be found at that location.* Because of the correspondence described in Section 4.1, there is a natural extension of this to quantum theory: we seek a continuous operator $\hat{\mathbf{x}}$ whose expectation values obey the same dynamical laws as $\mathbf{x}$. This is the

[53] It would not be a ridiculous proposal, however: our most sophisticated and well-established *classical* notion of location comes from the general theory of relativity, and this theory can be cast in a Hamiltonian form (*e.g.* [53]).

program we will be following for the next two Sections.

A side-effect of this attempt is that we can associate a *continuous basis element* with every point in space: $\mathbf{x} \mapsto |x\rangle$. If R is a spatial region, we have a map

$$R \mapsto \mathcal{H}_R \equiv \int_R d\mathbf{x}\, |x\rangle. \tag{4.29}$$

This $\mathcal{H}_R$ is a *subspace* of $\mathcal{H}$, and the projection operator $\hat{P}_R \equiv \int_R d\mathbf{x}\, |x\rangle\langle x|$ projects onto it. We have a map between arbitrarily small, non-overlapping regions of space and mutually orthogonal subspaces of $\mathcal{H}$.

Since we observe that classical particles move in three-dimensional Euclidean space and wish to maintain this correspondence, this means that our continuous operator $\hat{\mathbf{x}}$ imposes a three-dimensional Euclidean topology on the set of subspaces of $\mathcal{H}$, the space of states for a single particle.

5 Propagators

In this Section, our focus is on the Hamiltonian of a single particle. The notation $(\mathbf{x}, \mathbf{p})$ from the previous Section will be maintained and the calculations will be kept as general as possible, but we now wish to interpret $\mathbf{x}$ as the coordinates of a location in space. This will enable us to discuss **signalling** between spatial locations, and to identify the role of propagators, the coordinate space path integral and Green's functions in the causal (or otherwise) behaviour of quantum theory.

5.1 Canonical quantum mechanics and causality

We begin by applying the no-signalling condition from Section 3.3.1 to a general single-particle system.

Consider a binary measurement by Alice at time t_A to detect the particle in a spatial region R_A. An ideal detector would be represented by an observable of the form[54]

$$\hat{A} = \int_{R_A} d\mathbf{x}\, |x\rangle\langle x|. \tag{5.1}$$

If the state of the system at time t_A is $\hat{\rho}$, then the probability $p(+|R_A)$ for a positive detection in region R_A and the resulting state update are given by (3.31)

$$p(+|R_A) = \int_{R_A} d\mathbf{x}\, \langle x|\, \hat{\rho}\, |x\rangle \tag{5.2}$$

$$\hat{\rho} \to \hat{\rho}_+ = \frac{\int_{R_A} d\mathbf{x} \int_{R_A} d\mathbf{x}'\, |x\rangle\langle x|\, \hat{\rho}\, |x'\rangle\langle x'|}{\int_{R_A} d\mathbf{x}''\, \langle x''|\, \hat{\rho}\, |x''\rangle} \tag{5.3}$$

The probability of a negative result is $p(-|R_A) = 1 - p(+|R_A)$; the resulting update $\hat{\rho} \to \hat{\rho}_-$ has the same form as above but with the integrals over $X \setminus R_A$, the complement of R_A in X.

A similar position measurement $\hat{B}$ is made by Bob at time t_B and in region R_B. When this measurement takes place, the state has evolved to $\hat{U}_{BA}\, \hat{\rho}_\pm\, \hat{U}_{BA}^\dagger$, where $\hat{U}_{BA} = \hat{U}(t_B, t_A)$ is the evolution operator between times t_A and t_B.

[54] We have taken $\nu = 1$ here. We generalise to include non-classical degrees of freedom in Section 5.3

The total probability of Bob registering a positive detection is

$$\begin{aligned} p(+|R_B R_A) &= \sum_{\pm} p(+|R_B R_A \pm)\; p(\pm|R_A) \\ &= \int_{R_B} d\mathbf{x}''\, \langle x''|\, \hat{U}_{BA}\, \hat{\rho}_+\, \hat{U}_{BA}^\dagger\, |x''\rangle \int_{R_A} d\mathbf{x}\, \langle x|\, \hat{\rho}\, |x\rangle \\ &\qquad + \int_{R_B} d\mathbf{x}''\, \langle x''|\, \hat{U}_{BA}\, \hat{\rho}_-\, \hat{U}_{BA}^\dagger\, |x''\rangle \int_{X\setminus R_A} d\mathbf{x}\, \langle x|\, \hat{\rho}\, |x\rangle \\ &= \int_{R_B} d\mathbf{x}''\, \langle x''|\, \hat{U}_{BA} \left(\int_{R_A} d\mathbf{x} \int_{R_A} d\mathbf{x}'\, |x\rangle\langle x|\, \hat{\rho}\, |x'\rangle\langle x'| \right) \hat{U}_{BA}^\dagger\, |x''\rangle \\ &\qquad + \text{similar term with } R_A \to X\setminus R_A \\ &= \int_{R_A^2 \cup (X\setminus R_A)^2} d\mathbf{x} d\mathbf{x}' \int_{R_B} d\mathbf{x}''\; K_{BA}(\mathbf{x}'', \mathbf{x})\, \langle x|\, \hat{\rho}\, |x'\rangle\, K_{BA}^*(\mathbf{x}'', \mathbf{x}'), \end{aligned} \tag{5.4}$$

where K_{BA} is the **propagator** [54], defined by

$$K_{BA}(\mathbf{x_B}, \mathbf{x_A}) \equiv \langle x_B|\, \hat{U}(t_B, t_A)\, |x_A\rangle. \tag{5.5}$$

The integrals in (5.4) over $R_A \times R_A$ and $(X\setminus R_A)\times(X\setminus R_A)$ can be replaced by an integral over $X\times X$ less integrals over $R_A\times(X\setminus R_A)$ and $(X\setminus R_A)\times R_A$. This gives

$$p(+|R_B R_A) = p(+|R_B) - 2\,\Re\{\Delta p(+|R_B R_A)\} \tag{5.6}$$

where the first term is the $X \times X$ integration, which is independent of $\hat{A}$,

$$p(+|R_B) = \int_{R_B} d\mathbf{x}''\, \langle x''|\, \hat{U}_{BA}\, \hat{\rho}\, \hat{U}_{BA}^\dagger\, |x''\rangle, \tag{5.7}$$

and the second term contains all the $\hat{A}$-dependence,[55] with

$$\Delta p(+|R_B R_A) = \int_{R_A} d\mathbf{x} \int_{X\setminus R_A} d\mathbf{x}' \int_{R_B} d\mathbf{x}''\; K_{BA}(\mathbf{x}'', \mathbf{x})\, \langle x|\, \hat{\rho}\, |x'\rangle\, K_{BA}^*(\mathbf{x}'', \mathbf{x}'). \tag{5.8}$$

The probability, from (5.6), of Bob's measurement registering a pos-

[55] In the limit of small regions R_A and R_B, and employing a pure state $\hat{\rho} = |\psi\rangle\langle\psi|$ with wavefunction $\psi(\mathbf{x}, t) \equiv \langle x|\, \hat{U}(t, t_A)\, |\psi\rangle$, the $\hat{A}$-dependent term reduces to

$$\begin{aligned} \Delta p(+|R_B R_A) &= R_B R_A\, K_{BA}(\mathbf{x_B}, \mathbf{x_A}) \psi(\mathbf{x_A}, t_A) \int_{X\setminus R_A} d\mathbf{x}'\; \psi^*(\mathbf{x}', t_A)\, K_{BA}^*(\mathbf{x_B}, \mathbf{x}') \\ &= R_B R_A\, \psi^*(\mathbf{x_B}, t_B)\, K_{BA}(\mathbf{x_B}, \mathbf{x_A})\, \psi(\mathbf{x_A}, t_A) \;-\; \mathcal{O}\left(R_B (R_A)^2\right). \end{aligned}$$

itive response will in general depend on the location of Alice's measurement unless $K_{BA}(\mathbf{x_B}, \mathbf{x_A}) = 0$ for all $\mathbf{x_A} \in R_A$ and $\mathbf{x_B} \in R_B$.

In Appendix A.1, this result is generalised to any spatially-restricted operator of the form

$$\hat{A} = \int_{R_A} d\mathbf{x} \int_{R_A} d\mathbf{x}' \; |x'\rangle \hat{A}^{(x,x')} \langle x|, \tag{5.9}$$

where the operator $\hat{A}^{(x,x')}$ may be a function of $\mathbf{x}$ and $\mathbf{x}'$, or any series of finite order differential operators with functional coefficients.

If the propagator is non-zero for any $(\mathbf{x_B}, t_B)$ outside the future light cone of any $(\mathbf{x_A}, t_B)$, this would mean that operators of the form (5.9) permit superluminal signalling, which leads to significant problems in terms of causality (see Section 6.1.3). As we will see in the next Section, this is indeed the case – the propagator does not vanish for any finite interval.

The calculation above mirrors that leading to equation (3.19). If the off-diagonal terms $\hat{\Delta}_j^{(B,A_k)}$ do not vanish in that equation then the measurements A_k and B are causally linked. In the coordinate basis here, the 'off-diagonal' terms give rise to the Δp in (5.6), as can be seen from the asymmetric character of range of the $d\mathbf{x}d\mathbf{x}'$ integral. The original argument was shown to be equivalent to a commutation rule (3.20); the same argument applies for position measurements:[56]

$$K_{BA}(\mathbf{x_B}, \mathbf{x_A}) = 0 \;\; \forall \, \mathbf{x_A} \in R_A, \; \mathbf{x_B} \in R_B \quad \Leftrightarrow \quad \left[\hat{U}_{BA} \, \hat{A} \, \hat{U}_{BA}^\dagger \, , \, \hat{B}\right] = 0 \;\; \forall k. \tag{5.10}$$

The propagator result relies on the use of idealised projection operators corresponding to the detection or non-detection of a particle in a spatial region R_A. The commutator result, however, applies to *any* measurement $\hat{A}$ and $\hat{B}$ available to Alice and Bob (Section 3.3.1), so we may make a more general statement:

$$\left[\hat{U}_{BA} \, \hat{A} \, \hat{U}_{BA}^\dagger \, , \, \hat{B}\right] = 0 \quad \forall \;\; \hat{A}, \hat{B} \quad \Leftrightarrow \quad \text{no causal link.} \tag{5.11}$$

There is no causal link between Alice and Bob if and only if the time-evolved operator $\hat{U}(t_B, t_A) \, \hat{A} \, \hat{U}^\dagger(t_B, t_A)$ of every measurement available

[56] In the Heisenberg picture, the commutator condition would simply be $\left[\hat{A}(t_A), \hat{B}(t_B)\right] = 0$.

to Alice at time t_A commutes with the operator of every measurement $\hat{B}$ available to Bob at time t_B.

We may apply a smearing function $f(r)$ to the regions R_A and R_B by employing POVMs of the form described in Section 3.4, and using the probabilities and states given in (3.33) and (3.34). We may also introduce smearing to the time interval $t_B - t_A$. However, unless the functions $f(r)$ smear out any two events so far that they *always* overlap within a light cone, superluminal signalling will remain a part of this theory.

We are left with the choice of either:

1. Modifying quantum theory at the level of Postulates 1 & 2;
2. Accepting that superluminal signalling may occur to some degree and attempting to find a way to deal with the paradoxes this throws up;
3. Accepting that all physical measurements are necessarily smeared out over infinite space and/or infinite time; or
4. Accepting that position operators – and, by extension, wavefunctions in the position basis – are physically meaningful only as approximations, and being especially aware of this if they are introduced into any relativistic argument.

This is a statement about any operators constructed from a continuous basis $\{|\mathbf{x}\rangle\}$ of generalised coordinates in accordance with Postulate 3, regardless of any interpretation in terms of particles or otherwise.

This result will be explored in more detail throughout the remainder of this work. Having established the role of the propagator (5.5), our next task is to derive expressions for it in terms of the single-particle Hamiltonian.

5.2 The propagator in canonical quantum mechanics

The propagator $K_{BA} \equiv K(\mathbf{x_B}, t_B; \mathbf{x_A}, t_A)$ was defined in equation (5.5). With $\delta t \equiv (t_B - t_A)/N$, $t_s \equiv t_A + s\delta t$ and $t'_s \equiv t_A + (s - \frac{1}{2})\delta t$,[57] together with $\mathbf{x_N} = \mathbf{x_B}$

[57] The dashed notation t'_s refers to quantities that are averaged over the sth δt interval.

and $\mathbf{x_0} = \mathbf{x_A}$, we can use (4.6) to expand further:

$$\begin{aligned} K_{BA} &= \lim_{N\to\infty} \langle x_B|\, e^{\frac{1}{i\hbar}\hat{H}(t'_N)\delta t} e^{\frac{1}{i\hbar}\hat{H}(t'_{N-1})\delta t} \ldots e^{\frac{1}{i\hbar}\hat{H}(t'_2)\delta t} e^{\frac{1}{i\hbar}\hat{H}(t'_1)\delta t}\, |x_A\rangle \\ &= \lim_{N\to\infty} \int d\mathbf{x_{N-1}} \ldots \int d\mathbf{x_1} \langle x_B|\, e^{\frac{1}{i\hbar}\hat{H}(t'_N)\delta t} |x_{N-1}\rangle \ldots \langle x_1|\, e^{\frac{1}{i\hbar}\hat{H}(t'_1)\delta t} |x_A\rangle. \end{aligned} \tag{5.12}$$

If the Hamiltonian operator[58] can be expanded as a series

$$\hat{H}(t) = \sum_a\ f_a(\hat{\mathbf{x}}, t)\ g_a(\hat{\mathbf{p}}, t), \tag{5.13}$$

then, in n coordinate dimensions, each factor for $r \in \{1, \ldots, N\}$ has the following form to order δt:

$$\begin{aligned} &\langle x_r|\, e^{\frac{1}{i\hbar}\hat{H}(t'_r)\delta t} |x_{r-1}\rangle \\ &\quad\approx \langle x_r|\, \hat{1} + \frac{1}{i\hbar} \sum_a \delta t\ f_a(\hat{\mathbf{x}}, t'_r)\ g_a(\hat{\mathbf{p}}, t'_r)\, |x_{r-1}\rangle \\ &\quad= \int d\mathbf{p}\ \left(\langle x_r|p\rangle\langle p|x_{r-1}\rangle + \frac{\delta t}{i\hbar} \sum_a \langle x_r|f_a(\hat{\mathbf{x}}, t'_r)|p\rangle\langle p|g_a(\hat{\mathbf{p}}, t'_r)|x_{r-1}\rangle \right) \\ &\quad= \int d\mathbf{p}\ \frac{e^{i\mathbf{x_r}.\mathbf{p}/\hbar}}{(2\pi\hbar)^{n/2}} \frac{e^{-i\mathbf{x_{r-1}}.\mathbf{p}/\hbar}}{(2\pi\hbar)^{n/2}} \left(1 + \frac{\delta t}{i\hbar} \sum_a f_a(\mathbf{x_r}, t'_r)\ g_a(\mathbf{p}, t'_r) \right) \\ &\quad\approx \int \frac{d\mathbf{p}}{(2\pi\hbar)^n}\ \exp\left\{ \frac{i}{\hbar}\ (\mathbf{x_r} - \mathbf{x_{r-1}}).\mathbf{p} - \frac{i\,\delta t}{\hbar} \sum_a f_a(\mathbf{x_r}, t'_r)\ g_a(\mathbf{p}, t'_r) \right\} \\ &\quad= \int \frac{d\mathbf{p}}{(2\pi\hbar)^n}\ \exp\left[\frac{i\,\delta t}{\hbar}\ \left\{ \frac{\mathbf{x_r} - \mathbf{x_{r-1}}}{\delta t}.\mathbf{p}\ -\ H(\mathbf{x_r}, \mathbf{p}, t'_r) \right\} \right]. \end{aligned} \tag{5.14}$$

This analysis is valid provided the neglected terms of order δt^2 can be relied upon to vanish when the $N \to \infty$ limit is taken.[59]

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[58] The operator takes the same functional form as the classical Hamiltonian, per Postulate 3. A reordering of operators or functions of operators has no overall effect on the theory (see next footnote).

[59] The $\mathbf{x_r}$ appearing in the Hamiltonian in (5.14) would be $\mathbf{x_{r-1}}$ if the ordering of $f_a(\hat{\mathbf{x}}, t'_r)$ and $g_a(\hat{\mathbf{p}}, t'_r)$ were reversed in (5.13). This constitutes an ambiguity which would normally vanish as N^{-1} when the limit is taken. $\mathcal{O}(\delta t^2)$ corrections should be understood to be present in all lines of equation (5.14); they arise here from the implicit use of the Baker-Campbell-Hausdorff formula for exponential functions of non-commuting operators. Again, these corrections would normally vanish as N^{-1} when the limit is taken. Hamiltonians containing potentials that vary as a negative power of a coordinate, such as a Coulomb potential or a centrifugal barrier, are exceptions to this: the assumptions made here regarding limits are not applicable in those cases, although the result (5.15) remains valid [55, §2.1.4].

Thus

$$K_{BA} = \lim_{N\to\infty} \int \Big(\prod_{s=1}^{N-1} d\mathbf{x_s}\Big) \prod_{r=1}^{N} \frac{d\mathbf{p_r}}{(2\pi\hbar)^n} \exp\left[\frac{i\,\delta t}{\hbar}\left\{\dot{\mathbf{x}}'_{\mathbf{r}}.\mathbf{p_r} \;-\; H(\mathbf{x_r},\mathbf{p_r},t'_r)\right\}\right], \tag{5.15}$$

where $\dot{\mathbf{x}}'_{\mathbf{r}} \equiv (\mathbf{x_r} - \mathbf{x_{r-1}})/\delta t$.

5.2.1 If the Hamiltonian is a quadratic function of momentum

If the Hamiltonian (5.13) is quadratic in $\mathbf{p}$, *i.e.*

$$H(\mathbf{x},\mathbf{p},t) = f_0(\mathbf{x},t) + f_{1\,i}(\mathbf{x},t)\,p_i + f_{2\,ij}(\mathbf{x},t)\,p_i p_j\,, \tag{5.16}$$

then we can use a standard result for the Gaussian integral of a quadratic form (represented by a symmetric, non-singular $n\times n$ matrix a),

$$\int d\mathbf{p}\,\exp\left[-\tfrac{1}{2}i\mathbf{p}^{\mathbf{T}}a\mathbf{p} + i\mathbf{b}.\mathbf{p}\right] \;=\; \sqrt{\frac{(-2\pi i)^n}{\det a}}\,\exp\left[\tfrac{1}{2}i\,\mathbf{b}^{\mathbf{T}}a^{-1}\mathbf{b}\right], \tag{5.17}$$

to perform each momentum integral in (5.15):

$$\begin{aligned}
&\int \frac{d\mathbf{p_r}}{(2\pi\hbar)^n}\exp\left[-\tfrac{1}{2}i\,\mathbf{p_r}^{\mathbf{T}}\frac{2\delta t}{\hbar}f_2\mathbf{p_r} + i\frac{\delta t}{\hbar}\big(\dot{\mathbf{x}}'_{\mathbf{r}} - \mathbf{f}_1\big).\mathbf{p_r} - \frac{i\,\delta t}{\hbar}f_0\right] \\
&= \frac{1}{(2\pi\hbar)^n}\sqrt{\frac{(-2\pi i)^n}{(2\delta t/\hbar)^n\det f_2}}\exp\left[\tfrac{1}{2}i\frac{\delta t^2}{\hbar^2}\frac{(\dot{\mathbf{x}}'_{\mathbf{r}} - \mathbf{f}_1)^{\mathbf{T}} f_2^{-1}(\dot{\mathbf{x}}'_{\mathbf{r}} - \mathbf{f}_1)}{2\delta t/\hbar}\right]\exp\left[-\frac{i\,\delta t}{\hbar}f_0\right] \\
&= \sqrt{\frac{1}{(4\pi\hbar\, i\,\delta t)^n\det f_2}}\exp\left[\frac{i\,\delta t}{\hbar}\left\{\tfrac{1}{4}(\dot{\mathbf{x}}'_{\mathbf{r}} - \mathbf{f_1})^{\mathbf{T}} f_2^{-1}(\dot{\mathbf{x}}'_{\mathbf{r}} - \mathbf{f_1}) - f_0\right\}\right].
\end{aligned} \tag{5.18}$$

From (5.16), $\dot{x}_i = \frac{\partial H}{\partial p_i} = f_{1\,i} + 2f_{2\,ij}\,p_j$; so the classical Lagrangian is

$$L(\mathbf{x},\dot{\mathbf{x}},t) \equiv \dot{\mathbf{x}}.\mathbf{p} - H(\mathbf{x},\mathbf{p},t) = \left\{\tfrac{1}{4}\,(\dot{\mathbf{x}} - \mathbf{f_1})^{\mathbf{T}} f_2^{-1}(\dot{\mathbf{x}} - \mathbf{f_1}) - f_0\right\} \tag{5.19}$$

and the full propagator can be expressed as a coordinate space path integral:

$$\begin{aligned}
&K(\mathbf{x_B},t_B;\mathbf{x_A},t_A) \\
&= \lim_{N\to\infty}\int\Big(\prod_{s=1}^{N-1}d\mathbf{x_s}\Big)\prod_{r=1}^{N}\sqrt{\frac{1}{(4\pi\hbar\,i\,\delta t)^n\det f_2}}\exp\left[\frac{i\,\delta t}{\hbar}L(\mathbf{x_r},\dot{\mathbf{x}}'_{\mathbf{r}},t'_r)\right] \\
&= \lim_{N\to\infty}\int\left(\frac{\prod_{s=1}^{N-1}d\mathbf{x_s}}{\prod_{r=1}^{N}(4\pi\hbar\,i\,\delta t)^{n/2}\sqrt{\det f_2(\mathbf{x_r},t'_r)}}\right)\exp\left[\sum_{r=1}^{N}\frac{i\,\delta t}{\hbar}L(\mathbf{x_r},\dot{\mathbf{x}}'_{\mathbf{r}},t'_r)\right] \\
&\equiv \int\mathcal{D}\mathbf{x}(t)\exp\left[\frac{i}{\hbar}S_{BA}\right],
\end{aligned} \tag{5.20}$$

where S_{BA} is the classical action for the path $\mathbf{x}(t)$ between $(\mathbf{x}_A, t_A)$ and $(\mathbf{x}_B, t_B)$:

$$S_{BA} \equiv \int_{t_A}^{t_B} dt L(\mathbf{x}(t), \dot{\mathbf{x}}(t), t). \tag{5.21}$$

The path integral measure $\mathcal{D}\mathbf{x}(t)$ is defined here as the $N \to \infty$ limit of the product measure given in the line above.

Thus we find – at least in the case where the Hamiltonian is quadratic – that **the functional appearing in the path integral form of the canonical propagator is the same classical action that, via the stationary action principle, generates the Hamiltonian from which the canonical operators were constructed in Postulate 3.**

The circular character of this derivation[60] suggests that an alternative to Postulate 3, based on the action via equation (5.20), could be considered as more fundamental. Feynman proposed this in 1948 [56]; it has subsequently been made rigorous using *Itō calculus* to define the analytic continuation of a series of random processes [55, §18].

This **path integral formulation of quantum mechanics** is a generalisation of the stationary action principle, which is recovered in the limit $\hbar \to 0$ [55, §4].

5.2.2 free-particle propagators

Another useful case involves Hamiltonians that are functions of momentum alone, *i.e.* $H(\mathbf{x}, \mathbf{p}, t) = H(\mathbf{p})$. The general phase space path integral (5.15) is then

$$\begin{aligned} K_{BA} &= \lim_{N\to\infty} \int \Big(\prod_{s=1}^{N-1} d\mathbf{x_s}\Big) \prod_{r=1}^{N} \frac{d\mathbf{p_r}}{(2\pi\hbar)^n} \exp\left[\frac{i}{\hbar}(\mathbf{x_r} - \mathbf{x_{r-1}}).\mathbf{p_r} - \frac{i\,\delta t}{\hbar} H(\mathbf{p_r})\right] \\ &= \lim_{N\to\infty} \int \Big(\prod_{r=1}^{N} d\mathbf{p_r}\Big) \exp\left[-\frac{i\,\delta t}{\hbar} \sum_{r=1}^{N} H(\mathbf{p_r})\right] \exp\left[\frac{i}{\hbar}(-\mathbf{x_0}.\mathbf{p_1} + \mathbf{x_N}.\mathbf{p_N})\right] \\ &\qquad \times \frac{1}{(2\pi\hbar)^n} \int \prod_{s=1}^{N-1} \frac{d\mathbf{x_s}}{(2\pi\hbar)^n} \exp\left[\frac{i}{\hbar}\mathbf{x_s}.(\mathbf{p_s} - \mathbf{p_{s+1}})\right]. \end{aligned}$$

[60] The Hamiltonian formalism of classical mechanics, on which the canonical formalism of quantum mechanics is based, can be viewed as a structure that emerges from the more fundamental *stationary action principle* (or 'Hamilton's principle') [48, §3.7]. It is more fundamental in the sense that it is coordinate-free – this also makes it manifestly relativistically invariant, which the Hamiltonian formalism is not. For these reasons, the action is attractive as a starting point for approaches to quantum theory that seek to bypass the Hamiltonian altogether. The path integral is the key mathematical tool for this endeavour [54, 55].

Each of the $N-1$ coordinate space integrals gives an n-dimensional momentum delta function $\delta(\mathbf{p_s}-\mathbf{p_{s+1}})$, making all but one of the momentum integrals trivial:

$$\begin{aligned} K_{BA} &= \lim_{N\to\infty}\int \frac{d\mathbf{p_1}}{(2\pi\hbar)^n}\,\exp\!\left[-\frac{i\,\delta t}{\hbar}N\,H(\mathbf{p_1})\right]\exp\!\left[\frac{i}{\hbar}(-\mathbf{x_0}.\mathbf{p_1}+\mathbf{x_N}.\mathbf{p_1})\right] \\ &= \int \frac{d\mathbf{p}}{(2\pi\hbar)^n}\,\exp\!\left[\frac{i}{\hbar}(\mathbf{x_B}-\mathbf{x_A}).\mathbf{p}-\frac{i}{\hbar}(t_B-t_A)H(\mathbf{p})\right]. \end{aligned} \tag{5.22}$$

If the Hamiltonian is a function only of p, the *magnitude* of the momentum, the propagator is a function of $\Delta x = \mathbf{x_B}-\mathbf{x_A}$ and $\Delta t = t_B - t_A$:

$$K_{BA} = \begin{cases} \displaystyle\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\,\exp\!\left[\frac{i}{\hbar}(p\Delta x - H(p)\Delta t)\right] & n=1 \\ \displaystyle\int_0^{\infty} dp\,\frac{\Delta x}{\hbar}\left(\frac{p}{2\pi\hbar\Delta x}\right)^{\frac{n}{2}}\,J_{\frac{n}{2}-1}\!\left(\frac{p\Delta x}{\hbar}\right)\exp\!\left[-\frac{i}{\hbar}H(p)\Delta t\right] & n\geq 2. \end{cases} \tag{5.23}$$

Here $J_\nu(x)$ is the spherical Bessel function of order ν.

In $n=3$ spatial dimensions we may use the identity $z^{\frac{1}{2}}J_{\frac{1}{2}}(z) = (2/\pi)^{\frac{1}{2}}\sin z$. *Provided the Hamiltonian is an even function of* p, the integral simplifies considerably. By doubling the range of integration, the $\sin z$ is eliminated in favour of e^{iz}:

$$K(\mathbf{x_B},t_B;\mathbf{x_A},t_A) = \int_{-\infty}^{\infty}\frac{dp}{(2\pi\hbar)^2}\frac{p}{i\Delta x}\exp\!\left[\frac{i}{\hbar}(p\Delta x - H(p)\Delta t)\right]. \tag{5.24}$$

This expression will be used in Section 6 to evaluate the free-particle propagator for a relativistic scalar particle.

The Hamiltonian $H(\mathbf{p}) = \mathbf{p}^2/2m$ of a non-relativistic free scalar particle – or a set of non-interacting particles – in rectilinear coordinates $\mathbf{x}\in\mathbb{R}^n$ is another example. The momentum integral is Gaussian, so (5.17) can be used for general n. The result is[61]

$$K(\mathbf{x_B},t_B;\mathbf{x_A},t_A) = \left(\frac{m}{2\pi\hbar\,i\Delta t}\right)^{\frac{n}{2}}\exp\!\left[\frac{im}{2\hbar}\frac{\Delta x^2}{\Delta t}\right]. \tag{5.25}$$

[61] As the Hamiltonian is quadratic, this result can also be derived from the path integral expression (5.20) with $\det f_2 = \det(\delta_{ij}/2m) = (1/2m)^n$ and $L = \frac{1}{2}m[(\mathbf{x_r}-\mathbf{x_{r-1}})/\Delta t]^2$ [54, §3-1].

5.3 Propagators involving non-classical degrees of freedom

The propagators in Sections 5.1 and 5.2 can be generalised to include non-classical degrees of freedom and the associated ν-component wavefunctions.

The ideal detector of equation (5.1), capable of determining whether or not a particle is in a given region R_A, is generalised to one that can also discriminate between the components of the wavefunction:

$$\hat{A} = \sum_{\alpha\beta} \int_{R_A} d\mathbf{x}\, |x^\alpha\rangle \hat{A}^{(x)\alpha\beta} \langle x^\beta|. \tag{5.26}$$

If $\hat{A}^{(x)\alpha\beta} = \delta^{1\alpha}\delta^{1\beta}$, to take an idealised example, then the detector responds only to the 1st component of the wavefunction, $\psi^1(\mathbf{x})$. If the components of the wavefunction are to be interpreted as different types of particle at the same location, then this detector would respond to a single particle type.

If there are any non-classical degrees of freedom that an observer has some ability to distinguish experimentally, the reasoning in Section 5.1 must hold with regard to every element of the *matrix* of propagators $K^{\alpha\beta}_{BA}(\mathbf{x_A}, \mathbf{x_B}) \equiv \langle x^\beta_B | \hat{U}(t_B, t_A) | x^\alpha_A \rangle$: that is, the theory permits signalling between regions R_A and R_B unless $K^{\alpha\beta}_{BA}(\mathbf{x_A}, \mathbf{x_B}) = 0$ for all $\mathbf{x_A} \in R_A$ and $\mathbf{x_B} \in R_B$.

The general form of the Hamiltonian (4.19) can be expressed in the coordinate basis by means of a matrix with components $\hat{H}^{(x)\alpha\beta}(\mathbf{x}, t)$:

$$\hat{H}(t) = \sum_{\alpha\beta} \int_{R_A} d\mathbf{x}\, |x^\alpha\rangle \hat{H}^{(x)\alpha\beta} \langle x^\beta|. \tag{5.27}$$

The propagator may be calculated in the same way as Section 5.2. Following equation (5.13), we require it to be expressible as $\hat{H}(t) = \sum_a \hat{f}_a(\hat{\mathbf{x}}, t)\, \hat{g}_a(\hat{\mathbf{p}}, t)$.

$\hat{f}_a$ and $\hat{g}_a$ are now operators in the space of the non-classical degrees of freedom as well as functions of the canonical operators. We require that they can be expressed as a power series $\hat{f}_a = \sum_b \hat{f}_{ab} \hat{\mathbf{x}}^b$ and $\hat{g}_a = \sum_b \hat{g}_{ab} \hat{\mathbf{p}}^b$. Each coefficient can be expressed in matrix form in that space, as well as having a general rank-b tensor character with respect to the canonical operators, and being some function of the operators representing the non-classical degrees of freedom. In all its fully-indexed glory, this means

$$\left[\hat{f}_{ab}\right]_{i_1 i_2 \ldots i_b} \hat{x}_{i_1} \hat{x}_{i_2} \ldots \hat{x}_{i_b} = \sum_{\alpha\beta} \int d\mathbf{x}\, |x^\alpha\rangle \left[f^{\alpha\beta}_{ab}(\hat{a}, \hat{b}, \hat{c}, \ldots; t)\right]_{i_1 i_2 \ldots i_b} \hat{x}_{i_1} \hat{x}_{i_2} \ldots \hat{x}_{i_b} \langle x^\beta| \tag{5.28}$$

and similarly for $\hat{g}_{ab}$.

From this, we can define a matrix $H^{\alpha\beta}(\mathbf{x}, \mathbf{p}, t)$ that will play the role of

the classical Hamiltonian in the coordinate space while remaining an operator in the space of the non-classical degrees of freedom:

$$H^{\alpha\beta}(\mathbf{x},\mathbf{p},t) \equiv \sum_a \left(\sum_b f_{ab}^{\alpha\gamma}(t)\mathbf{x}^b \right) \left(\sum_c g_{ac}^{\gamma\beta}(t)\mathbf{p}^c \right). \tag{5.29}$$

With the application of (4.22): $\langle x^\alpha | p^\beta \rangle = (2\pi\hbar)^{-n/2}\, \delta^{\alpha\beta}\, e^{i\mathbf{x}.\mathbf{p}/\hbar}$, the reasoning that leads to equation (5.14) continues to hold and we arrive at a full generalisation of the phase space expression (5.15) for the propagator:[62]

$$K^{\alpha\beta}(\mathbf{x_B},t_B;\mathbf{x_A},t_A) = \lim_{N\to\infty} \int \Big(\prod_{s=1}^{N-1} d\mathbf{x_s}\Big) \prod_{r=1}^{N} \frac{d\mathbf{p_r}}{(2\pi\hbar)^n} \exp\left[\frac{i\Delta t}{\hbar} \left\{ \dot{\mathbf{x}}'_{\mathbf{r}}.\mathbf{p_r}\, \delta^{\alpha\beta} - H^{\alpha\beta}(\mathbf{x_r},\mathbf{p_r},t'_r) \right\} \right]. \tag{5.30}$$

For Hamiltonians that are quadratic in the momentum operator, such as the Pauli–Schrödinger Hamiltonian (4.26), the standard Gaussian integral (5.17) is no longer enough. Our expression for a single momentum integral now has the form

$$\int \Big(\prod_{i=1}^{n} dp_i\Big)\, \exp\left[-\tfrac{1}{2} i\, p_i\, a_{ij}^{\alpha\beta} p_j + i\, b_i^{\alpha\beta} p_i + i\, c^{\alpha\beta} \right]. \tag{5.31}$$

If $a_{ij}^{\alpha\beta}$, $b_i^{\alpha\beta}$ and $c^{\alpha\beta}$ can be diagonalised simultaneously with respect to the non-classical degrees of freedom (the Greek indices), then this integral can be performed using the standard Gaussian result for each element on the diagonal, and a coordinate space path integral emerges as we saw in (5.20). For our Hamiltonian, this is equivalent to the requirement that a basis $\{|x^\alpha\rangle\}$ exists in which each component of a wavefunction $\psi^\alpha(\mathbf{x}) = \langle x^\alpha|\psi\rangle$ evolves independently. In other words, the system would be equivalent to a set of independent systems each of which evolves unitarily with no non-classical degrees of freedom.

To derive a coordinate space path integral by this method, we must attempt to find a position representation in which the Hamiltonian itself is diagonal.

5.4 Propagators as Green's functions

All propagators discussed in Section 5 rely on the notion of a time evolution operator (Postulate 3), and the equivalent path integral procedure relies on an ordered time-slicing. A propagator $K(\mathbf{x_B},t_B;\mathbf{x_A},t_A) \equiv \langle x_B|\, \hat{U}(t_B,t_A)\, |x_A\rangle$

[62] The right-hand side of (5.30) and (5.31) are to be understood as the $\alpha\beta$ element of the exponential of the matrix, rather than the exponential of the $\alpha\beta$ element.

in this context is therefore defined for $t_B > t_A$ only.

Let us now define

$$G_R(\mathbf{x}, t; \mathbf{x_0}, t_0) \equiv \theta(t-t_0)\, K(\mathbf{x}, t; \mathbf{x_0}, t_0), \tag{5.32}$$

which has the following property:

$$\begin{aligned} \int d\mathbf{x}'\, G_R(\mathbf{x}, t; \mathbf{x}', t_0)\psi(\mathbf{x}', t_0) &= \theta(t-t_0) \int d\mathbf{x}'\, \langle x|\, \hat{U}(t, t_0)\, |x'\rangle\langle x'|\psi(t_0)\rangle \\ &= \theta(t-t_0)\langle x|\hat{U}(t, t_0)|\psi(t_0)\rangle \\ &= \begin{cases} 0 & \text{if } t < t_0 \\ \psi(\mathbf{x}, t) & \text{if } t > t_0. \end{cases} \end{aligned} \tag{5.33}$$

Let us also define a differential operator

$$\hat{S} = \frac{\partial}{\partial t} - \frac{\hat{H}}{i\hbar}. \tag{5.34}$$

This is an operator that gives zero in and only if that state is evolving according to the laws of quantum mechanics. (The Schrödinger equation (4.7) implies $\hat{S}|\psi\rangle = 0 \;\; \forall |\psi\rangle \in \mathcal{H}$.) If we apply the operator to $G_R(\mathbf{x}, t; \mathbf{x_0}, t_0)$ and refer to (4.5), we find

$$\begin{aligned} \hat{S}\, G_R &= \theta(t-t_0)\, \langle x| \left(\frac{\partial}{\partial t} - \frac{\hat{H}}{i\hbar} \right) \hat{U}(t, t_0)\, |x_0\rangle \;+\; \delta(t-t_0)\, \langle x|\, \hat{U}(t, t_0)\, |x_0\rangle \\ &= \delta(t - t_0)\, \delta(\mathbf{x}-\mathbf{x_0}) \end{aligned} \tag{5.35}$$

This is the defining condition for G_R to be a **Green's function** of $\hat{S}$. Because it evolves *from* a given state, it is known as the retarded Green's function. A Green's function that evolves *to* a given state – the advanced Green's function – also exists for $\hat{S}$:

$$G_A(\mathbf{x}, t; \mathbf{x_0}, t_0) \equiv \theta(t_0-t)\, K(\mathbf{x_0}, t_0; \mathbf{x}, t), \tag{5.36}$$

for which

$$\begin{aligned} \int d\mathbf{x}\, G_A(\mathbf{x}, t; \mathbf{x}', t_0)\psi(\mathbf{x}, t) &= \theta(t_0-t) \int d\mathbf{x}\, \langle x'|\, \hat{U}(t_0, t)\, |x\rangle\langle x|\psi(t)\rangle \\ &= \theta(t_0-t)\langle x'|\hat{U}(t_0, t)|\psi(t)\rangle \\ &= \begin{cases} \psi(\mathbf{x}', t_0) & \text{if } t < t_0 \\ 0 & \text{if } t > t_0. \end{cases} \end{aligned} \tag{5.37}$$

The existence of a retarded and an advanced Green's function is a general property of differential operators $\hat{S}$ that are **first order in time**. Once they are known, they can be used to solve equations of the form

$$(\hat{S}\psi)(\mathbf{x},t) = j(\mathbf{x},\mathbf{t}) \quad \forall \mathbf{x} \in V,\ t_1 \leq t \leq t_2 \tag{5.38}$$

where $j(\mathbf{x},t)$ is any function of space and time. The solution can be expressed in terms of $\psi(\mathbf{x},t_0)$ where $t_1 \leq t_0 \leq t_2$. For $t > t_0$ it takes the following form, of which (5.33) is a special case:

$$\begin{aligned} \psi(\mathbf{x},t) \;\; = \;\; & \int_V d\mathbf{x}'\, G_R(\mathbf{x},t;\mathbf{x}',t_0)\, \psi(\mathbf{x}',t_0) \\ & + \;\; \int_{t_0}^{t} dt' \int_V d\mathbf{x}'\, G_R(\mathbf{x},t;\mathbf{x}',t')\, j(\mathbf{x}',t') \;\; + \;\; \text{surface term} \end{aligned}$$

The surface term, integrated over the boundary of V from time t_0 to t, depends on the form of $\hat{S}$. If $\hat{S}$ contains second order spatial derivatives, this term includes the components of $\nabla\psi$ and ∇G_R normal to the boundary in addition to the boundary values of ψ and G_R themselves.

6 Relativistic free particles and their propagators

Note: we set $c = 1$ and $\hbar = 1$ in this and subsequent discussions concerning relativistic quantum theory.

6.1 The relativistic scalar particle propagator

The Hamiltonian of a relativistic particle of mass m and charge q is well-defined in classical mechanics:

$$\begin{aligned} H(\mathbf{x},\mathbf{p},t) &= \sqrt{[\mathbf{p}-q\mathbf{A}(\mathbf{x},t)]^2+m^2}+q\phi(\mathbf{x},t) \\ &= \sqrt{\mathbf{p}^2+m^2} \quad \text{for a free particle.} \end{aligned} \tag{6.1}$$

As per Postulate 3, in the absence of non-classical degrees of freedom (as we assume to be the case for a scalar particle) we propose a free-particle Hamiltonian operator with the same functional form as the classical Hamiltonian. In the coordinate representation, the identification $\hat{p}_i^{(x)} = \partial/\partial x_i$ inside the square root is problematic: we will return to this in Section 6.2. For now, we make use of the fact that the Hamiltonian is a function of momentum alone, so that the propagator takes the form (5.22):

$$K(\mathbf{x_B},t_B;\mathbf{x_A},t_A) = \int \frac{d\mathbf{p}}{2\pi}\,\exp\left[i\Delta\mathbf{x}.\mathbf{p} - i\Delta t\sqrt{\mathbf{p}^2+m^2}\right], \tag{6.2}$$

where $\Delta\mathbf{x} \equiv \mathbf{x_B}-\mathbf{x_A}$ and $\Delta t \equiv t_B - t_A$.

The propagator calculation below includes the negative as well as the positive square root Hamiltonian:

$$H_\pm(\mathbf{p},t) = \pm\sqrt{\mathbf{p}^2+m^2}. \tag{6.3}$$

We will make use of both results in later Sections.

6.1.1 Positive and negative energy propagators

In three spatial dimensions, the propagator is given by (5.24). Applying the substitution $p = m\sinh\chi$,

$$\begin{aligned} K_\pm(\mathbf{x_B},t_B;\mathbf{x_A},t_A) &= \int_{-\infty}^{\infty}\frac{dp}{(2\pi)^2}\frac{p}{i\Delta x}\exp\left[i(p\,\Delta x \mp (p^2+m^2)^{\frac{1}{2}}\Delta t)\right] \\ &= \frac{m^2}{(2\pi)^2 i\Delta x}\int_{-\infty}^{\infty}\sinh\chi\cosh\chi\,d\chi\,\exp[\mp im\tau\cosh(\chi\mp\phi)], \end{aligned}$$

where $\tau = (\Delta t^2 - \Delta x^2)^{\frac{1}{2}}$ and $\sinh\phi = \Delta x/\tau$. Changing variables again to $\chi' = \chi \mp \phi$, the integral becomes

$$\tfrac{1}{2}\cosh 2\phi \int_{-\infty}^{\infty} \sinh 2\chi'\, d\chi'\, e^{\mp im\tau\cosh\chi'} \pm \tfrac{1}{2}\sinh 2\phi \int_{-\infty}^{\infty} \cosh 2\chi'\, d\chi'\, e^{\mp im\tau\cosh\chi'}.$$

The first term has an odd integrand and therefore vanishes; the second is even. Since $\frac{1}{2}\sinh 2\phi = \Delta t\Delta x/\tau^2$, we have

$$K_{\pm}(\mathbf{x_B}, t_B; \mathbf{x_A}, t_A) = \frac{\pm m^2\,\Delta t}{(2\pi)^2\, i\,\tau^2}\; 2\int_0^{\infty} d\chi'\, \cosh 2\chi'\, e^{\mp im\tau\cosh\chi'}. \tag{6.4}$$

If a small appropriately-signed imaginary part is added to t, the integral converges to give a modified Bessel function. To this end, we redefine τ as:

$$\equiv \lim_{\epsilon\to 0^+} [(\Delta t \mp i\epsilon)^2 - \Delta x^2]^{\frac{1}{2}} \tag{6.5}$$

and, with $z = \pm im\tau$, make use of the standard result

$$K_\nu(z) = \int_0^{\infty} \cosh\nu t\, e^{-z\cosh t} \quad \text{provided } \Re(z) > 0 \tag{6.6}$$

to arrive at a general expression for the propagator:

$$K_{\pm}(\mathbf{x_B}, t_B; \mathbf{x_A}, t_A) = \frac{m^2}{2\pi^2}\,\frac{\pm\Delta t}{i\,\tau^2}\, K_2(\pm im\tau). \tag{6.7}$$

When the interval from $(\mathbf{x_A}, t_A)$ to $(\mathbf{x_B}, t_B)$ is timelike – that is, if $\Delta t > \Delta x$ – the variation with τ is revealed more clearly as a Hankel function via the relation[63] $K_2(\pm im\tau) = -i\frac{\pi}{2}H_2^{(1)}(\mp m\tau)$. When the interval is spacelike, we note that the ϵ prescription implies $\pm i\tau = \sqrt{-\tau^2}$.

Hence, **for a relativistic free scalar particle in three spatial dimen-**

[63] The relationship between modified Bessel functions and Hankel functions is [57, §9.6]

$$K_\nu(z) \equiv \begin{cases} (i)^{\nu+1}\dfrac{\pi}{2}H_\nu^{(1)}(iz) & \text{if } -\pi < \arg(z) \le \pi/2, \\ (-i)^{\nu+1}\dfrac{\pi}{2}H_\nu^{(2)}(-iz) & \text{if } -\pi/2 < \arg(z) \le \pi. \end{cases}$$

In (6.7), $z = \pm im\tau$, and $-\pi/2 < \arg(z) < \pi/2$ for finite $\epsilon > 0$. As $\epsilon \to 0^+$, $\arg(z) \to \pm\pi/2$ for the timelike case, and $\arg(z) \to 0$ for the spacelike case. Therefore the $H_\nu^{(1)}(iz)$ result is necessary for the timelike propagator in the negative energy case, and is sufficient for the positive energy case also.

sions, we obtain from (6.7),[64]

$$K_{\pm}(\mathbf{x_B},t_B;\mathbf{x_A},t_A) = \begin{cases} \dfrac{m^2}{4\pi}\,\dfrac{\mp\Delta t}{\tau^2}\,H_2^{(1)}(\mp m\tau) & \text{if } \Delta t > \Delta x \ \ \text{(timelike)} \\ \dfrac{im^2}{2\pi^2}\,\dfrac{\pm\Delta t}{-\tau^2}\,K_2(m\sqrt{-\tau^2}) & \text{if } \Delta t < \Delta x \ \ \text{(spacelike).} \end{cases} \tag{6.8}$$

In the lightlike limit $\tau^2 \to 0$, approaching the light cone surface from either the timelike or spacelike side, and also in the massless limit $m \to 0$, this becomes

$$K_{\pm}(\mathbf{x_B},t_B;\mathbf{x_A},t_A) = \frac{\pm i\,\Delta t}{\pi^2\tau^4}\left[1+\frac{m^2\tau^2}{4}+\mathcal{O}(m^4\tau^4)\right] \quad \text{as } \ |m\tau|\to 0. \tag{6.9}$$

Away from the surface of the light cone (for massive particles) in either the timelike or spacelike limit $|m\tau| \to \infty$,

$$K_{\pm}(\mathbf{x_B},t_B;\mathbf{x_A},t_A) = \sqrt{\frac{m^3}{8\pi^3}\frac{1}{\pm i\tau}}\,\frac{\pm i\Delta t}{-\tau^2}\,e^{\mp im\tau}\left[1+\frac{15}{8}\frac{1}{\pm im\tau}+\mathcal{O}\Big(\frac{1}{m^2\tau^2}\Big)\right]. \tag{6.10}$$

In the spacelike case, $e^{\mp im\tau} = e^{-m\sqrt{-\tau^2}}$ drops off exponentially away from the light cone surface for both positive and negative energy propagators. Within the light cone, $e^{\mp im\tau}$ is a phase.

For a particle **in one spatial dimension**, the process of integration is very similar, resulting in[65]

$$K_{\pm}(x_B,t_B;x_A,t_A) \;=\; \frac{m}{\pi}\,\frac{\Delta t}{\tau}\,K_1(\pm im\tau) \tag{6.11}$$

$$\;=\; \begin{cases} -\dfrac{m}{2}\,\dfrac{\Delta t}{\tau}\,H_1^{(1)}(\mp m\tau) & \text{if } \Delta t > \Delta x \ \ \text{(timelike)} \\ \dfrac{m}{\pi}\,\dfrac{\pm i\Delta t}{\sqrt{-\tau^2}}\,K_1(m\sqrt{-\tau^2}) & \text{if } \Delta t < \Delta x \ \ \text{(spacelike)} \end{cases} \tag{6.12}$$

In the $|m\tau| \to 0$ limit,

$$K_{\pm}(\mathbf{x_B},t_B;\mathbf{x_A},t_A) = \frac{\mp i\,\Delta t}{\pi\tau^2}\left[1-\frac{m^2\tau^2}{4}\Big(\ln(\frac{-m^2\tau^2}{4})+2\gamma-1\Big)+\mathcal{O}\big(m^4\tau^4\big)\right], \tag{6.13}$$

where $\gamma \approx 0.5772$ is Euler's constant and the logarithm takes the principle

[64] In the 3D timelike positive energy propagator, $-H_2^{(1)}(-m\tau)$ may be replaced by $+H_2^{(2)}(m\tau)$.

[65] In the 1D timelike positive energy propagator, $-H_1^{(1)}(-m\tau)$ may be replaced by $-H_1^{(2)}(m\tau)$. The 1D positive energy propagator here (6.11) agrees with that in [58].

value. When $|m\tau| \to \infty$,

$$K_{\pm}(\mathbf{x_B}, t_B; \mathbf{x_A}, t_A) = \sqrt{\frac{m}{2\pi}\frac{1}{\pm i\tau}}\,\frac{\Delta t}{\tau}\,e^{\mp im\tau}\left[1 + \frac{3}{8}\frac{1}{\pm im\tau} + \mathcal{O}\Big(\frac{1}{m^2\tau^2}\Big)\right]. \tag{6.14}$$

Again, in the spacelike case, $e^{\mp im\tau} = e^{-m\sqrt{-\tau^2}}$ drops off exponentially for both propagators.

The limits (6.10) and (6.14) in particular illustrate that propagation beyond the light cone is a feature of any theory with a square root Hamiltonian of the form (6.1).

6.1.2 The path integral for a relativistic particle

We know from Sections 5.2.1 and 5.3 that when the Hamiltonian is quadratic in the momentum operator (after having been diagonalised with respect to any intrinsic degrees of freedom), there is an equivalence between the canonical propagator $K(\mathbf{x_B}, t_B; \mathbf{x_A}, t_A)$ and the coordinate space path integral representation (5.20)

$$K(\mathbf{x_B}, t_B; \mathbf{x_A}, t_A) = \int \mathcal{D}\mathbf{x}\; e^{iS_{BA}}, \tag{6.15}$$

where S_{BA} is the classical action for a path between $(\mathbf{x_A}, t_A)$ and $(\mathbf{x_B}, t_B)$. This allows for a very attractive picture of quantum mechanics in terms of particles taking all conceivable paths through space.

The relativistic Hamiltonian, however, is not quadratic, so we must refer back to the more general phase space path integral (5.15), which may be written

$$K(\mathbf{x_B}, t_B; \mathbf{x_A}, t_A) = \int \mathcal{D}\mathbf{x}\frac{\mathcal{D}\mathbf{p}}{(2\pi)^n}\,\exp\left[\,i\int_{t_a}^{t_b} dt\,\big\{\dot{\mathbf{x}}.\mathbf{p} - H(\mathbf{x}, \mathbf{p}, t)\big\}\right]. \tag{6.16}$$

Nevertheless, the coordinate space equation (6.15) is worth investigating, with a view to introducing some ways in which it can be generalised to the relativistic case.

The classical action for a free relativistic particle is simply $S_{BA} = -m\tau$, where $\tau^2 = \Delta t^2 - \Delta\mathbf{x}^2$. For timelike intervals, this is a real quantity; for spacelike intervals it is imaginary. If anything like equation (6.15) holds in this case, we should expect iS_{BA} to be unambiguously negative for spacelike intervals so that propagation is exponentially suppressed rather than amplified. An initial glance at $iS_{BA} = -im\sqrt{-(\Delta\mathbf{x}^2 - \Delta t^2)}$ is not reassuring.

Let us consider free relativistic particles (for completeness, I include the negative as well as the positive energy case, following on from Section 6.1.1) by taking a Lagrangian of

$$L_{\pm}(\mathbf{x},\dot{\mathbf{x}}) \;=\; \mp m\sqrt{1-\dot{\mathbf{x}}^2} \;=\; \mp m\sqrt{\frac{dx^\mu}{dt}\frac{dx_\mu}{dt}}. \tag{6.17}$$

This implies $S_{BA} = \mp m\tau$. The ith component of momentum is then

$$p_i \;\equiv\; \frac{\partial L_\pm}{\partial \dot{x}_i} \;=\; \frac{\pm m\,\dot{x}_i}{\sqrt{1-\dot{\mathbf{x}}^2}} \;=\; \frac{\pm m\dot{x}_i}{\sqrt{\frac{dx^\mu}{dt}\frac{dx_\mu}{dt}}} \tag{6.18}$$

which makes $\dot{\mathbf{x}}(\mathbf{p}) = \pm\mathbf{p}/\sqrt{\mathbf{p}^2+m^2}$, and the Hamiltonian is

$$H_\pm(\mathbf{x},\mathbf{p}) \;\equiv\; \mathbf{p}.\dot{\mathbf{x}}(\mathbf{p}) - L_\pm(\mathbf{x},\dot{\mathbf{x}}(\mathbf{p})) \;=\; \pm\sqrt{\mathbf{p}^2+m^2} \tag{6.19}$$

in correspondence with (6.3).

If we adopt the same $i\epsilon$ prescription as was employed in (6.5), the action becomes

$$\begin{aligned} S_{BA} \;&=\; \lim_{\epsilon\to 0^+} \mp m\left[(\Delta t \mp i\epsilon)^2 - \Delta\mathbf{x}^2\right]^{\frac{1}{2}} \\ &=\; \lim_{\epsilon\to 0^+} \mp m\sqrt{(\Delta t^2-\Delta\mathbf{x}^2)\left(1 \mp \frac{i\epsilon'}{\Delta t^2-\Delta\mathbf{x}^2}\right)} \\ &=\; \begin{cases} \mp m\sqrt{\Delta t^2-\Delta\mathbf{x}^2} & \text{if } \Delta t > \Delta x \;\; \text{(timelike)} \\ im\sqrt{\Delta\mathbf{x}^2-\Delta t^2} & \text{if } \Delta t < \Delta x \;\; \text{(spacelike)} \end{cases} \end{aligned} \tag{6.20}$$

The weight of a path in (6.15) over a spacelike interval is then $e^{-m\sqrt{\Delta\mathbf{x}^2-\Delta t^2}}$, which is indeed exponentially suppressed in both positive and negative energy cases. Equivalently, if *any part* of a path involves a spacelike interval, the contribution of that path to the propagator will be exponentially suppressed.

In Section 6.1.1, the $i\epsilon$ prescription was required to carry out a basic integral, but here the choice is not so inevitable. If we do not wish to rely on the results of the canonical calculation, it may be motivated by demanding that spacelike contributions to the propagator be suppressed rather than amplified.

The evaluation below illustrates that this prescription is sufficient to maintain the equivalence between the two approaches for the case of a free relativistic particle.

The positive energy propagator – see (6.7) and (6.11) – has been derived in the path integral representation by Jizba and Kleinert [59]. The authors

first derive the conditions for an identity relating the path integrals of pairs of Hamiltonians $H(\mathbf{p},\mathbf{x})$ and $\overline{H}(\mathbf{p},\mathbf{x})$ via a distribution function $\omega(v,t_{ba})$:

$$\int \mathcal{D}\mathbf{x}\mathcal{D}\mathbf{p}\,\exp\Big[\int_{t_a}^{t_b} dt\,\big(i\mathbf{p}.\dot{\mathbf{x}} - \overline{H}\big)\Big] \\ = \int_0^\infty dv\,\omega(v,t_{ba}) \int \mathcal{D}\mathbf{x}\mathcal{D}\mathbf{p}\,\exp\Big[\int_{t_A}^{t_B} dt\,\big(i\mathbf{p}.\dot{\mathbf{x}} - vH\big)\Big]. \quad (6.21)$$

The integral is over all paths fixed at the two points $\mathbf{x}(t_a) = \mathbf{x_a}$ and $\mathbf{x}(t_b) = \mathbf{x_b}$, and $t_{ba} \equiv t_b - t_a$.

In particular, they find that the path integral for a square root Hamiltonian $\overline{H}(\mathbf{p},\mathbf{x}) = a\sqrt{\mathbf{p}^2+m^2}$ can be transformed into a superposition of path integrals for a quadratic Hamiltonian $vH(\mathbf{p},\mathbf{x}) = v(\mathbf{p}^2+m^2)$ by means of the following distribution:[66]

$$\omega(v,t_{ba}) = \frac{a\,e^{-a^2 t_{ba}/4v}}{2\sqrt{\pi v^3/t_{ba}}}. \quad (6.22)$$

The propagator discussed here (6.2) is related to (6.21) by a Wick rotation $t_A \to it_A \equiv t_a$ and $t_B \to it_B \equiv t_b$

$$K(\mathbf{x_b}, -it_b; \mathbf{x_a}, -it_a) = \int \frac{d\mathbf{p}}{2\pi}\,\exp\Big[i\Delta\mathbf{x}.\mathbf{p} - t_{ba}\sqrt{\mathbf{p}^2+m^2}\Big] \\ = \int \mathcal{D}\mathbf{x}\mathcal{D}\mathbf{p}\,\exp\Big[\int_{t_a}^{t_b} dt\,\big(i\mathbf{p}.\dot{\mathbf{x}} - \overline{H}\big)\Big] \quad (6.23)$$

provided a suitable analytic continuation exists for $t \in \mathbb{C}$ throughout the calculation, which is the case here.

The transformation to a quadratic Hamiltonian allows us to recover a

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[66] This is the 'Weibull distribution' of order a. The case of $a = 1$ is sufficient here. The invariance of this identity with a corresponds to the global reparametrisation invariance of the action over a parametrised path [60, §V].

If an arbitrary parametrisation $x^\mu(\lambda)$ is applied to a path, one may consider the intrinsic (0+1)-dimensional metric $g_{00}(\lambda) = \frac{\partial x^\mu}{\partial\lambda}\frac{\partial x_\mu}{\partial\lambda}$ (or the 'einbein' $e(\lambda) = \sqrt{g_{00}}$) induced by that parametrisation. The requirement that the action be independent of the parametrisation then dictates how this metric must vary if the parametrisation is changed [61, 6.2]. Invariance with respect to $a \to ka$ corresponds to a small subset of this reparametrisation invariance – namely the global invariance of the action with respect to $\lambda \to \lambda/k$ and $e(\lambda) \to ke(\lambda)$ everywhere along the path.

The full local gauge freedom of reparametrisation is explored in [60, §V], and it is shown that the distribution over v can be re-expressed as an integral over path lengths L together with a functional integral over einbeins $\mathcal{D}e$, putting $e(\lambda)$ on the same footing as $\mathbf{x}(\lambda)$.

coordinate space expression. With $a=1$, the integrals over $\mathbf{p}$ give

$$K(\mathbf{x_b}, -it_b; \mathbf{x_a}, -it_a) = \int_0^\infty dv \frac{e^{-t_{ba}/4v}}{2\sqrt{\pi v^3/t_{ba}}} \int \mathcal{D}\mathbf{x}\, e^{S_{BA,v}} \tag{6.24}$$

where

$$S_{BA,v} = -v \int_{t_a}^{t_b} dt \Big(m^2 + \frac{\dot{\mathbf{x}}^2}{4v^2} \Big). \tag{6.25}$$

After the final integral over v, their general result for D spatial dimensions is[67]

$$K(\mathbf{x_b}, -it_b; \mathbf{x_a}, -it_a) = 2t_{ba} \left(\frac{m\gamma}{2\pi t_{ba}} \right)^{(D+1)/2} K_{(D+1)/2}\Big(\frac{m t_{ba}}{\gamma} \Big) \tag{6.26}$$

where $\gamma = (1 + x_{ba}^2/t_{ba}^2)^{-1/2}$. We can continue the expression to real Δt while maintaining $\Re(t_{ba}) > 0$ by employing the same $i\epsilon$ prescription (6.5): $t_{ba} = i(\Delta t - i\epsilon)$. This gives $t_{ba}/\gamma = i\tau$ for both timelike and spacelike intervals, and hence

$$K(\mathbf{x_B}, t_B; \mathbf{x_A}, t_A) = 2i\Delta t \left(\frac{m}{2\pi i \tau} \right)^{(D+1)/2} K_{(D+1)/2}(im\tau). \tag{6.27}$$

This expression agrees with the positive energy cases in (6.7) and (6.11) for $D=3$ and $D=1$ respectively.

6.1.3 Propagation backwards in time?

As discussed in Section 5.4, the derivations of propagators above rely on the notion of a time evolution operator. They therefore apply only for $t_B > t_A$.

We have seen that $K_{AB} \neq 0$ between spacelike-separated spacetime points $(\mathbf{x_A}, t_A)$ and $(\mathbf{x_B}, t_B)$. As this is proposed as a relativistic theory, what are we to make of this from the point of view of an observer for whom $t_B < t_A$? The propagator in its current form lacks self-consistency.

One option is to argue that we have sufficient grounds to abandon the attempt to use a single-particle Hamiltonian to define a position operator and move on, perhaps to a field theory (Section 7). In the context of special relativity itself, it is not difficult to show that where superluminal signalling is possible, it is also possible for an observer to transmit information to him or herself at an earlier time, would constitute the worst kind of violation of

[67] Equation (82) in [59]. The paper incorrectly shows $D+\frac{1}{2}$ in the exponent and in the order of the Bessel function.

causality:

In 1+1 dimensions: A stationary observer, Alice, at $x^\mu_A = \binom{0}{0}$ sends a signal at speed w_1 to Bob, who is stationary relative to Alice. He receives the signal at $x^\mu_B = b^\mu \equiv \binom{b/w_1}{b}$ where $b>0$. Bob immediately hands this information to Charlie, who is travelling away from Alice at speed $v<w_1$ relative to Bob. In Charlie's frame of reference, this takes place at $x'^\mu_B = \Lambda^\mu_\nu b^\nu$, where $\Lambda^\mu_\nu = \begin{pmatrix} \gamma_v & -v\gamma_v \\ -v\gamma_v & \gamma \end{pmatrix}$ and $\gamma_v \equiv (1-v^2)^{-1/2}$. Charlie immediately transmits a signal in the opposite direction, this time at signal speed $w_2 > v$, to Dan who is stationary relative to Charlie. He receives it at $x'^\mu_D = \Lambda^\mu_\nu b^\nu - d^\mu$ where $d^\mu \equiv \binom{d/w_2}{-d}$ and $d>0$. Dan hands the information immediately back to Alice, so that she receives it at $x^\mu_D = (\Lambda^{-1})^\mu_\nu x^\nu_D$ in her own frame of reference. Thus,

$$x^\mu_D = (\Lambda^{-1})^\mu_\nu(\Lambda^\nu_\rho b^\rho - d^\nu) = b^\mu - (\Lambda^{-1})^\mu_\nu d^\nu = \begin{pmatrix} b/w_1 + \gamma_v d/w_2 - v\gamma_v d \\ b + v\gamma_v d/w_2 - \gamma_v d \end{pmatrix}.$$

As she is stationary, $x^1_D = 0$, $\Rightarrow$ $b = \gamma_v d(1-\frac{v}{w_2})$. The time at which she receives the information is therefore

$$x^0_D = \frac{\gamma_v d}{w_1 w_2}\Big((w_1+w_2) - v(1+w_1 w_2)\Big), \tag{6.28}$$

which means the causal condition $x^0_D > 0$ for her to receive it *after* she sent it is equivalent to $v < \frac{w_1+w_2}{1+w_1 w_2}$. In other words, if there exist solutions to

$$\frac{w_1 + w_2}{1 + w_1 w_2} \;<\; v \;<\; \min(w_1, w_2) \tag{6.29}$$

then Alice will be able to receive – and act on – the information before she chooses to send it. If *either* of the signals is not superluminal, *i.e.* if $\min(w_1, w_2) \leq 1$, then $\frac{w_1+w_2}{1+w_1 w_2} \geq \min(w_1, w_2)$ and no such solutions for v exist; but if *both* are superluminal, *i.e.* if $\min(w_1, w_2) > 1$, then subluminal speeds v exist that satisfy (6.29).

There is no limit on how far into the past the message can be sent – the time (6.28) is proportional to d (and therefore to b) – so unless there is an absolute restriction on signalling distance, any delays in the transmission process can in principle be compensated for.

We have assumed here that the sending and receiving of signals occur at spacetime points, but the argument extends trivially to a

case in which the sending and receiving of signals takes place within finite regions of spacetime, such as that discussed in Section 5.1.

A theory of nature that permits bi-directional signalling over spacelike intervals therefore also makes it possible for someone to alter the information she sends after having already received it from herself, or for a device to be programmed to signal to itself in the past if and only if it does not receive a signal from itself. This proves by *reductio* that either some very contrived new laws apply (*viz.* special relativity is false, or there are absolute restrictions on free will and programmable devices, or signal speed is limited in different ways in different directions) or signalling over spacelike intervals cannot occur in nature.

The second option is to keep going and see what happens. This alternative is what I intend to do here, in the spirit of investigating how far the single-particle theory can be taken. If we were to really take this seriously, we would have to admit that either

(a) all observables relating to the particle are spread over infinite space,[68] or

(b) the transmission of signals backwards in time is possible: that it is exponentially suppressed rather than forbidden.

We must then seek a consistent means of extending the domain of the propagator from its present requirement ($t_B - t_A > 0$) at least as far as the backwards light cone ($t_B - t_A > -|\mathbf{x_B} - \mathbf{x_A}|$), so that time-ordering is not restricted for spacelike-separated events.

One clue is evident from the forms (6.8) and (6.12) taken by the propagators for the positive and negative energy Hamiltonians: they are time-reversed images of each other.[69] We will see in Section 6.4 that the Feshbach–Villars theory unites the positive and negative energy Hamiltonians, making it possible to exploit this symmetry, at least to some extent. We will return to the relativistic particle propagator in this context in Section 6.4.7.

[68] Because we know from Section 5.1 that any observable defined within a finite region (5.9) makes signalling possible whenever the propagator is non-zero.

[69] The reason for this can be traced back to the emergence of the Hamiltonian as the generator of time evolution in Section 4.1, in particular the invariance of (4.5) under $\delta t \to -\delta t$ and $\hat{H} \to -\hat{H}$.

6.2 The square root Hamiltonian

For the calculation above, we avoided the question of what form the Hamiltonian operator takes in coordinate space by making use of a general result for free-particle Hamiltonians. Here we look at what form this Hamiltonian could take.[70]

An operator that is identical to (6.1) for at least *some* region of Hilbert space (see below for the domain) can be constructed by using a Taylor expansion:

$$\begin{aligned}\hat{H}_{\surd} &= m\sum_{n=0}^{\infty}\frac{-1}{2n-1}\frac{(2n)!}{(2^n n!)^2}\left(-\frac{\hat{\mathbf{p}}^2}{m^2}\right)^n \\ &= m\,\hat{1}+\frac{\hat{\mathbf{p}}^2}{2m}-\frac{\hat{\mathbf{p}}^4}{8m^3}+\frac{\hat{\mathbf{p}}^6}{16m^5}-\frac{5\,\hat{\mathbf{p}}^8}{128m^7}+\ldots \end{aligned} \tag{6.30}$$

Writing $\hat{H}_{\surd} = \int d\mathbf{x}\,|x\rangle\,\hat{H}^{(x)}_{\surd}\langle x|$, and employing the simplest coordinate representation (4.13),

$$\hat{H}^{(x)}_{\surd} = m\sum_{n=0}^{\infty}\frac{-1}{2n-1}\frac{(2n)!}{(2^n n!)^2}\left(\frac{1}{m^2}\nabla^2\right)^n. \tag{6.31}$$

The square of this Hamiltonian converges to

$$\hat{H}^2_{\surd}|\psi\rangle = (\hat{\mathbf{p}}^2 + m^2\hat{1})|\psi\rangle, \tag{6.32}$$

mirroring the classical Hamiltonian perfectly, but only if $|\psi\rangle$ can be decomposed as $\int_0^m d|\mathbf{p}|\int d\Omega\ \psi(\mathbf{p})\,|p\rangle$. That is, the domain of $\hat{H}_{\surd}$ is limited to a subset of Hilbert space satisfying $\langle p|\psi\rangle = 0$ for all $|p\rangle$ with $|\mathbf{p}| \geq m$.[71]

We can construct an equivalent operator for the set of all *analytic* wavefunctions by using a convolution operation, as set out in Appendix A.2. The

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[70] It can be proven that for every positive self-adjoint operator $\hat{T}$ on a Hilbert space there exists a *unique* positive self-adjoint square root operator $\hat{T}^{\frac{1}{2}}$ such that $(\hat{T}^{\frac{1}{2}})^2 = \hat{T}$ [62].

[71] There can be no non-trivial *analytic* functions in momentum space satisfying $\psi(\mathbf{p}) = 0\ \forall|\mathbf{p}| \geq m$, because by definition an analytic function is equal to its Taylor expansions, and a Taylor expansion of such a function about a point $\mathbf{p}'$ with $|\mathbf{p}'| > m$ would be zero everywhere. (The Hilbert space of square-integrable functions does include non-analytic functions.)

The equivalence between (6.31) and (6.32) would also apply if $\psi(\mathbf{x})$ were polynomial in $\mathbf{x}$, but no non-trivial polynomials are square-integrable over $\mathbb{R}^3$.

result for three spatial dimensions, (A.28), is

$$\hat{H}_{\vee}^{(x)}\psi(\mathbf{x}) = m\psi(\mathbf{x}) + \frac{m}{2\pi^2}\int_{\mathbb{R}^3} d\mathbf{r}\; r\frac{\partial}{\partial r}\left(\frac{K_1(mr)}{r^2}\right)[\psi(\mathbf{x}+\mathbf{r}) - \psi(\mathbf{x})]\,. \tag{6.33}$$

The function in the integrand has the following character for large r

$$\lim_{r\to\infty} r\frac{\partial}{\partial r}\left(\frac{K_1(mr)}{r^2}\right) \propto \frac{e^{-mr}}{(mr)^{\frac{3}{2}}}. \tag{6.34}$$

In one spatial dimension, the equivalent expression (A.15) is

$$\hat{H}_{\vee}^{(x)}\psi(x) = m\psi(x) - \frac{m}{\pi}\int_{-\infty}^{\infty} dr\,\frac{K_1(m|r|)}{|r|}\,[\psi(x+r) - \psi(x)]\,. \tag{6.35}$$

It may be verified numerically that these operators satisfy $(\hat{H}_{\vee}^{(x)})^2\psi = (-\nabla^2 + m^2)\psi$ for a variety of square-integrable functions of $\mathbf{x}$.

The action of the operator (6.35) on Gaussian functions is illustrated in Figure 1. The even character of the function is retained in the low-momentum limit, where the Hamiltonian is dominated by the mass. In the high-momentum limit, the operator converts an even function into an odd one. Between these limits, the function $\hat{H}_{\vee}^{(x)}\psi(x)$ is neither even nor odd.

Does this square root Hamiltonian act 'locally'? At first glance, the convolution operation above may appear to be non-local.[72] However, the appearance of $[\psi(\mathbf{x}+\mathbf{r}) - \psi(\mathbf{x})]$ rather than just $\psi(\mathbf{x}+\mathbf{r})$ indicates that this is not a convolution in the strict sense (A.8).

It can be seen in Figure 1 that wherever $\psi(x) \to 0$ in coordinate space, it is also the case that $\hat{H}_{\vee}^{(x)}\psi(x) \to 0$. This remains true in the limit, represented in Figure 2. So in this sense at least, this Hamiltonian is a 'local' operator, even though it is not expressed in a manifestly local form.

Nevertheless, propagation does occur over spacelike intervals under this Hamiltonian, as was shown in Section 6.1.

[72] If at $t = 0$ we have a localised wavefunction such as $\delta(\mathbf{x}-\mathbf{x_0})$, a convolution operation with a function $g(\mathbf{x})$ that is non-zero throughout coordinate space gives a result which is no longer localised, such as $\delta(\mathbf{x}-\mathbf{x_0}) * g(\mathbf{x}) = g(\mathbf{x}-\mathbf{x_0})$. The Schrödinger equation (4.7) tells us that the Hamiltonian operator gives the rate of change of a wavefunction with time; therefore under a Hamiltonian of this form, a highly localised wavefunction would have non-zero time derivatives for all $\mathbf{x}$ at $t = 0$. This is not the case for the Hamiltonians discussed in this Section.

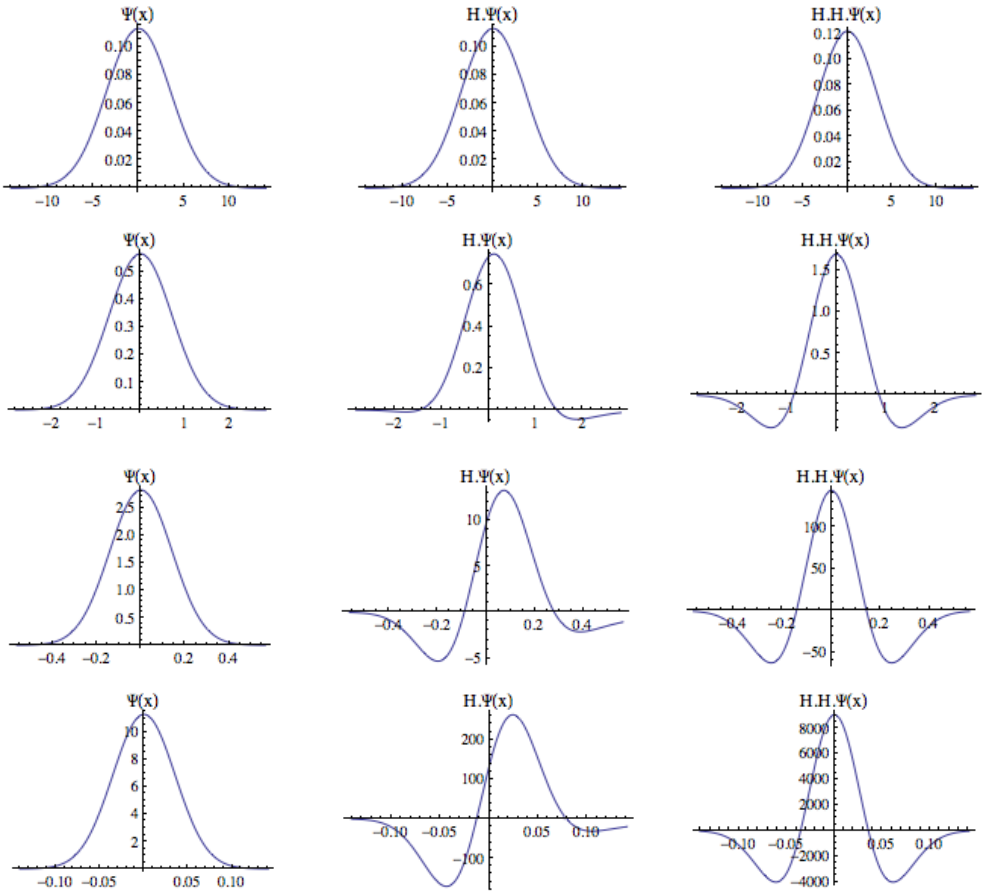

Figure 1: The action of the square root Hamiltonian (6.35) on Gaussian wavefunctions $\psi(x) = \frac{a}{\sqrt{\pi}} e^{-(ax)^2}$, with $a = 0.2$, 1, 5 and 20 respectively, and $m = 1$. The broadest functions, representing high mass or low momentum, are at the top of the Figure. In the limit of broad Gaussians, $\hat{H}^{(x)}_{\surd}\psi(x) \to m\psi(x)$. In the limit of narrow Gaussians, $\hat{H}^{(x)}_{\surd}\psi(x) \to -d\psi/dx$ (see Figure 2).

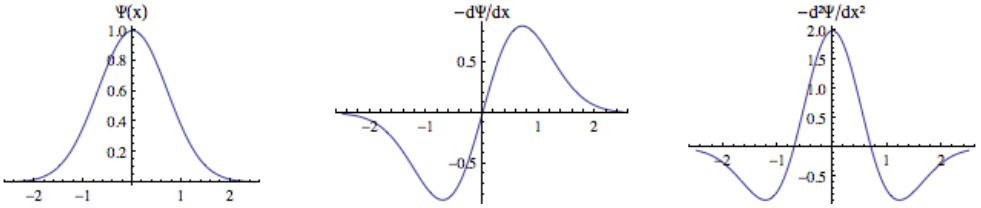

Figure 2: A Gaussian function and its 1st and 2nd derivatives

6.3 Other relativistic Hamiltonians

It is possible to construct Hamiltonians in accord with Postulate 3 that obey the Klein–Gordon relation $\hat{H}^2 = \hat{\mathbf{p}}^2 + m^2\hat{1}$ without resorting to convolution functions or infinite sums of momentum operators.

The most general *finite* sum of products of momentum operators, employing a series of rank-r tensors, is

$$\frac{\hat{H}}{m} = \sum_{r=0}^{N} A^{(r)}_{i_1 i_2 \ldots i_r} \frac{\hat{p}_{i_1}}{m}\frac{\hat{p}_{i_2}}{m}\ldots\frac{\hat{p}_{i_r}}{m} \quad \text{such that} \quad \left(\frac{\hat{H}}{m}\right)^2 = \left(\frac{\hat{\mathbf{p}}}{m}\right)^2 + \hat{1}. \tag{6.36}$$

There are no solutions for $N=0$. For $N=1$, we require

$$\frac{\hat{H}}{m} = A^{(0)}\hat{1} + A^{(1)}_i \frac{\hat{p}_i}{m} \text{ such that } (A^{(0)})^2=1;\ \{A^{(0)}, A^{(1)}_i\}=0;\ \{A^{(1)}_i, A^{(1)}_j\}=\delta_{ij}.$$

This anticommutator algebra defines the Dirac theory, which will be discussed in Section 6.5. It requires at least a $\nu=4$-dimensional representation, which may be self-adjoint.

For $N=2$, there is some redundancy. In the the case $A^{(1)}_i = 0$, we have

$$A^{(2)}_{ij} = \alpha\,\delta_{ij} \text{ and } A^{(0)} = \beta \text{ with } \{\alpha,\beta\} = 1;\ \alpha^2 = 0;\ \beta^2 = 1.$$

This algebra defines the Feshbach–Villars theory, which will be discussed in the next Section. It requires at least a 2-dimensional representation, and the matrices in this representation cannot be self-adjoint because of the nilpotency requirement $\alpha^2 = 0$.[73]

If we set $A^{(1)}_i = \epsilon_i$ and allow all the coefficients to vary a small amount from the elements of the Feshbach–Villars algebra, we obtain to lowest order in ϵ_i the following anticommutation relations:

$$\{\epsilon_i, \epsilon_j\} = 0;\ \{\epsilon_i, A^{(2)}\} = 0;\ \{\epsilon_i, A^{(0)}\} = 0.$$

These restrict ϵ_i somewhat, in particular the nilpotency relations $\epsilon_i^2 = 0$, and are rather suggestive of $\epsilon_i = 0$. Another set of zero relations arises if we start from the Dirac algebra and introduce $A^{(2)}_{ij} = \epsilon_{ij}$.

For $N \geq 3$, the number of zero anticommutation relations and nilpotent elements increases, and the algebra becomes progressively more contrived.

The conclusion here is that the set of single-particle theories in line with the

[73] If A is self-adjoint, $A^2 = 0 \Rightarrow \sum_j A_{ij}A_{jk} = 0\ \forall\ i,k \Rightarrow \sum_j |A_{ij}|^2 = 0\ \forall\ i \Rightarrow A = 0$.

three postulates for a particle with manifestly locally-generated time evolution that could give rise to the relativistic energy-momentum relation we observe classically is effectively exhausted by two cases. I discuss the Feshbach–Villars theory in some detail below, and follow this with a brief examination of the similarities and differences that arise for the Dirac theory.

6.4 The Feshbach–Villars Hamiltonian

6.4.1 Introduction

The simplest represention of the Feshbach–Villars algebra uses two of the Pauli matrices, giving the following Hamiltonian [63, §1.6]:

$$\hat{H}_{FV} = (\sigma_3 + i\sigma_2)\frac{\hat{\mathbf{p}}^2}{2m} + \sigma_3 m. \tag{6.37}$$

Appreciating the nature of position in this theory requires some care. There is clearly a momentum operator $\hat{\mathbf{p}}$, which must be self-adjoint (as it is an observable) with a continuous spectrum of eigenvalues. A position operator can be constructed from momentum along the lines of the argument outlined for constructing momentum from position in Section 4.2, but I will postpone this until Section 6.4.5. The intention is to begin by exploring the character of this theory as far as possible without relying on any particular notion of position.

We proceed as follows. First, the time evolution equation is found in the momentum representation, with basis elements denoted by $|p^\alpha\rangle$. Its solutions are used to generate a *second* momentum representation, with basis elements denoted by $|p^{(\pm)}\rangle$, in which the free-particle Hamiltonian is diagonal and the two components of the wavefunction evolve independently. These can then naturally be identified with a pair of particle types, which we will see is a particle-antiparticle pair. After a brief examination of the space of states for physical particles, we will be equipped to consider what is required for a meaningful position observable, and to use this to derive propagators and investigate the causal implications of the theory.

In Section 6.5 we will see that significant aspects of this Section apply also to Dirac theory.

6.4.2 Notation

A few words are required to clarify the notation in this Section.

As the momentum representation is two-dimensional, there is a pair of

momentum basis elements $|p^\alpha\rangle$ for each momentum eigenvalue $\mathbf{p}$, and consequently a pair of wavefunctions. I refer to these explicitly in component form with superscripts $\psi^\alpha(\mathbf{p},t)$, or collectively using a capital $\Psi(\mathbf{p},t)$, and also in column vector form. The relations between these are defined in (6.39) below; the t-dependence will only be made explicit when it is relevant. 'Ket' notation $|\psi\rangle$ is reserved for expressions that are representation-independent.

Operators in the standard momentum representation, which I shall refer to as the **canonical momentum representation**, carry a superscript $^{(p)}$. When given explicitly as elements of a matrix in relation to vector components they also carry two matrix superscripts, for example $\hat{H}_{FV}^{(p)\alpha\beta}$. Operators without any superscript are representation-independent. A subscript on vectors a_i runs from 1 to 3, and refers to a Cartesian basis. A vector operator $\hat{\mathbf{A}}$ is an operator that has vector eigenvalues, here labelled by n: $\hat{\mathbf{A}}|A^{(n)}\rangle = \mathbf{A}^{(\mathbf{n})}|A^{(n)}\rangle$. In component form, it may be expressed as $(\hat{A}_1, \hat{A}_2, \hat{A}_3)$ where $\hat{A}_i|A^{(n)}\rangle = A_i^{(n)}|A^{(n)}\rangle$. It is understood that $\hat{p}_i^{(p)} = p_i$.

A second momentum representation, known as the **Φ-representation**, will be introduced, in which the two components of the wavefunction are written as $\phi^{(+)}(\mathbf{p})e^{-iE_pt}$ and $\phi^{(-)}(\mathbf{p})e^{iE_pt}$, or collectively as $\Phi(\mathbf{p},t)$, as defined in (6.45) and (6.49). Operators in this representation are distinguished by a further superscript $^\Phi$, for example $\hat{H}^{(p\Phi)}$.

Vectors $|\psi\rangle$ and wavefunctions $\psi^\alpha(\mathbf{p},t)$ carrying superscripts $^{(+)}$ and $^{(-)}$ refer to states that have only a single non-zero component (upper and lower respoectively) when expressed in the Φ-representation. These correspond to particle and antiparticle states respectively. The subspaces of these states are denoted $\mathcal{H}_{FV}^{(+)}$ and $\mathcal{H}_{FV}^{(-)}$, and are spanned by the continuous momentum bases $|p^{(+)}\rangle$ and $|p^{(-)}\rangle$ respectively.

Any equation in which the $\pm$ symbol is used, whether in superscript or otherwise, should be regarded as a pair of equations.

6.4.3 The two momentum representations

Any continuous momentum representation for the space of states $\mathcal{H}_{FV}$ may be expressed as follows:

$$\hat{p}_i = \sum_{\alpha=1}^{2} \int d\mathbf{p}\, p_i\, |p^\alpha\rangle\langle p^\alpha| \tag{6.38}$$

$$\Psi(\mathbf{p}) \equiv \begin{pmatrix} \psi^1(\mathbf{p}) \\ \psi^2(\mathbf{p}) \end{pmatrix} \equiv \begin{pmatrix} \langle p^1|\psi\rangle \\ \langle p^2|\psi\rangle \end{pmatrix}. \tag{6.39}$$

We define the *canonical* momentum representation to be that in which the Hamiltonian has the form prescribed in (6.37):

$$\hat{H}^{(p)}_{FV} \;=\; (\sigma_3 + i\sigma_2)\frac{\mathbf{p}^2}{2m} + \sigma_3 m \;=\; \begin{pmatrix} \frac{\mathbf{p}^2}{2m}+m & \frac{\mathbf{p}^2}{2m} \\ -\frac{\mathbf{p}^2}{2m} & -\frac{\mathbf{p}^2}{2m}-m \end{pmatrix}. \tag{6.40}$$

Continuous unitary time evolution (Section 3.1) can only be generated by a self-adjoint Hamiltonian operator (Section 4.1). The Hamiltonian in (6.37) has $\hat{H}^{\dagger}_{FV} = \sigma_3 \hat{H}_{FV} \sigma_3$; but it can be made self-adjoint on $\mathcal{H}_{HV}$ if the inner product on $\mathcal{H}_{HV}$ is suitably defined. Requiring

$$\langle \psi_2 | \hat{H}_{FV} \psi_1 \rangle = \langle \psi_1 | \hat{H}_{FV} \psi_2 \rangle^* \quad \forall |\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}_{FV} \tag{6.41}$$

implies the following inner product in the momentum basis:

$$\langle \psi_1 | \psi_2 \rangle \equiv \int d\mathbf{p}\, \psi_1{}^{\dagger}(\mathbf{p}) \sigma_3\, \psi_2(\mathbf{p}). \tag{6.42}$$

Since σ_3 has eigenvalues of ± 1, the cost of introducing this inner product is that it cannot be positive-definite: that is, there are $|\psi\rangle \in \mathcal{H}_{FV}$ such that $\langle \psi | \psi \rangle < 0$. This means the vector space $\mathcal{H}_{FV}$ is **not a Hilbert space**. From Section 3.1, the necessity for using a Hilbert space arises from the requirement that all probabilities in the theory be positive, if Postulate 1 is to hold.

This is not necessarily as serious a problem as it appears. A proposal for generalising a theory need not satisfy all the postulates of that theory provided it can demonstrate that those postulates could emerge from it. As we will see below, a subspace $\mathcal{H}^{(+)}_{FV} \subset \mathcal{H}_{FV}$ exists which *is* a Hilbert space. We can identify this as the space of states of a 'particle', and apply the postulates to those states. (The remainder of the full space of states would then be open to interpretation and phenomenological investigation.)

The time evolution generated by this Hamiltonian in the momentum representation, with $\hat{H}_{FV} \equiv \sum_{\alpha\beta} \int d\mathbf{p}\, |p^\alpha\rangle \hat{H}^{(p)\alpha\beta}_{FV} \langle p^\beta|$, is

$$\sum_{\alpha\beta} \int d\mathbf{p}\, |p^\alpha\rangle \hat{H}^{(p)\alpha\beta}_{FV} \psi^\beta(\mathbf{p}, t) = i\frac{\partial}{\partial t} \sum_{\alpha} \int d\mathbf{p}\, |p^\alpha\rangle \psi^\alpha(\mathbf{p}, t). \tag{6.43}$$

Pre-multiplying by $\langle p'^\gamma|$, this yields the Feshbach–Villars equation:

$$\begin{aligned} \hat{H}^{(p)\gamma\beta}_{FV} \psi^\beta(\mathbf{p}', t) \;&=\; i\frac{\partial}{\partial t}\psi^\gamma(\mathbf{p}', t) \\ \Rightarrow \quad \begin{pmatrix} \frac{\mathbf{p}^2}{2m}+m & \frac{\mathbf{p}^2}{2m} \\ -\frac{\mathbf{p}^2}{2m} & -\frac{\mathbf{p}^2}{2m}-m \end{pmatrix} \begin{pmatrix} \psi^1 \\ \psi^2 \end{pmatrix} \;&=\; \begin{pmatrix} i\,\partial\psi^1/\partial t \\ i\,\partial\psi^2/\partial t \end{pmatrix}. \end{aligned} \tag{6.44}$$

This has the pair of solutions

$$\Psi^{(\pm)}(\mathbf{p},t) \equiv \begin{pmatrix} \psi^{1(\pm)}(\mathbf{p},t) \\ \psi^{2(\pm)}(\mathbf{p},t) \end{pmatrix} = \frac{1}{\sqrt{4mE_p}} \begin{pmatrix} m \pm E_p \\ m \mp E_p \end{pmatrix} \phi^{(\pm)}(\mathbf{p})\, e^{\mp i\, E_p t}, \quad (6.45)$$

where $E_p \equiv \sqrt{p^2+m^2}$. These are normalised to $\int d\mathbf{p}\, |\phi^{(\pm)}(\mathbf{p})|^2 = 1$, so that a state constructed from either positive states only or negative states only would satisfy[74]

$$\langle \psi^{(+)} | \psi^{(+)} \rangle = 1\,; \qquad \langle \psi^{(-)} | \psi^{(-)} \rangle = -1\,. \quad (6.46)$$

We know that at any given point in $\mathbf{p}$ in momentum space, there exists a two-dimensional space spanned by the two basis vectors $|p^1\rangle$ and $|p^2\rangle$. What this tells us is that **there are only two combinations of basis vectors from which unitarily-evolving states can be constructed.** These are $|p^{(+)}\rangle$ and $|p^{(-)}\rangle$, given by

$$|p^{(\pm)}\rangle \;\equiv\; \frac{(m \pm E_p)}{\sqrt{4mE_p}} |p^1\rangle + \frac{(m \mp E_p)}{\sqrt{4mE_p}} |p^2\rangle. \quad (6.47)$$

Any physical wavefunction in this basis then has only one non-zero component:

$$\begin{aligned} \langle p^{(\pm)} | \psi^{(\pm)} \rangle &= \phi^{(\pm)}(\mathbf{p})\, e^{\mp i\, E_p t} \\ \langle p^{(\mp)} | \psi^{(\pm)} \rangle &= 0. \end{aligned} \quad (6.48)$$

---

[74] This can be made explicit by considering a state in the limit of well-defined momentum $\mathbf{p}'$, taking $\phi^{(\pm)}(\mathbf{p})$ in (6.45) to be the limit of a rectangular function:

$$\begin{aligned} \Psi^{(\pm)}_{\mathbf{p}'}(\mathbf{p},t) &= \lim_{K\to 0} \frac{1}{\sqrt{4mE_p}} \begin{pmatrix} m \pm E_p \\ m \mp E_p \end{pmatrix} \frac{1}{K^{3/2}} \mathrm{rect}^3\!\left(\frac{\mathbf{p}-\mathbf{p}'}{K}\right) e^{\mp i\, E_p t} \\ |\psi^{(\pm)}_{\mathbf{p}'}\rangle &\equiv \sum_\alpha \int d\mathbf{p}\, \psi^{\alpha(\pm)}_{\mathbf{p}'}(\mathbf{p},t) |p^\alpha\rangle \\ &= \lim_{K\to 0} \int d\mathbf{p}\, \frac{1}{K^{3/2}} \mathrm{rect}^3\!\left(\frac{\mathbf{p}-\mathbf{p}'}{K}\right) e^{\mp i\, E_p t} \left(\frac{(m \pm E_p)}{\sqrt{4mE_p}} |p^1\rangle + \frac{(m \mp E_p)}{\sqrt{4mE_p}} |p^2\rangle \right). \end{aligned}$$

The 'rect' function allows us to translate between discrete and continuous bases: it takes the value 1 when all components of its vector argument lie in the range $(-\frac{1}{2}, +\frac{1}{2})$, and zero otherwise. In terms of the Heaviside function, $\mathrm{rect}^3(\mathbf{a}) = \prod_{i=1}^3 (\theta(a_i + \frac{1}{2}) - \theta(a_i - \frac{1}{2}))$. Here it specifies a box in momentum space of volume K^3.

The integral over $\mathbf{p}$ in the final line may appear to be redundant in the limit $K \to 0$, but this is not the case – the continuous basis elements $|p^\alpha\rangle$ must be integrated to give a state in $\mathcal{H}_{FV}$. It would be a mistake to regard the $|p^\alpha\rangle$ themselves as equivalent to states in the limit of well-defined momenta, as one might in non-relativistic quantum mechanics.

Now if we consider a mutually exclusive and complete set of these boxes in momentum space, then the orthogonality relation $\langle p'^\alpha | p''^\beta \rangle = \delta^{\alpha\beta} \delta(\mathbf{p}' - \mathbf{p}'')$ leads directly to $\langle \psi^{(\pm)}_{\mathbf{p}'} | \psi^{(\pm)}_{\mathbf{p}''} \rangle = \pm \delta_{\mathbf{p}'\mathbf{p}''}$. General solutions to the Feshbach–Villars equation (6.44) may be constructed from superpositions of these states.

We can express a general wavefunction $\Phi(\mathbf{p},t) \equiv \begin{pmatrix} \langle p^{(+)}|\psi\rangle \\ \langle p^{(-)}|\psi\rangle \end{pmatrix}$ in this basis:

$$\begin{aligned} \Phi^{(+)}(\mathbf{p},t) &\equiv U_p \Psi^{(+)}(\mathbf{p},t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \phi^{(+)}(\mathbf{p})\, e^{-iE_p t} \\ \Phi^{(-)}(\mathbf{p},t) &\equiv U_p \Psi^{(-)}(\mathbf{p},t) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \phi^{(-)}(\mathbf{p})\, e^{iE_p t}, \end{aligned} \tag{6.49}$$

where the matrix U_p is given by

$$U_p \equiv \frac{(m+E_p)I - (m-E_p)\sigma_1}{\sqrt{4mE_p}} \tag{6.50}$$

and[75]

$$U_p^{-1} \equiv \frac{(m+E_p)I + (m-E_p)\sigma_1}{\sqrt{4mE_p}}. \tag{6.51}$$

This is the Φ-representation [63, §1.6]. Notably, the Hamiltonian is diagonalised in this representation:

$$\hat{H}^{(p\Phi)} \equiv U_p \hat{H}^{(p)}_{FV} U_p^{-1} = \begin{pmatrix} E_p & 0 \\ 0 & -E_p \end{pmatrix} = E_p\, \sigma_3. \tag{6.52}$$

The diagonalising matrix U_p is *pseudo-unitary*: that is, from $\hat{H}^{(p)\dagger}_{FV} = \sigma_3 \hat{H}^{(p)}_{FV} \sigma_3$ it follows that $U_p^\dagger = \sigma_3 U_p^{-1} \sigma_3$.

6.4.4 The structure of the space of states

We may now define each of the pair of vector spaces $\mathcal{H}^{(\pm)}_{FV}$ as the set of states $\int d\mathbf{p}\, \phi(\mathbf{p})\, |p^{(\pm)}\rangle$ such that $\phi(\mathbf{p})$ is any square-integrable function over momentum space.

The 'positive energy space' $\mathcal{H}^{(+)}_{FV}$ is a Hilbert space. It possesses a positive norm-squared for all states. Any state in the limit of well-defined momentum is an eigenstate of the Hamiltonian $\hat{H}_{FV}$ with positive eigenvalue E_p. The 'negative energy space' $\mathcal{H}^{(-)}_{FV}$ has a consistently negative norm-squared.[76]

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[75] Note that $\begin{pmatrix} |p^{(+)}\rangle \\ |p^{(-)}\rangle \end{pmatrix} = U_p^{-1} \begin{pmatrix} |p^{1}\rangle \\ |p^{2}\rangle \end{pmatrix}$, *i.e.* the matrix transforming the basis states is the inverse of the one transforming the wavefunctions. This is as should be expected for two representations of the same state.

[76] It can readily be seen that the expectation value of the Hamiltonian $\int d\mathbf{p}\, \Phi^\dagger(\mathbf{p}) \sigma_3 \hat{H}^{(p\Phi)} \Phi(\mathbf{p})$ remains strictly positive. In this sense at least, the term 'negative energy' is something of a misnomer.

The two spaces are quite distinct. This suggests, as we will see below, that every physical observable in this single-particle theory should be represented by an operator in $\mathcal{H}_{FV}$ that does not mix states between the positive and negative energy spaces. Any operator $\hat{A}$ for which $\hat{A}^{(p\Phi)} \equiv U_p \hat{A}^{(p)} U_p^{-1}$ is diagonal has this property, so I will refer to such operators as Φ-diagonal.

The significance of this pair of spaces $\mathcal{H}_{FV}^{(\pm)}$ is that they are stable under free-particle evolution. This means they can be considered as representing two distinct *particle types*.

The operator that distinguishes between the two is called $\hat{Q}$, defined such that $\hat{Q}|\psi^{(\pm)}\rangle = \pm|\psi^{(\pm)}\rangle$ for all $|\psi^{(\pm)}\rangle \in \mathcal{H}_{FV}^{(\pm)}$. In the Φ-representation, therefore, $\hat{Q}^{(p\Phi)} = \sigma_3$. It is shown in Appendix A.4.1, where an electromagnetic field is introduced into the Hamiltonian, that the eigenvalues of $\hat{Q}$ are directly proportional to the charge of the particle type. As both $\hat{Q}$ and $\hat{H}_{FV}$ are simultaneously diagonal in the Φ representation, they commute and therefore charge is conserved as the state evolves.

The operator $\hat{C}$ that switches between the two charges is defined in the momentum representation by $\hat{C}^{(p)}\Psi(\mathbf{p}) = \sigma_1 \Psi^*(\mathbf{p})$. The state $\hat{C}|\psi\rangle$ is referred to as the charge conjugate of $|\psi\rangle$, and where one refers to a particle, the other is its antiparticle. The two sets of states $\mathcal{H}_{FV}^{(+)}$ and $\hat{C}\mathcal{H}_{FV}^{(-)}$ are therefore both Hilbert spaces, and in both of these spaces we will see that Postulates 1, 2 and 3 continue to hold. It is therefore natural to consider this theory as a particle theory, with antiparticles.

The statement that a measurement performed on a particle should be represented by operators $\hat{A}$ that are diagonal in the Φ representation is equivalent to the statement that **the process of making this measurement does not switch of the sign of the charge of the particle**. This would normally be seen as a reasonable requirement for a measurement – in particular for a measurement of the particle's position, which is what we will consider below.

A discussion of the structure of the full space $\mathcal{H}_{FV}$ is presented in Appendix A.3.

6.4.5 The two position operators and their eigenstates

In Feshbach and Villars' paper [64], they employ a coordinate representation for which $\hat{p}_i^{(x)} = -i\partial/\partial x_i$, so that the equation of motion (6.37) becomes a wave equation:

$$\hat{H}_{FV}^{(x)} = (\sigma_3 + i\sigma_2)\frac{-\nabla_x^2}{2m} + \sigma_3 m\,. \tag{6.53}$$

I will refer to this representation as the **canonical position representation**, and denote it with a subscript C.

The only possible position operator in this representation (up to an additive constant) satisfying $[\hat{x}_{i_C}, \hat{p}_j] = i\,\delta_{ij}$ is the familiar $\hat{x}^{(x)}_{i_C} = x_i$. It follows that

$$\hat{x}^{(p)}_{i_C} = \; i\frac{\partial}{\partial p_i} I. \tag{6.54}$$

This operator is clearly diagonal (when the 2×2 unit matrix I is made explicit) in the canonical momentum representation. If we move to the Φ-representation, however, we find that it is not Φ-diagonal:

$$\begin{aligned} \hat{x}^{(p\Phi)}_{i_C} &= U_p\,\hat{x}^{(p)}_{i_C} U_p^{-1} \\ &= U_p\, i\,\frac{\partial U_p^{-1}}{\partial p_i} + U_p\, i\, U_p^{-1}\frac{\partial}{\partial p_i} \\ &= -\frac{ip_i}{2E_p^2}\sigma_1 + i\,I\frac{\partial}{\partial p_i}. \end{aligned} \tag{6.55}$$

If the canonical position operator represented a measurement, it would be one that caused particle and antiparticle states (of a single particle) to intermix. This could be taken as reasonable grounds to reject it as a physical observable in this theory. But it is not without significance, as we will see.

By demanding that a position operator "preserves the positive character of the wavefunction" – that is, does not transform particle states into antiparticle states – we are following the specification set out by Newton and Wigner in their 1949 landmark paper [65]. Position operators of this form are referred to as **Newton–Wigner operators**; I will denote the operator we seek with a subscript NW.

The requirements are that $[\hat{x}_{i_{NW}}, \hat{p}_j] = i\,\delta_{ij}\hat{1}$, and that $\hat{\mathbf{x}}^{(p\Phi)}_{NW}$ be diagonal.

In Section 4.2, a general expression for a momentum operator was derived from the commutation relation in the position basis. Here we have established a momentum basis and seek a position operator. Switching the roles of position and momentum involves only a change of sign in the commutator. Mirroring (4.21), we have

$$\hat{x}^{(p)\alpha\beta}_{i_{NW}}\psi(\mathbf{p},t) = \left[a_i^{\alpha\beta}(\mathbf{p}) + i\,\delta^{\alpha\beta}\frac{\partial}{\partial p_i}\right]\psi(\mathbf{p},t), \tag{6.56}$$

from which

$$\begin{aligned}\hat{x}^{(p\Phi)}_{i_{NW}} &= U_p\, a_i(\mathbf{p})\, U_p^{-1} + U_p\, i\, \frac{\partial U_p^{-1}}{\partial p_i} + U_p\, i\, U_p^{-1} \frac{\partial}{\partial p_i} \\ &= U_p\, a_i(\mathbf{p})\, U_p^{-1} - \frac{ip_i}{2E_p^2}\sigma_1 + i\, I \frac{\partial}{\partial p_i}. \end{aligned} \tag{6.57}$$

The requirement that $\hat{\mathbf{x}}^{(p\Phi)}_{NW}$ be diagonal then amounts to[77]

$$\begin{aligned} U_p\, a_i(\mathbf{p})\, U_p^{-1} - \frac{ip_i}{2E_p^2}\sigma_1 &= \kappa_i(\mathbf{p}) I + \lambda_i(\mathbf{p})\sigma_3 \\ \Rightarrow \qquad a_i(\mathbf{p}) &= \frac{ip_i}{2E_p^2}\sigma_1 + \kappa_i(\mathbf{p}) I + \lambda_i(\mathbf{p}) U_p^{-1}\sigma_3 U_p\,, \end{aligned} \tag{6.58}$$

where $\kappa_i(\mathbf{p})$ and $\lambda_i(\mathbf{p})$ are arbitrary functions.

The simplest form of the position operator, $\hat{x}^{(p\Phi)}_{i_{NW}} = iI\frac{\partial}{\partial p_i}$, is obtained by choosing the momentum basis in which these arbitrary functions are zero, just as we were free to choose a convenient coordinate basis in Section 4.2. This leaves us with

$$\hat{x}^{(p)}_{i_{NW}} = i\sigma_1 \frac{p_i}{2E_p^2} + iI\frac{\partial}{\partial p_i}. \tag{6.59}$$

This operator has its own continuous basis, with two basis elements for each spatial position $\mathbf{x}$ – one from which particle states may be constructed, and one for antiparticle states:

$$\hat{\mathbf{x}}_{NW} |x^{(\pm)}_{NW}\rangle = \mathbf{x} |x^{(\pm)}_{NW}\rangle. \tag{6.60}$$

In this basis, the Hamiltonian and *all physical measurements* (that do not involve transforming particles into antiparticles) are represented in diagonal form.

The disadvantage is that the Hamiltonian does not have manifestly local form. As we will see below, in the Newton–Wigner basis the Feshbach–Villars theory reverts to that of the square root Hamiltonian discussed earlier.

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[77] Any 2×2 diagonal matrix can be expressed as a sum of terms proportional to the unit matrix and σ_3. The relation $U_p \sigma_1 U_p^{-1} = \sigma_1$ has been employed here; the equivalent relations for σ_2 and σ_3 are less trivial:

$$\begin{aligned} U_p \sigma_2 U_p^{-1} &= \frac{E_p}{2m}(\sigma_2 + i\sigma_3) + \frac{m}{2E_p}(\sigma_2 - i\sigma_3) \\ U_p \sigma_3 U_p^{-1} &= \frac{E_p}{2m}(\sigma_3 - i\sigma_2) + \frac{m}{2E_p}(\sigma_3 + i\sigma_2) \;=\; U_p^2 \sigma_3\,. \end{aligned}$$

In the Φ representation, $\hat{x}^{(p\Phi)}_{i_{NW}}\langle p^{\pm}|x^{\pm}_{NW}\rangle = i\frac{\partial}{\partial p}\langle p^{\pm}|x^{\pm}_{NW}\rangle$, and $\langle p^{\pm}|x^{\mp}_{NW}\rangle = 0$. Normalising to $\langle x'^{\pm}_{NW}|x^{\pm}_{NW}\rangle = \delta(\mathbf{x}-\mathbf{x}')$ and discarding an arbitrary constant phase, it follows that

$$\langle p^{\pm}|x^{\pm}_{NW}\rangle = (2\pi)^{-3/2}e^{-i\mathbf{x}.\mathbf{p}}. \tag{6.61}$$

With Greek indices now running over the + and − states, and sums over repeated indices implied,

$$\begin{aligned}
\hat{H}^{(x\Phi)\alpha\beta}\phi^{\beta}(\mathbf{x}) &= \langle x^{\alpha}|\hat{H}_{FV}|\psi\rangle \\
&= \int d\mathbf{p}\,\langle x^{\alpha}|p^{\rho}\rangle\hat{H}^{(p\Phi)\rho\sigma}\langle p^{\sigma}|\psi\rangle \\
&= \int d\mathbf{p}\,\frac{e^{i\mathbf{x}.\mathbf{p}}}{(2\pi)^{3/2}}E_p\sigma_3^{\alpha\sigma}\int d\mathbf{x}'\,\langle p^{\sigma}|x'^{\gamma}\rangle\langle x'^{\gamma}|\psi\rangle \\
&= \sigma_3^{\alpha\sigma}\int d\mathbf{p}\,\frac{e^{i\mathbf{x}.\mathbf{p}}}{(2\pi)^{3/2}}(\mathbf{p}^2+m^2)^{\frac{1}{2}}\int d\mathbf{x}'\,\frac{e^{-i\mathbf{x}'.\mathbf{p}}}{(2\pi)^{3/2}}\,\langle x'^{\sigma}|\psi\rangle \\
&= \sigma_3^{\alpha\sigma}\int d\mathbf{p}\,\hat{H}^{(x)}_{\surd}\int d\mathbf{x}'\,\frac{e^{i(\mathbf{x}-\mathbf{x}').\mathbf{p}}}{(2\pi)^3}\,\phi^{\sigma}(\mathbf{x}') \\
&= \sigma_3^{\alpha\sigma}\,\hat{H}^{(x)}_{\surd}\int d\mathbf{x}'\,\delta^3(\mathbf{x}-\mathbf{x}')\,\phi^{\sigma}(\mathbf{x}')
\end{aligned} \tag{6.62}$$

Hence,

$$\begin{aligned}
\hat{H}^{(x\Phi)}\phi^{(\pm)}(\mathbf{x}) &= \pm\hat{H}^{(x)}_{\surd}\phi^{(\pm)}(\mathbf{x}) \\
&= \pm\left\{m\phi^{(\pm)}(\mathbf{x}) + \frac{m}{\pi}\int_{-\infty}^{\infty}d\mathbf{r}\,r\frac{\partial}{\partial r}\left(\frac{K_1(mr)}{r^2}\right)\Big[\phi^{(\pm)}(\mathbf{x}+\mathbf{r}) - \phi^{(\pm)}(\mathbf{x})\Big]\right\}.
\end{aligned} \tag{6.63}$$

The square root operator $\hat{H}^{(x)}_{\surd}$ was introduced in Section 6.2 in the context of single-component wavefunctions. The final step follows from (6.33).

In the Newton–Wigner basis, the dynamics are therefore the same as those described in Sections 6.1 and 6.2. The free particle$^{(+)}$ and antiparticle$^{(-)}$ propagators between eigenstates of the Newton–Wigner operator in this theory are therefore also given by (6.7) and (6.8):

$$\begin{aligned}
\langle x^{(\pm)}_B|\hat{U}(t_B,t_A)|x^{(\pm)}_A\rangle &= \frac{m^2}{2\pi^2}\,\frac{\pm\Delta t}{i\,\tau^2}\,K_2(\pm im\tau) \\
&= \begin{cases} \dfrac{m^2}{4\pi}\,\dfrac{\mp\Delta t}{\tau^2}\,H_2^{(1)}(\mp m\tau) & \text{if } \Delta t^2 > \Delta x^2 \\ \dfrac{im^2}{2\pi^2}\,\dfrac{\pm\Delta t}{-\tau^2}\,K_2(m\sqrt{-\tau^2}) & \text{if } \Delta t^2 < \Delta x^2\,. \end{cases}
\end{aligned} \tag{6.64}$$

Once again, it is non-zero for spacelike separations.

To conclude this Section, the eigenstates of the Newton–Wigner operator are calculated in the canonical position representation.

We start by establishing some basic relations in the canonical representations. Basis states are defined such that $\hat{\mathbf{x}}_C|x_C^\alpha\rangle = \mathbf{x}|x_C^\alpha\rangle$. Using $\hat{p}_i^{(x)}\langle x_C^\alpha|p^\beta\rangle = -i\frac{\partial}{\partial x_i}\langle x_C^\alpha|p^\beta\rangle$ and normalising to $\langle x_C'^\alpha|x_C^\beta\rangle = \delta(\mathbf{x}-\mathbf{x}')\,\delta^{\alpha\beta}$, it follows[78] that $\langle x_C^\alpha|p^\beta\rangle = (2\pi)^{-3/2}\delta^{\alpha\beta}e^{-i\mathbf{x}.\mathbf{p}}$.

Now let us compare basis elements representing the point $\mathbf{x}$ in the Newton–Wigner basis and the point $\mathbf{y}$ in the canonical basis:

$$\begin{aligned}\hat{\mathbf{x}}_{NW}|x_{NW}^{(\pm)}\rangle &= \mathbf{x}\,|x_{NW}^{(\pm)}\rangle \\ \hat{\mathbf{x}}_C\,|y_C^\alpha\rangle &= \mathbf{y}\,|y_C^\alpha\rangle, \quad \alpha\in\{1,2\}.\end{aligned} \tag{6.65}$$

Inserting a complete set of momentum basis elements in the Φ-representation and employing (6.47) and (6.61),

$$\begin{aligned}\langle y^\alpha|x_{NW}^{\pm}\rangle &= \int d\mathbf{p}\,\langle y^\alpha|p^{\pm}\rangle\langle p^{\pm}|x_{NW}^{\pm}\rangle \\ &= \int d\mathbf{p}\,\langle y^\alpha|\left[\frac{(m\pm E_p)}{\sqrt{4mE_p}}|p^1\rangle + \frac{(m\mp E_p)}{\sqrt{4mE_p}}|p^2\rangle\right]\frac{e^{-i\mathbf{x}.\mathbf{p}}}{(2\pi)^{3/2}} \\ \Rightarrow\quad \begin{pmatrix}\langle y^1|x_{NW}^{\pm}\rangle\\ \langle y^2|x_{NW}^{\pm}\rangle\end{pmatrix} &= \int\frac{d\mathbf{p}}{(2\pi)^3}\begin{pmatrix}\frac{(m\pm E_p)}{\sqrt{4mE_p}}\\ \frac{(m\mp E_p)}{\sqrt{4mE_p}}\end{pmatrix}e^{-i(\mathbf{x}-\mathbf{y}).\mathbf{p}}\,.\end{aligned} \tag{6.66}$$

These integrals are performed in [63, §1.12]. The results, in terms of $r\equiv|\mathbf{x}-\mathbf{y}|$

[78] Strictly, it follows that $\langle x_C^\alpha|p^\beta\rangle = (2\pi)^{-3/2}\hat{U}^{\alpha\beta}e^{-i\mathbf{x}.\mathbf{p}}$, with $\hat{U}$ pseudo-unitary. The choice $\hat{U}^{\alpha\beta}=\delta^{\alpha\beta}$ aligns the bases so that states represented by wavefunctions $\Psi(\mathbf{p})$ with zero in one component are represented by wavefunctions $\Psi(\mathbf{x})$ with zero in the same component.

for the exact case and for the approximation for $r \gg 1/m$ are as follows:[79]

$$\begin{aligned}
&\begin{pmatrix} \langle y^1 | x^{\pm}_{NW} \rangle \\ \langle y^2 | x^{\pm}_{NW} \rangle \end{pmatrix} \\
&\quad = \frac{1}{4\pi^2 mr} \frac{d}{dr} \left(\frac{d^2}{dr^2} - m^2 \right) \begin{pmatrix} \frac{\sqrt{\pi}(mr)^{3/4}}{\Gamma(5/4)} K_{3/4}(mr) \pm \frac{\sqrt{\pi}(mr)^{1/4}}{\Gamma(3/4)} K_{1/4}(mr) \\ \frac{\sqrt{\pi}(mr)^{3/4}}{\Gamma(5/4)} K_{3/4}(mr) \mp \frac{\sqrt{\pi}(mr)^{1/4}}{\Gamma(3/4)} K_{1/4}(mr) \end{pmatrix} \\
&\quad \approx \frac{m^3}{8\pi\sqrt{2}\,\Gamma(\frac{5}{4})} \frac{e^{-mr}}{(mr)^{7/4}} \left\{ \begin{pmatrix} 1 \\ 1 \end{pmatrix} \pm \frac{\Gamma(\frac{5}{4})}{\Gamma(\frac{3}{4})} \frac{1}{\sqrt{mr}} \begin{pmatrix} -1 \\ 1 \end{pmatrix} + \mathcal{O}\Big(\frac{1}{mr}\Big) \right\}. \qquad (6.67)
\end{aligned}$$

To clarify what this means, consider a particle state $|\psi^{(+)}_{\mathbf{x}'}\rangle$ that is well-localised at a point $\mathbf{x}'$ with respect to the Newton–Wigner coordinate basis. That is, a state for which an ideal position measurement would give a well-defined outcome: $\hat{\mathbf{x}}_{NW} |\psi^{(+)}_{\mathbf{x}'}\rangle = \mathbf{x}' \, |\psi^{(+)}_{\mathbf{x}'}\rangle$. In the Newton–Wigner representation, this state would be a delta function. For simplicity let us represent it by a rectangular function:

$$\Phi^{(+)}_{\mathbf{x}'}(\mathbf{x}) \;\equiv\; \begin{pmatrix} 1 \\ 0 \end{pmatrix} \langle x^{+}_{NW} | \psi^{(+)}_{\mathbf{x}'} \rangle \;=\; \lim_{L\to\infty} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \frac{1}{L^{3/2}} \,\mathrm{rect}^3\Big(\frac{\mathbf{x}-\mathbf{x}'}{L}\Big). \qquad (6.68)$$

In the canonical representation, its wavefunction would be (in the $r \gg 1/m$ approximation)

$$\begin{aligned}
\Psi^{(+)}_{\mathbf{x}'}(\mathbf{y}) \;&\equiv\; \begin{pmatrix} \langle y^1 | \psi^{(+)}_{\mathbf{x}'} \rangle \\ \langle y^2 | \psi^{(+)}_{\mathbf{x}'} \rangle \end{pmatrix} \\
&=\; \int d\mathbf{x} \begin{pmatrix} \langle y^1 | x^{+}_{NW} \rangle \langle x^{+}_{NW} | \psi^{(+)}_{\mathbf{x}'} \rangle \\ \langle y^2 | x^{+}_{NW} \rangle \langle x^{+}_{NW} | \psi^{(+)}_{\mathbf{x}'} \rangle \end{pmatrix} \\
&\approx\; L^{3/2} \frac{m^3}{8\pi\sqrt{2}\,\Gamma(\frac{5}{4})} \frac{e^{-m|\mathbf{y}-\mathbf{x}'|}}{(m|\mathbf{y}-\mathbf{x}'|)^{7/4}} \begin{pmatrix} 1-\ldots \\ 1+\ldots \end{pmatrix}. \qquad (6.69)
\end{aligned}$$

It is an idealised localised particle state at $\mathbf{x}'$, yet it has a two-component extended wavefunction in the canonical representation. The Hamiltonian (6.53) acts locally at every point $\mathbf{y}$ in the infinite domain of this function.

At this point, we may make a general diagnosis of **what has brought**

[79] The standard integral exploited in the calculation is:

$$\int_0^\infty dq \, \frac{\cos qz}{(q^2+1)^{\nu+\frac{1}{2}}} = \frac{z^\nu}{\Gamma(\nu+\frac{1}{2})} K_\nu(z).$$

about the split between these two physical representations of position. This same split will arise whenever the Hamiltonian is specified in the form of a non-diagonal matrix involving the momentum operator, and the process of diagonalisation requires a momentum-dependent operator such as (6.50). This inevitably introduces an off-diagonal momentum-dependent term to the Newton–Wigner operator (6.59), making the Newton–Wigner operator non-local in the canonical basis. Likewise, the canonical operator is non-local in the Newton–Wigner basis. The two bases are 'out of focus' with respect to one another.

The principles involved in ideal localised preparations and measurements of states were outlined in Section 5.1. I have argued that only the Newton–Wigner operator can be responsible for a physical determination of the position of a particle in this theory, so if a localised state were prepared at a position $\mathbf{x_A}$ and a subsequent localised measurement were taken at position $\mathbf{x_B}$, the outcome would be determined by the Newton–Wigner propagator (6.64). The non-zero values of this propagator for spacelike intervals makes clear that the evolution generated by the Hamiltonian gives rise to superluminal spreading of the wavefunction in the Newton–Wigner representation.

Since this affects subsequent measurements outside the light cone, the theory violates relativistic causality with respect to observables defined on bounded spatial regions at particular times, if those observables have the general form given in (5.9).

6.4.6 A theory with two position spaces

It has been shown above that there are two position representations – corresponding to two position operators – with direct physical relevance in this theory. We have also seen (Section 4.3) that in a single-particle theory, position space emerges in the form of a representation of the space of states derived from the position operator. There are therefore two definitions of position space in Feshbach–Villars theory.

On scales significantly larger than the Compton wavelength of the particle, the Newton–Wigner and canonical 'spaces' are indistinguishable for all practical purposes; but at smaller scales, if a point in one of the 'spaces' is brought into sharp focus, points in the other become smeared. The smear has the form of a Bessel function (6.67) with unlimited spatial extent.

In the Newton–Wigner space, local measurements take place. A particle or an antiparticle can be located, in principle to any accuracy. If a

particle is prepared or created or detected somewhere, then that somewhere is a region of the Newton–Wigner space; but time evolution is non-local (6.63).

In the canonical space, the local unitary evolution of the state takes place. The Hamiltonian acts point-wise, but any measurement that can locate a particle within a finite spatial region gives rise to a mixing of particle and antiparticle states.

To illustrate the fact that localised measurements clearly relate to the one of these representations rather than the other, we may look to the correspondence principle. In the Newton–Wigner representation, the expectation value of the position operator satisfies

$$\begin{aligned}
\frac{d}{dt}\langle \hat{x}_{i_{NW}} \rangle &= -i \, \langle \, [\hat{x}_{i_{NW}}, \hat{H}_{FV}] \, \rangle \\
&= -i \int d\mathbf{p} \; \Phi^\dagger(\mathbf{p}) \, \sigma_3 \left[i \frac{\partial}{\partial p_i}, E_p \sigma_3 \right] \Phi(\mathbf{p}) \\
&= \int d\mathbf{p} \; \Phi^\dagger(\mathbf{p}) \, \sigma_3 \frac{p_i}{E_p} \sigma_3 \Phi(\mathbf{p}) \\
&= \langle \hat{v}_i \rangle, \qquad (6.70)
\end{aligned}$$

where $\hat{v}_i$ is defined by its Φ-representation $\hat{v}_{i\Phi}^{(p)} \equiv (p_i/E_p)\sigma_3$, in correspondence with the velocity $\frac{\partial}{\partial p_i} H(\mathbf{x}, \mathbf{p})$ in the classical Hamiltonian formalism for a relativistic particle. This operator has eigenvalue p'_i/E'_p for any state $|\psi^{(\pm)}_{p'}\rangle$ in the limit of well-defined momentum $\mathbf{p}'$.

In contrast, the equivalent operator in the canonical representation is

$$\begin{aligned}
\frac{d}{dt}\langle \hat{x}_{i_C} \rangle &= -i \, \langle \, [\hat{x}_{i_C}, \hat{H}_{FV}] \, \rangle \\
&= -i \int d\mathbf{p} \; \Psi^\dagger(\mathbf{p}) \, \sigma_3 \left[i \frac{\partial}{\partial p_i}, \left((\sigma_3 + i\sigma_2) \frac{\mathbf{p}^2}{2m} + \sigma_3 m \right) \right] \Psi(\mathbf{p}) \\
&= \int d\mathbf{p} \; \Psi^\dagger(\mathbf{p}) \, \sigma_3 \left((\sigma_3 + i\sigma_2) \frac{p_i}{m} \right) \Psi(\mathbf{p}) \\
&= \langle \, (\sigma_3 + i\sigma_2) \frac{\hat{p}_i}{m} \, \rangle \, . \qquad (6.71)
\end{aligned}$$

This operator has no non-zero eigenvalues (both of the eigenvalues of $\sigma_3 + i\sigma_2$ are zero). Thus, the measurements involved in determining what we recognise the velocity of a relativistic particle in the classical limit are well-described only in the Newton–Wigner representation.

6.4.7 A small adjustment to restore Lorentz invariance

The Newton–Wigner operator clearly has attractive features, but the causality violation still present in Section 6.4.5 is very serious for a relativistic theory (see Section 6.1.3).

One approach is to modify the propagator from that given in (6.64) to this:

$$\begin{aligned} K'^{(+)}_{NW}(\mathbf{x_A}, t_A; \mathbf{x_B}, t_B) &\equiv G_R(\mathbf{x_A}, t_A; \mathbf{x_B}, t_B) \\ &= \begin{cases} 0 & \text{if } t_B < t_A \\ K^{(+)}_{NW}(\mathbf{x_A}, t_A; \mathbf{x_B}, t_B) & \text{if } t_B > t_A \end{cases} \\ K'^{(-)}_{NW}(\mathbf{x_A}, t_A; \mathbf{x_B}, t_B) &\equiv G_A(\mathbf{x_A}, t_A; \mathbf{x_B}, t_B) \\ &= \begin{cases} K^{(+)}_{NW}(\mathbf{x_B}, t_B; \mathbf{x_A}, t_A) & \text{if } t_B < t_A \\ 0 & \text{if } t_B > t_A, \end{cases} \end{aligned}$$

which gives

$$K'^{(\pm)}_{NW}(\mathbf{x_A}, t_A; \mathbf{x_B}, t_B) = \begin{cases} \theta\big(\pm(t_B - t_A)\big)\, \dfrac{m^2}{4\pi}\, \dfrac{-|\Delta t|}{\tau^2}\, H^{(1)}_2(-m|\tau|) & \text{if } \Delta t^2 > \Delta x^2 \\ \theta\big(\pm(t_B - t_A)\big)\, \dfrac{im^2}{2\pi^2}\, \dfrac{|\Delta t|}{-\tau^2}\, K_2(m\sqrt{-\tau^2}) & \text{if } \Delta t^2 < \Delta x^2. \end{cases} \tag{6.72}$$

For positive states $|\psi^{(+)}\rangle \in \mathcal{H}^{(+)}$, this changes nothing. The result (6.64) is valid only for $t_B > t_A$, because it is based at root on Postulate 3 – the unitary evolution of states in the Hilbert space – and this still holds.

For the negative states, $|\psi^{(-)}\rangle \in \mathcal{H}^{(-)}$, the retarded propagator has been replaced by the advanced propagator (see Section 5.4). Because of the symmetry of the propagator with interchange of $\mathbf{x_A}$ and $\mathbf{x_B}$, this is equivalent to postulating that the unitary evolution of negative states $|\psi^{(-)}\rangle \in \mathcal{H}^{(-)}$ occurs 'backwards in time'. (As previously noted, we cannot require the negative-energy states to conform to the same postulates that we have assumed for everything else, as $\mathcal{H}^{(-)}$ isn't a Hilbert space. Provided the postulates hold for $\mathcal{H}^{(+)}$ and $\hat{C}\mathcal{H}^{(-)}$, the theory remains in good health.)

The canonical propagator is related to this via the overlap functions $\langle x^\alpha_C | x'^{\pm}_{NW} \rangle$ given in (6.67):

$$K'^{\alpha\beta}_C(\mathbf{x_A}, t_A; \mathbf{x_B}, t_B) \;=\; \sum_{\pm} \int d\mathbf{x}'\, d\mathbf{x}''\, \langle x^\alpha_C | x'^{\pm}_{NW} \rangle K'^{(\pm)}_{NW}(\mathbf{x}', t_A; \mathbf{x}'', t_B) \langle x''^{\pm}_{NW} | x^\beta_C \rangle \tag{6.73}$$

Kleinert and Jizba [60] use distributions over path integrals (see Section 6.1.2)

to derive this propagator, and obtain[80]

$$K'^{\pm}_{NW}(\mathbf{x_A}, x^0_A; \mathbf{x_B}, x^0_B) = \int \frac{d^4p}{(2\pi)^4} \left[-ip^0 \mp iE_p\right] \frac{e^{-ip.(x_A - x_B)}}{-p^2 - i\epsilon + m^2} \quad (6.74)$$

$$K'^{\alpha\beta}_{C}(\mathbf{x_A}, x^0_A; \mathbf{x_B}, x^0_B) = \int \frac{d^4p}{(2\pi)^4} \left[-ip^0\, \delta^{\alpha\beta} - i\hat{H}^{(p)\alpha\beta}_{FV}\right] \frac{e^{-ip.(x_A - x_B)}}{-p^2 - i\epsilon + m^2} \quad (6.75)$$

The latter of these (the expression for $K'^{\alpha\beta}_{C}$), they state, is Lorentz invariant.[81] Both propagators, however, remain non-zero for spacelike $x_A - x_B$.

It might be suggested that the Lorentz invariance of the canonical expression should have been expected – after all, the Schrödinger equation with (6.53) squares to $(-\partial^2/\partial t^2)\Psi(\mathbf{x}, t) = (-\nabla^2_x + m^2)\Psi(\mathbf{x}, t)$, which is Lorentz invariant. However, in the Newton–Wigner representation, although considerably less transparently, (6.63) also squares to give $(-\partial^2/\partial t^2)\Phi(\mathbf{x}, t) = (-\nabla^2_x + m^2)\Phi(\mathbf{x}, t)$ (see Section 6.2).

The fact that *both* propagators $K'^{\alpha\beta}_{C}$ and $K'^{\alpha\beta}_{NW}$ are not simultaneously Lorentz invariant is a consequence of the fact that the function (6.67) that translates between the two representations is not Lorentz invariant.

The results presented in this Section are motivated by quantum field theory (the relationship of (6.75) to field theory propagators is discussed below) rather than single-particle theory. Although the symmetry of the single particle theory under $t \leftrightarrow -t$, $K_+ \leftrightarrow K_-$ was noted in Section 6.1.3, our quantum postulates are insufficient to give rise to an 'adjustment' of the type made in this section – it would have to be made ad hoc.

To conclude, let us take a brief look at the resemblance between (6.75) and the **Feynman propagator** $G_F(x - y)$ of quantum field theory, to be introduced in Section 7.2. The Green's functions, G_1 and G_2, for the first-order (in time derivatives) operator $\hat{S}_1 \equiv \left(\frac{\partial}{\partial t} + i\hat{H}^{(x)}\right)$ and the second-order

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[80] Their equations (46), translated from Euclidean to real time; also their equation (28).

[81] From [60, p. 10]: *"These difficulties* [notably loss of relativistic invariance] do not arise when the full matrix structure of the Weibull distribution [equivalent to the use of retarded and advanced propagators described here, in the context of the Feshbach–Villars formalism] *is taken into account. Such a matrix structure takes complete care of both particles and antiparticles. And it highlights the key role of the Feynman–Stuckelberg boundary condition."* The Feynman–Stuckelberg boundary condition is the postulate *"that negative-energy solutions propagate backwards in time." Ibid.,* p.7.

Note that the Lorentz invariance is manifest in the equivalent expression in Dirac theory (6.87). The reason is more straightforward in that case: unlike the Feshbach–Villars Hamiltonian, the Dirac Hamiltonian immediately gives a Lorentz invariant equation in the canonical position representation (6.83).

operator $\hat{S}_2 \equiv \left(\frac{\partial^2}{\partial t^2} - (\hat{H}^{(x)})^2\right)$ respectively, satisfy

$$\left(\frac{\partial}{\partial t} + i\hat{H}^{(x)}\right) G_1(\mathbf{x}, t; \mathbf{x}', t') \;=\; \delta(\mathbf{x}-\mathbf{x}')\delta(t-t') \tag{6.76}$$

$$\left(\frac{\partial}{\partial t} + i\hat{H}^{(x)}\right)\left(\frac{\partial}{\partial t} - i\hat{H}^{(x)}\right) G_2(\mathbf{x}, t; \mathbf{x}', t') \;=\; \delta(\mathbf{x}-\mathbf{x}')\delta(t-t') \tag{6.77}$$

Any wavefunction satisfying $\hat{S}_1\psi(\mathbf{x},\mathbf{t}) = 0$ also satisfies $\hat{S}_2\psi(\mathbf{x},\mathbf{t}) = 0$, just as any wavefunction satisfying the Feshbach–Villars equation also satisfies the Klein–Gordon equation.

All of the propagators discussed so far satisfy an equation of the form (6.76) (see Section 5.4), whereas the Feynman propagator satisfies the second-oder equation (7.18). If $\hat{H}^2 = \hat{p}^2 + m^2\hat{1}$, the Feynman propagator supplies a solution to (6.77) in the form $G_2(\mathbf{x}, x^0; \mathbf{y}, y^0) = G_F(x-y)$.

A sufficient[82] condition for (6.76) to follow from (6.77) is

$$G_1(\mathbf{x}, t; \mathbf{x}', t') \;=\; \left(\frac{\partial}{\partial t} - i\hat{H}^{(x)}\right) G_2(\mathbf{x}, t; \mathbf{x}', t'). \tag{6.78}$$

This allows us to generate a Green's function for the first-order equation from a Green's function for the second. If we apply this to G_F given in (7.24), and $\hat{H}^{(x)}_{FV}$ in the canonical position representation from (6.53), what we obtain is the canonical propagator of (6.75):

$$K'_C(\mathbf{x_A}, x^0_A; \mathbf{x_B}, x^0_B) \;=\; \left(\frac{\partial}{\partial t} - i\hat{H}^{(x)}_{FV}\right) G_F(x_A - x_B). \tag{6.79}$$

Similarly, taking G_R and G_A from (7.24) and the Newton–Wigner representation of the Hamiltonian (6.62),

$$\begin{aligned} K'^{+}_{NW}(\mathbf{x_A}, x^0_A; \mathbf{x_B}, x^0_B) \;&=\; \left(\frac{\partial}{\partial t} - i\hat{H}^{(x\Phi)}_{FV}\right) G_R(x_A - x_B) \\ K'^{-}_{NW}(\mathbf{x_A}, x^0_A; \mathbf{x_B}, x^0_B) \;&=\; \left(\frac{\partial}{\partial t} - i\hat{H}^{(x\Phi)}_{FV}\right) G_A(x_A - x_B) \end{aligned} \tag{6.80}$$

These two Green's functions can be obtained using the square root Hamil-

[82] A necessary condition is that any function ψ' of the form

$$\psi'(\mathbf{x}, t) \equiv \int d\mathbf{x}' \left\{ (\frac{\partial}{\partial t} - i\hat{H}^{(x)}) G_2(\mathbf{x}, t; \mathbf{x}', t') - G_1(\mathbf{x}, t; \mathbf{x}', t') \right\} f(\mathbf{x}', t'),$$

where $f(\mathbf{x}, t)$ is an arbitrary smooth function, is a solution to the Schrödinger equation $\hat{S}_1\psi'(\mathbf{x}, t) = 0$.

tonian of Section 6.2, which acts on a single-component wavefunction. The two-dimensional representation of the Feshbach–Villars formalism allows us to obtain equivalences with all four of the second-order Green's functions in (7.24).

6.5 The Dirac Hamiltonian

A third operator satisfying the Klein–Gordon relation (6.32) is the Dirac Hamiltonian:

$$\hat{H}_{D} = \gamma_0 \boldsymbol{\gamma}.\hat{\mathbf{p}} + \gamma_0 m \tag{6.81}$$

which satisfies $\hat{H}_{D}^2 = (\hat{\mathbf{p}}^2 + m^2\hat{1})$ provided the γ operators satisfy the commutation relation $[\gamma_\rho, \hat{p}_i] = 0$ and the anticommutation relation $\{\gamma_\rho, \gamma_\sigma\} = 2\eta_{\rho\sigma}$ for any $\rho, \sigma \in \{0, 1, 2, 3\}$. A self-adjoint momentum operator with a continuous spectrum of eigenvalues must have a ν-dimensional momentum basis $|p^\alpha\rangle$, from which we can construct a wavefunction $\Psi(\mathbf{p})$ for every state $|\psi\rangle$, with ν components $\psi^\alpha(\mathbf{p}) \equiv \langle p^\alpha|\psi\rangle$. This gives us a representation in which each γ_ρ is a $\mathbf{p}$-independent, $\nu \times \nu$ matrix.

A minimum of $\nu = 4$ is required to satisfy the anti-commutation relations. One convenient choice of basis gives

$$\gamma_0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}; \quad \gamma_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}. \tag{6.82}$$

The Dirac Hamiltonian has two properties that make it significantly more appealing for a relativistic quantum theory than the Feshbach–Villars Hamiltonian. Firstly, it is manifestly self-adjoint under the straightforward inner product $\langle\psi_1|\psi_2\rangle \equiv \int d\mathbf{p}\, \Psi_1^\dagger(\mathbf{p})\Psi_2(\mathbf{p})$, which makes the space of states $\mathcal{H}$ an uncomplicated Hilbert space. And secondly, in the simplest coordinate representation for which the Hamiltonian is a local operator, the Dirac equation[83] $\hat{H}_{D}^{(x)}\Psi(\mathbf{x}, t) = i\frac{\partial}{\partial t}\Psi(\mathbf{x}, t)$ is manifestly Lorentz invariant:

$$i\gamma^\mu \partial_\mu \Psi(x) - m\Psi(x) = 0. \tag{6.83}$$

In the non-relativistic limit, both theories revert to a particle theory with $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m}$, but they differ when an electromagnetic field is introduced. While the Feshbach–Villars theory reverts to the single-component non-relativistic Schrödinger theory (see Appendix A.4.2), the Dirac theory becomes equivalent

[83] This is the Schrödinger equation (4.7) for the Dirac Hamiltonian

to the two-component Pauli–Schrödinger theory (4.26), with the components differing in their response to a magnetic field.

In common with the Feshbach–Villars equation, the Dirac equation allows us to define a coordinate representation such that we either have a manifestly local Hamiltonian or we have a local position operator, but not both. We may analyse these two representations and the class of transformations that connect them by proceeding along similar lines to Section 6.4.

The momentum space wavefunction has four components that are mixed by time evolution under a non-diagonal Hamiltonian. Using a unitary matrix $U_{FW} = e^{(\boldsymbol{\gamma}.\mathbf{p}/p)\theta_p}$ with $\tan(2\theta_p) = p/m$, known as a Foldy-Wouthuysen transformation [66], the Hamiltonian can be diagonalised:[84]

$$\hat{H}^{(p)}_{FW} \equiv U_{FW}\hat{H}^{(p)}_{D}U^{-1}_{FW} = E_p\gamma^0, \tag{6.85}$$

In this representation, we can interpret the four components of the wavefunction $\Psi_{FW}(\mathbf{p}) \equiv U_{FW}\Psi(\mathbf{p})$ as representing types of particle – types that are preserved in the time evolution of the system. Employing the Dirac–Pauli representation (6.82) for the γ_ρ matrices, in relation to some chosen z-axis, the four particle types are, respectively, spin-up particle, spin-down particle, spin-up antiparticle and spin-down antiparticle.

A position operator $\hat{\mathbf{x}}_{NW}$ satisfying $[\hat{x}_{i_{NW}}, \hat{p}_j] = i\delta_{ij}$ can then be defined which is diagonal, and we have a Newton–Wigner representation for the Dirac particle. This defines position to be an observable of a particle that doesn't flip its charge or affect its spin.

The simplest such operator is again $i\partial/\partial p_i$ in this representation, which transforms back to the Dirac representation to give

$$\begin{aligned}
\hat{x}^{(p)}_{i_{NW}} &= U^{-1}_{FW}\, i\frac{\partial}{\partial p_i} U_{FW} \\
&= i\frac{\partial}{\partial p_i} + i\frac{E_p + m - \boldsymbol{\gamma}.\mathbf{p}}{\sqrt{(E_p+m)^2 + \mathbf{p}^2}}\left(\frac{\partial}{\partial p_i}\frac{E_p + m + \boldsymbol{\gamma}.\mathbf{p}}{\sqrt{(E_p+m)^2 + \mathbf{p}^2}}\right) \\
&= i\frac{\partial}{\partial p_i} + i\frac{(E_p + m - \boldsymbol{\gamma}.\mathbf{p})\,\gamma_i - (1 + \boldsymbol{\gamma}.\mathbf{p}/E_p)\,p_i}{2E_p(E_p+m)}.
\end{aligned} \tag{6.86}$$

[84] Expressing the even and odd powers of the series expansion in terms of $\sin\theta = \sqrt{\frac{1}{2}(1 - m/E_p)}$ and $\cos\theta = \sqrt{\frac{1}{2}(1 + m/E_p)}$, the unitary operator can be written

$$U_{FW} = \frac{E_p + m + \boldsymbol{\gamma}.\mathbf{p}}{\sqrt{(E_p+m)^2 + \mathbf{p}^2}}; \quad U^{-1}_{FW} = \frac{E_p + m - \boldsymbol{\gamma}.\mathbf{p}}{\sqrt{(E_p+m)^2 + \mathbf{p}^2}}. \tag{6.84}$$

The departure from $\partial/\partial p_i$ indicates that the eigenfunctions of position are not delta functions, but are irreducibly smeared in the canonical coordinate representation.

Once again, **there are in effect two position spaces for a Dirac particle, in the sense discussed in Section 6.4.6 – one in which local unitary evolution takes place, and one in which local measurements can be made.**

And again, the motion of the free particle in the Newton–Wigner representation satisfies $\frac{d}{dt}\langle\hat{\mathbf{x}}_{NW}\rangle = \langle\hat{\mathbf{v}}\rangle$ where $\hat{\mathbf{v}}$ has eigenvalues of $\hat{\mathbf{p}}/E_p$ for states in the limit of well-defined momentum, in correspondence with classical observations. No such corresponence exists in the canonical representation.

The propagators for the two position representations (compare (6.75)) may be written[85]

$$\begin{aligned} K_{NW}(\mathbf{x_A}, t_A; \mathbf{x_B}, t_B) &= \int \frac{d^4p}{(2\pi)^4} \left[-ip^0 - iE_p\gamma_0\right] \gamma_0 \frac{e^{-ip.(x-x')}}{-p^2+m^2} \\ K_{C}(\mathbf{x_A}, t_A; \mathbf{x_B}, t_B) &= \int \frac{d^4p}{(2\pi)^4} \left[-ip^0 - i\hat{H}_D^{(p)}\right] \gamma_0 \frac{e^{-ip.(x-x')}}{-p^2+m^2} \end{aligned} \quad (6.87)$$

As with the Feshbach–Villars propagator, a Lorentz invariant form of the canonical representation can be obtained by taking a $p^2 + i\epsilon$ prescription:

$$K_{C}(\mathbf{x_A}, t_A; \mathbf{x_B}, t_B) = -i \int \frac{d^4p}{(2\pi)^4} \gamma_0 \left[\gamma_\mu p^\mu + m\right] \gamma_0 \frac{e^{-ip.(x-x')}}{-p^2-i\epsilon+m^2}. \quad (6.88)$$

This prescription again corresponds to the use of the *advanced* propagator for the negative energy states – the lower pair of components in the Foldy–Wouthuysen representation that correspond to anti-particles. Equivalently, it corresponds to postulating that the unitary evolution of the negative energy states takes place 'backwards in time' (see Section 6.4.7).

Following Postulate 3 as expressed in Section 4.1 leads to the retarded propagator throughout, which does not give a Lorentz invariant theory. And once again, the Lorentz invariance does not extend to the Newton–Wigner representation in which precise measurements may be defined.

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[85] Equations (55) of [60], translated from Euclidean time to real time. Note that, from (6.81),

$$\gamma_0(\gamma_\mu p^\mu + m) = p^0 + \hat{H}_D^{(p)}.$$

With regard to electromagnetic interactions, the Dirac theory is a theory of point-like interactions with classical fields in the canonical representation. The fields are minimally coupled to the Hamiltonian, making them part of the unitary evolution:

$$i\frac{\partial\psi}{\partial t} = \left[\gamma_0\boldsymbol{\gamma}.\big(\hat{\mathbf{p}} - \mathbf{A}(\hat{\mathbf{x}}_C)\big) + \gamma_0 m + \phi(\hat{\mathbf{x}}_C)\right]\psi. \tag{6.89}$$

In the Newton–Wigner representation, a particle is an extended object with respect to electromagnetic interactions. Foldy and Wouthuysen [66] use this extended object to account for terms that arise in the energy spectrum of a Dirac particle in a Coulomb potential – in particular the term proportional to the divergence of the electric field, now known as the Darwin or Darwin–Foldy term, which corresponds to the first-order correction that would arise if the point-like charge were replaced by a multipole expansion.

Almost all textbooks discussing Dirac theory implicitly employ the canonical position representation, and describe the Darwin term as being a consequence of unlocalisability [42, §20.2], or more specifically of Zitterbewegung[86] [67, §4.3], [63, §11.1].

6.6 The breakdown of relativistic quantum particle mechanics

This exhausts the possibilities for creating a Hamiltonian that satisfies the Klein–Gordon relation.

If a free Hamiltonian (4.19) involves discrete operators $\hat{\tau}_i$, and takes a matrix form as a function of momentum, then it must be diagonalised in order to establish the basis for physical states and to identify these as particle types. If the diagonalising matrix is also function of momentum, then the canonical position operator will cease to be diagonal and the Newton–Wigner operator will be distinct from it.

A non-diagonal Hamiltonian that is a function of *both* position and momentum does not have a momentum basis, because it no longer commutes with the momentum operator. Unless a canonical transformation exists that diagonalises the Hamiltonian with respect to both position and momentum

[86] Zitterbewegung is a fluctuation in position that results from the interference between positive and negative energy states (see Appendix A.4.1). There is no such interference for a free particle in the Newton–Wigner representation.

simultaneously, there is no Newton–Wigner operator.[87]

The violations of relativistic causality with respect to any kind of local measurements of the form (5.9) by relativistic particle theories is just one of many signs of a theory being pushed beyond its sphere of applicability. Other signs include the Klein paradox, the existence of photons, and the failure of the Dirac theory to account for the Lamb shift in the hydrogen spectrum.

Any theory with a fixed number of pairs of canonical coordinates, as stipulated by Postulate 3, if interpreted as representing the dynamics of particles, necessarily describes systems in which the *numbers* of particles with each type of dynamics are fixed. The premise of the theory contradicts observations such as the creation and annihilation of electrons and positrons in pairs, or that the emission and absorption of bosons, so it should be no surprise that it breaks down at scales or energies where such processes might occur.

A largely successful resolution, as is well-known, comes about with the transition from particle degrees of freedom to field degrees of freedom, and the development of quantum field theory.

[87] In perturbation theory, where the position-dependent 'interaction' part of the Hamiltonian is small in comparison to the momentum-dependent 'free' part, a Newton–Wigner operator may be defined with respect to the free Hamiltonian. Because of the interaction, a measurement of position that doesn't change the type of particle being measured in the process can no longer be defined.

7 Quantum Field Theory

We saw in Section 4.1 that a classical–quantum correspondence exists if we can express the generator of time evolution and other observables as functions of operators with continuous eigenvalue spectra and their canonical conjugates. The equations of classical mechanics emerge as the time evolution equations of the expectation values of those observables, the Hamiltonian emerges as the generator of time evolution, and position and momentum emerge from the conjugate pairs of operators.

We then saw in Section 5.1 that if that theory admits of measurements that are confined within a finite region (5.9), no matter how large that region, these measurements can be used to signal between a spatial region R_A at time t_A and a second region R_B at t_B if and only if the propagator $K_{BA}(\mathbf{x_B}, \mathbf{x_A}) \equiv \langle x_B|\hat{U}(t_B, t_A)|x_A\rangle$ (constructed from the set of basis elements $|x\rangle$ of the position operator) is nonzero for some $\mathbf{x_A} \in R_A$ and $\mathbf{x_B} \in R_B$.

And finally, we have seen that, for $t_B > t_A$, this propagator is never zero in quantum mechanics, and that when special relativity is taken into account, this implies a breakdown in causality for the theory (see Section 6.1.3).

We wish to attempt to restore causality to the theory without abandoning the Hilbert space formulation that was argued for in Section 2. To do this, we need to find a way of guaranteeing that an evolving vector $\hat{U}(t_B, t_A)\,|\psi_A\rangle$ can remain *orthogonal* to a fixed vector $|\psi_B\rangle$ for a finite time. We could then attempt to interpret this inner product as a propagator between to locations.

The following toy model might suggest itself as a way in which relativistic causality could be restored.

In a system with discrete time-steps, we can guarantee that a state initially parallel to a basis vector $|e_\alpha\rangle$ remains orthogonal to a basis vector $|e_{\alpha+n}\rangle$ at least until n time steps have elapsed by employing a *tridiagonal* time evolution operator.[88] Given an initial state of $|\psi(0)\rangle = |e_k\rangle$, the state after one application of a tridiagonal operator will be $|\psi(1)\rangle = a|e_{k-1}\rangle + b|e_k\rangle + c|e_{k+1}\rangle$,

[88] In an orthonormal basis $\{|e_\alpha\rangle\}$, a tridiagonal operator has the form

$$\hat{U}(t_i) = \sum_{\beta\gamma} |e_\beta\rangle \Big(U^{(0)}_\gamma(t_i)\,\delta_{\beta,\gamma} + U^{(+)}_\gamma(t_i)\,\delta_{\beta+1,\gamma} + U^{(-)}_\gamma(t_i)\,\delta_{\beta-1,\gamma} \Big) \langle e_\gamma|.$$

The use of '+1' and '-1' in the labels means there is an implicit *topology* to the set of basis elements: each element has neighbours, and a metric can be defined giving a measure of 'distance' between elements. This is the kind of property one would expect for a mathematical representation of position.

which maintains orthogonality with every basis element having a label further than 1 from k. The influence of initial conditions propagates at a rate of no more than one basis vector per time step. It is a one-dimensional system with a guaranteed speed limit.

The fatal flaw in this model is that the only tridagonal matrices that are *unitary* are block-diagonal in 1×1 or 2×2 blocks [68].[89] This means propagation among the basis states in this model can progress no further than a perpetual interchange between neighbouring pairs. If the bases were to represent positions in space, there wouldn't be scope for much movement.

Generalising the time evolution matrices from tri-diagonal to $(2N+1)$-diagonal does not fix the flaw. The objective of employing basis vectors to represent position and having non-orthogonality propagate at a finite rate appears to be fundamentally at fault.

In classical physics, on the other hand, a theory that generates precisely this kind of spacetime propagation already exists: **covariant field theory**. What's more, it is built on exactly the same foundations as classical mechanics, making it amenable to the quantum postulates that we already have.

7.1 Covariant field theory

7.1.1 Classical fields

Classical covariant field theory is derived from the stationary action principle over a set of infinite sets of classical variables $\phi_a(x)$ where the continuous label $x \equiv (x^0, \mathbf{x})$ ranges throughout Minkowski space $\mathbb{R}^{1,3}$ and the discrete label a distinguishes between fields. The theory is covariant if the action is a Lorentz invariant functional of the fields.[90]

For an observer using coordinates $(t, \mathbf{x})$, the defining equations in the

[89] Each block must be $e^{i\theta}$ if 1×1 or $e^{i(n_0 I + \mathbf{n}.\boldsymbol{\sigma})}$ if 2×2 ($n_i \in \mathbb{R}$).

[90] The action $S[\phi_a] = \int d^4x\, \mathcal{L}[\phi_a, \partial_\mu\phi_a; x]$ is the spacetime integral of the Lagrangian density $\mathcal{L}$; minimising this leads to the Euler-Lagrange equations $\partial_\mu(\partial\mathcal{L}/\partial(\partial_\mu\phi_a)) - \partial\mathcal{L}/\partial\phi_a = 0$. The conjugate fields are defined by $\pi_a(x) \equiv \partial\mathcal{L}/\partial(\partial_0\phi_a)$, and the Hamiltonian density is $\mathcal{H} \equiv \pi_a\partial_0\phi_a - \mathcal{L}$, which is also the time-time component of the energy-momentum tensor

$$\mathcal{H} = \mathcal{T}^0_0, \text{ where } \mathcal{T}^\nu_\mu \equiv \sum_a \frac{\partial\mathcal{L}}{\partial(\partial_\nu\phi_a)}\partial_\mu\phi_a - \delta^\nu_\mu\mathcal{L}.$$

With the Hamiltonian of the field given by $H[\phi_a, \pi_a; t] \equiv \int d^3\mathbf{x}\, \mathcal{H}[\phi_a(\mathbf{x}), \pi_a(\mathbf{x}); \mathbf{x}, t]$, Hamilton's field equations (7.1) follow directly from the Euler–Lagrange equations [69, §12.4], [70, §2.1].

We may extend the Lorentz invariance of the action further to *Poincaré invariance* by removing explicit x-dependence from $\mathcal{L}$, which also removes explicit $\mathbf{x}$-dependence from $\mathcal{H}$.

Hamiltonian formulation, with fields $\phi_a(\mathbf{x})$ and conjugate fields $\pi_a(\mathbf{x})$ (defined over space rather than spacetime), are

$$\frac{\partial \pi_a(\mathbf{x})}{\partial t} = \frac{\delta H}{\delta \phi_a(\mathbf{x})}; \qquad \frac{\partial \phi_a(\mathbf{x})}{\partial t} = -\frac{\delta H}{\delta \pi_a(\mathbf{x})}. \tag{7.1}$$

Defining a Poisson bracket for functions of the fields $A[\phi_a, \pi_a; t]$ and $B[\phi_a, \pi_a; t]$,

$$\{A, B\}_{P} \equiv \int d^3\mathbf{x} \sum_a \left(\frac{\delta A}{\delta \phi_a(\mathbf{x})} \frac{\delta B}{\delta \pi_a(\mathbf{x})} - \frac{\delta A}{\delta \pi_a(\mathbf{x})} \frac{\delta B}{\delta \phi_a(\mathbf{x})} \right), \tag{7.2}$$

it follows that

$$\begin{aligned} \{\phi_a(\mathbf{x}), \pi_b(\mathbf{y})\}_{P} &= \delta_{ab}\, \delta^3(\mathbf{x}-\mathbf{y}); \\ \frac{dA}{dt} &= \{A, H\}_{P} + \frac{\partial A}{\partial t}. \end{aligned} \tag{7.3}$$

The situation precisely parallels that of Section 4.1; therefore if we apply Postulate 3 to a set of infinite sets of continuous operators labeled by $\mathbf{x} \in \mathbb{R}^3$ together with conjugate operators, we are guaranteed a correspondence between the dynamics of expectation values and their counterparts in a classical covariant field theory.

7.1.2 Quantum scalar fields and observables

We start with the most basic type of field: one that has a scalar character with respect to Lorentz transformation, so we need not apply any particular constraints on how it may appear in the action.

A field operator $\hat{\phi}(\mathbf{x})$ is an *operator-valued distribution* over space, such that an integral $\int_R d^3\mathbf{x}\, \hat{\phi}(\mathbf{x})$ over any spatial region R is an operator in a Hilbert space $\mathcal{H}$. Postulate 3 requires that the Hamiltonian be a function of these operators; a sufficient condition (and a necessary one for a covariant theory) is to employ a Hamiltonian density $\mathcal{H}$ defined at each point $\mathbf{x}$ as a function of field operators and their conjugates at that point. Thus, with

$$\begin{aligned} \hat{H}(t) &= \int d^3\mathbf{x}\, \mathcal{H}[\hat{\phi}_a(\mathbf{x}), \hat{\pi}_a(\mathbf{x}); t, \mathbf{x}] \\ \left[\hat{\phi}_a(\mathbf{x}), \hat{\phi}_b(\mathbf{y})\right] &= \left[\hat{\pi}_a(\mathbf{x}), \hat{\pi}_b(\mathbf{y})\right] = 0 \\ \left[\hat{\phi}_a(\mathbf{x}), \hat{\pi}_b(\mathbf{y})\right] &= i\, \delta_{ab}\, \delta^3(\mathbf{x}-\mathbf{y}), \end{aligned} \tag{7.4}$$

yhe expectation values of any operator that is a function of the field operators throughout space $\hat{A}(t) = A[\hat{\phi}_a(\mathbf{x} \in \mathbb{R}^3), \hat{\pi}_a(\mathbf{x} \in \mathbb{R}^3); t]$ then automatically

satisfies

$$\frac{d}{dt}\langle \hat{A} \rangle = \frac{1}{i} \langle\, [\hat{A}, \hat{H}]\, \rangle + \langle \frac{\partial \hat{A}}{\partial t} \rangle \tag{7.5}$$

for an observer employing coordinates $(t, \mathbf{x})$, mirroring the classical result.

These operators, now defined at every point in space, are examples of the continuous operators described in Section 4.1: the operators of which the generator of time evolution is a function (Postulate 3). By analogy with (4.9), the field operators have a continuous basis $\{|\phi\rangle\}$ satisfying

$$\hat{\phi}_a(\mathbf{x})|\phi)\rangle = \phi_a(\mathbf{x})|\phi\rangle \quad \forall\, \mathbf{x} \in \mathbb{R}^3 \tag{7.6}$$

where $\phi_a(\mathbf{x})$ is the equivalent of a spectral eigenvalue of the operator at a given point in space. For any state $|\Psi\rangle$ in the Hilbert space of the system, we can now define a *wave functional* $\Psi[\phi(\mathbf{x}), t] \equiv \langle \phi | \Psi \rangle$. For a given Hamiltonian we could present the Schrödinger equation in this basis [71, §2.10], showing the evolution of the state over time in the Schrödinger picture.

There is no reason to require the field itself to be self-adjoint, although an observable $\hat{A}$ constructed as a function of field operators clearly must be. For the purposes of establishing a direct correspondence with a real classical scalar field we would consider $\hat{\phi}_a$ to be self-adjoint. Beyond this purpose, significant generalisations are open to us, as will be seen in Section 7.1.3.

For a relativistic field theory, it is convenient to work in the *Heisenberg picture* in relation to some base time t_0, defining, for $x \equiv (t, \mathbf{x})$,

$$\hat{\phi}_a(x) \equiv \hat{U}^\dagger(t, t_0)\hat{\phi}_a(\mathbf{x})\hat{U}(t, t_0) \tag{7.7}$$

The state vector $|\Psi\rangle$ in the Heisenberg picture must then be fixed for all t to be equal to the Schrödinger state vector $|\Psi(t_0)\rangle$.

It follows from the definition that the commutation relations (7.4) continue to apply provided they are evaluated at *equal times*. As the theory is Lorentz invariant, it follows immediately that any two field operators $\hat{\phi}_a(x)$ and $\hat{\phi}_b(y)$ necessarily commute if x and y are spacelike separated. This condition is referred to as **microcausality**.

Further, if two operators $\hat{A}$ and $\hat{B}$ are functions of the field operators $\hat{\phi}_a(x)$ and $\hat{\pi}_a(x)$ within the bounded spacetime regions $\mathcal{R}_A$, and $\mathcal{R}_B$ respectively,

then

$$\left[\,\hat{A}\,,\,\hat{B}\,\right] = 0 \;\text{ if } \mathcal{R}_A \text{ and } \mathcal{R}_B \text{ are entirely spacelike separated.}^{91} \qquad (7.8)$$

If we were to assert that all observables have the form of functions of field operators over bounded spacetime regions, then quantum field theory is guaranteed to be a causal theory with respect to pairs of measurements over those regions.[92]

7.1.3 Non-scalar fields and observables

If the equal time commutation rules are modified by a phase,

$$\begin{aligned}
\hat{\phi}_a(t,\mathbf{x})\hat{\phi}_b(t,\mathbf{y}) - e^{2\pi i/\nu}\hat{\phi}_b(t,\mathbf{y})\hat{\phi}_a(t,\mathbf{x}) &= 0 \\
\hat{\pi}_a(t,\mathbf{x})\hat{\pi}_b(t,\mathbf{y}) - e^{2\pi i/\nu}\hat{\pi}_b(t,\mathbf{y})\hat{\pi}_a(t,\mathbf{x}) &= 0 \\
\hat{\phi}_a(t,\mathbf{x})\hat{\pi}_b(t,\mathbf{y}) - e^{2\pi i/\nu}\hat{\pi}_b(t,\mathbf{y})\hat{\phi}_a(t,\mathbf{x}) &= i\,\delta_{ab}\,\delta^3(\mathbf{x}-\mathbf{y}),
\end{aligned} \qquad (7.9)$$

where $\nu \in \mathbb{N}$, then (7.5) and (7.8) continue to hold provided $\hat{A}$, $\hat{B}$ and $\hat{H}$ each involve a multiple of ν one-point products of field operators.

The requirement that the action be Lorentz invariant, however, requires that the fields must transform as representations of the Lorentz group [72, §4]. For some representation $D[\Lambda]$ (which, by definition, satisfies $D[\Lambda_1]_{ab}\,D[\Lambda_2]_{bc} = D[\Lambda_1\Lambda_2]_{ac}$), the fields must transform under $x^\mu \to \Lambda^\mu{}_\nu x^\nu$ as

$$\hat{\phi}_a(x) \;\to\; D[\Lambda]_{ab}\;\hat{\phi}_b(\Lambda^{-1}x). \qquad (7.10)$$

In 3+1 dimensions, two classes of representation exist for the Lorentz group: bosonic representations with $\nu = 1$, and fermionic representations with

[91] Spacetime regions $\mathcal{R}_A$ and $\mathcal{R}_B$ are entirely spacelike separated if $\mathbf{x_A}$ is spacelike separated from $\mathbf{x_B}$ for all $\mathbf{x}_A \in \mathcal{R}_A$ and all $\mathbf{x}_B \in \mathcal{R}_B$.

[92] See, however, Section 7.5.1.

with $\nu = 2$.[93]

A field with a rank-p tensor character is called a **boson field**. $D[\Lambda]$ is a product of p Lorentz tensors, and (7.4) continue to apply. The results of Section 7.1.2 generalise straightforwardly to vector and other tensor fields.

The other type of field is a **fermion field**. Fermionic representations include the **spinor representation**, which has the form $S[\Lambda] = \exp(\frac{1}{8}[\gamma^\mu, \gamma^\nu]\,\omega_{\mu\nu})$ for infinitesimal Lorentz transformations $\Lambda^\mu{}_\nu = \delta^\mu_\nu + \omega^\mu{}_\nu$. The indices for spinor fields $\hat{\psi}_\alpha$ and the representation $S[\Lambda]_{\alpha\beta}$ correspond to the indices of the matrix representation chosen for the γ^μ, for example (6.82).

From (7.9), all fermion fields and their conjugates $\hat{\pi}$ satisfy the anticommutation relations

$$\begin{aligned} \big\{\hat{\psi}_a(t,\mathbf{x}), \hat{\psi}_b(t,\mathbf{y})\big\} &= \big\{\hat{\pi}_a(t,\mathbf{x}), \hat{\pi}_b(t,\mathbf{y})\big\} = 0 \\ \big\{\hat{\psi}_a(t,\mathbf{x}), \hat{\pi}_b(t,\mathbf{y})\big\} &= i\,\delta_{ab}\,\delta^3(\mathbf{x}-\mathbf{y}), \end{aligned} \tag{7.11}$$

The relations (7.5) and (7.8) therefore continue to hold provided $\hat{H}$, $\hat{A}$ and $\hat{B}$ are composed of an even number of field operators, $\hat{\psi}_a(x)$ and/or $\hat{\pi}_a(x)$.

It is instructive to look more closely at the kind of operator that could represent an observable in a fermion field.

In the spinor representation, there are five Lorentz covariant objects that can be formed from the fields. They are constructed using the γ^μ matrices

[93] The group $SO(n,1)^+$ of proper (non-reflecting) orthochronous (non-time-reversing) Lorentz transformations in n spatial dimensions is a Lie group, and therefore has a topological structure. The set of closed paths in a topological space can be divided into equivalence classes by continuous deformation, and the set of transformations between those equivalence classes forms a group, called the fundamental homotopy group of that space. $SO(n,1)^+$ has a homotopy group that is trivial for $n = 1$, $\mathbf{Z}$ for $n = 2$ and $\mathbf{Z}_2$ for $n \geq 3$. For each $SO(n,1)^+$, a 'universal covering group' exists that is simply connected (has a trivial homotopy group) and has $SO(n,1)^+$ as a subgroup. In three dimensions, the universal covering group is $SL(2,\mathbb{C})$. By exploiting the homomorphism $SL(2,\mathbb{C}) \to SO(3,1)^+$, all of the representations of $SO(3,1)^+$ can be found. The two classes of representations, bosonic ($\nu = 1$) and fermionic ($\nu = 2$), correspond to the two elements of the homotopy group $\mathbf{Z}_2$, which is the kernel of the homomorphism.

In one spatial dimension, only bosonic representations exist. In two spatial dimensions, ν may take any integer value, and the resulting representations are *anyonic*. However, the relations (7.9) do not generate a local field theory. The quantum theory of anyons relies on representations of the braid group rather than the homotopy group, so commutation relations of the form (7.9) do not apply [73, §5].

along with $\bar{\psi} \equiv \psi^\dagger \gamma^0$ and $\gamma^5 \equiv i\gamma^0\gamma^1\gamma^2\gamma^3$, and are all bilinear in the fields:[94]

$$\bar{\psi}\,\psi, \qquad \bar{\psi}\,\gamma^\mu\psi, \qquad \bar{\psi}\,[\gamma^\mu,\gamma^\nu]\psi, \qquad \bar{\psi}\,\gamma^\mu\gamma^5\psi, \qquad \bar{\psi}\,\gamma^5\psi. \tag{7.12}$$

If the field theory is to be covariant, then any spinor field may only appear in the action in the form of these objects.

Setting aside the Lorentz character of these bilinears, what we have here is a set of 1+4+6+4+1 = 16 matrices – let us call them $\Gamma^i_{\alpha\beta}$, $i \in \{1, ..., 16\}$. As the Lagrangian density $\mathcal{L}$ must be built from these, the conjugate field $\hat{\pi}_a(x) = \partial\mathcal{L}/\partial(\partial_0\psi_a)$ must also. Each one of these bilinears $\bar{\psi}\,\Gamma^i\psi$ is a self-adjoint operator [72, §4]. As we have 16 linearly independent operators, they constitute a complete basis for **self-adjoint bilinears** on the spinor fields.

The most general observable we may define using a spinor field is therefore a self-adjoint[95] operator function $f(\hat{A}, \hat{B}, \ldots)$ of operators of the form:

$$\hat{A} = \int_{\mathcal{R}_A} d^4x \bar{\psi}_\alpha(x)\, \hat{A}^{(x)}_i \Gamma^i_{\alpha\beta}\, \psi_\beta(x), \tag{7.13}$$

where $\hat{A}^{(x)}_i$ is a set of self-adjoint differential operators with respect to x (or functions of x, or numbers). The differential operator may act to the right on $\psi_\beta(x)$, to the left on $\bar{\psi}_\alpha(x)$, or both. The integration takes place over a spacetime region $\mathcal{R}_A$.

The anticommutation relations (7.11) for these fields give zero for different points at equal times in any reference frame. Since the sign changes inherent in manipulating anticommutators come in pairs when applied to pairs of operators, we may restate (7.8) for spinor fields:

$$\left[\,\hat{A}\,,\,\hat{B}\,\right] = 0 \;\text{ if } \mathcal{R}_A \text{ and } \mathcal{R}_B \text{ are entirely spacelike separated.} \tag{7.14}$$

If we were to assert that all observables on a spinor field have the form of functions of integrals of self-adjoint bilinears over bounded spacetime regions, then a quantum field theory of spinors would be guaranteed to be causal with respect to pairs of measurements in those regions.

Result (7.14) is proven for the general case in Appendix A.5

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[94] For reasons of clarity, I have dropped the caret notation for fermion fields.

[95] Any function $f(\hat{A}, \hat{B})$ of self-adjoint operators can be made self-adjoint by symmetrising or antisymmetrising. Examples include the symmetric product $\frac{1}{2}(\hat{A}\hat{B} + \hat{B}\hat{A})$ and the antisymmetric product $\frac{1}{2}i(\hat{A}\hat{B} - \hat{B}\hat{A})$.

7.2 A field theory with a classical source

One way of representing an external influence on a quantum field is by adding a classical source term to the action. A simple example using an otherwise free real scalar field is discussed in [74, §2.4]:

$$\hat{S}[x] \equiv \int d^4x\, \mathcal{L}[\hat{\phi}, \partial_\mu\hat{\phi}; x] = \int d^4x \left(\tfrac{1}{2}(\partial_\mu\hat{\phi})(\partial^\mu\hat{\phi}) - \tfrac{1}{2}m^2\hat{\phi}^2 + j(x)\hat{\phi}\right) \quad (7.15)$$

where $j(x)$ is a scalar function of x that is zero outside of a finite region $\mathcal{R}_j$, and $\hat{\phi}(x)$ is a real scalar field. The last term breaks the Poincaré invariance of the action, but not the Lorentz invariance.

The equivalent action in classical field theory gives the equation of motion of a scalar field with a source $j(x)$. In quantum field theory, with $j(x)$ a function of x, the equation is identical:

$$(\partial_\mu\partial^\mu + m^2)\hat{\phi} = j(x)\hat{1}. \quad (7.16)$$

This 'classical source' $j(x)$ does not evolve along with the system's equations of motion. It is an influence *on* the system, but isn't affected by anything within it. If it represents a physical influence, it must be one that is determined externally.

A general solution to (7.16) can be expressed as

$$\hat{\phi}(x) = \hat{\phi}_0(x) + \int d^4y\, \hat{G}(x,y)j(y) \quad (7.17)$$

for some two-point operator $\hat{G}(x,y)$, where $\hat{\phi}_0(x)$ is a solution for the homogeneous equation $(\partial_\mu\partial^\mu + m^2)\hat{\phi}_0 = 0$.

Substituting (7.17) into (7.16), we find that $\hat{G}(x,y) = G(x-y)\hat{1}$ must be a distribution proportional to the unit operator on the Hilbert space, satisfying the differential equation:

$$(\partial_\mu\partial^\mu + m^2)G(x-y) = \delta^4(x-y). \quad (7.18)$$

This marks $G(x-y)$ as a **Green's function** of the Klein–Gordon operator $\partial_\mu\partial^\mu + m^2$ in (7.16). In [74, §2.4], it is taken to be the *retarded* Green's function; in this Section, I will consider whether this is necessarily the case.

If the inhomogeneous Klein–Gordon equation $(\partial_\mu\partial^\mu{+}m^2)\phi{=}j(x)$ is known to hold in a given spacetime region $\mathcal{R}\supset\mathcal{R}_j$, then the general solution is[96]

$$\phi(x) \;=\; \int_R d^4y\, G(x{-}y)j(y) - \int_{\partial R}(d^3y)^\mu\,\left[G(x{-}y)\frac{\partial\phi}{\partial y^\mu} - \frac{\partial G}{\partial y^\mu}\phi(y)\right]. \quad (7.19)$$

Comparing with (7.17), this gives a source-independent relation between $\hat{\phi}_0(x)$ and the conditions at a boundary ∂R, in terms of a given Green's function:

$$\hat{\phi}_0(x) \;=\; -\int_{\partial R}(d^3y)^\mu\,\left[G(x{-}y)\frac{\partial\hat{\phi}}{\partial y^\mu} - \frac{\partial G}{\partial y^\mu}\hat{\phi}(y)\right]. \quad (7.20)$$

Returning to the Green's function itself, the Fourier Transform of (7.18) is

$$(-k_\mu k^\mu + m^2)\tilde{G}(k) = 1 \quad (7.21)$$

which has the general (distribution) solution[97]

$$\tilde{G}(k) = \frac{1}{-k^2+m^2} + \tilde{G}_0(k)\,\delta(-k^2+m^2). \quad (7.22)$$

---

[96]This can be shown using, in turn, the inhomogeneous Klein–Gordon equation, the product rule for differentiation, Stokes' theorem and the definition of a Green's function (7.18):

$$\begin{aligned}
\int_R d^4y\, G(x{-}y)j(y) &= \int_R d^4y\, G(x{-}y)\left[\frac{\partial^2}{\partial y_\mu\partial y^\mu}+m^2\right]\phi(y)\\
&= \int_R d^4y\,\left\{\frac{\partial}{\partial y_\mu}\left[G\frac{\partial\phi}{\partial y^\mu}\right] - \frac{\partial}{\partial y_\mu}\left[\frac{\partial G}{\partial y^\mu}\phi\right] + \frac{\partial^2 G}{\partial y_\mu\partial y^\mu}\phi + m^2G\phi\right\}\\
&= \int_{\partial R}(d^3y)^\mu\,\left[G\frac{\partial\phi}{\partial y^\mu} - \frac{\partial G}{\partial y^\mu}\phi\right] + \int_R d^4y\,\left\{\left[\frac{\partial}{\partial^2 y_\mu\partial y^\mu}+m^2\right]G\right\}\phi\\
&= \int_{\partial R}(d^3y)^\mu\,\left[G\frac{\partial\phi}{\partial y^\mu} - \frac{\partial G}{\partial y^\mu}\phi\right] + \int_R d^4y\,\delta^4(x{-}y)\,\phi(y)
\end{aligned}$$

which leads directly to (7.19) [75, §6]. In the boundary term, $(d^3y)^\mu$ is an outward-directed three-dimensional element of the boundary of the Minkowski spacetime region R. At an initial time boundary, for example, $(d^3y)^\mu\frac{\partial}{\partial y^\mu} = -d^3\mathbf{y}\frac{\partial}{\partial t}$. At a spatial boundary, in terms of an outward-directed area element $d\mathbf{A}$, $(d^3y)^\mu\frac{\partial}{\partial y^\mu} = -dt\,d\mathbf{A}.\nabla$. (Here, $t{\equiv}y^0$.)

[97]A distribution solution to $A(x){=}B(x)$ is one for which $\int dx\,A(x)f(x) = \int dx\,B(x)f(x)$ for any smooth function $f(x)$ that vanishes outside of a finite region. For a straightforward introduction to distributions, including the reason for this definition, see [76, §2]. (Some authors, *e.g.* [77, §2.1], use the slightly less restrictive condition that $f(x)$ must vanish at infinity faster than any power of x. Distributions defined in this way are said to be 'tempered'.)

Hence

$$\begin{aligned} G(x-y) &= \int \frac{d^4k}{(2\pi)^4}\,\frac{e^{-ik.(x-y)}}{-k^2+m^2} + \int \frac{d^4k}{(2\pi)^4}\,e^{-ik.(x-y)}\tilde{G}_0(k)\,\delta(-k^2+m^2) \\ &= \int \frac{d^4k}{(2\pi)^4}\,\frac{e^{-ik.(x-y)}}{-k^2+m^2} + \Phi(x-y) \end{aligned} \tag{7.23}$$

where $\Phi(x)$ is a solution of the homogeneous Klein–Gordon equation $(\partial_\mu\partial^\mu+m^2)\Phi(x)=0$.

Because of the singularities at $k^\mu k_\mu = m^2$, the integral does not converge to a unique solution. It can be performed using complex analysis, treating the singularities as poles in the complex k^0 plane [74, §2.4]. By taking a contour clockwise or anticlockwise about each of the two poles, one may obtain four distinct results – all of which ultimately differ only in terms of the Φ in (7.23), but which are appropriate for particular types of boundary conditions.

With $\tau \equiv \sqrt{x^\mu - y^\mu)(x_\mu - y_\mu)}$, and using the notation $x \succ y$ and $x \prec y$ to refer to x being in the future and past light cones of y respectively, the four

Green's functions are as follows: [78, §2], [79, §App. II][98]

$$
\begin{aligned}
G_R(x-y) &\equiv \lim_{\epsilon\to 0^+}\int \frac{d^4k}{(2\pi)^4}\frac{e^{-ik.(x-y)}}{-k^2-i\epsilon k^0+m^2} = \begin{cases} \dfrac{\delta(\tau^2)}{2\pi} - \dfrac{m}{4\pi\tau}J_1(m\tau) & \text{if } x\succ y \\ 0 & \text{otherwise} \end{cases} \\
G_A(x-y) &\equiv \lim_{\epsilon\to 0^+}\int \frac{d^4k}{(2\pi)^4}\frac{e^{-ik.(x-y)}}{-k^2+i\epsilon k^0+m^2} = \begin{cases} \dfrac{\delta(\tau^2)}{2\pi} - \dfrac{m}{4\pi\tau}J_1(m\tau) & \text{if } x\prec y \\ 0 & \text{otherwise} \end{cases} \\
G_F(x-y) &\equiv \lim_{\epsilon\to 0^+}\int \frac{d^4k}{(2\pi)^4}\frac{e^{-ik.(x-y)}}{-k^2-i\epsilon+m^2} = \begin{cases} \dfrac{\delta(\tau^2)}{4\pi} - \dfrac{m}{8\pi\tau}H_1^{(2)}(m\tau) & \text{if } \tau^2\geq 0 \\ \dfrac{im}{4\pi^2\sqrt{-\tau^2}}\,K_1(m\sqrt{-\tau^2}) & \text{if } \tau^2<0 \end{cases} \\
G_D(x-y) &\equiv \lim_{\epsilon\to 0^+}\int \frac{d^4k}{(2\pi)^4}\frac{e^{-ik.(x-y)}}{-k^2+i\epsilon+m^2} = \begin{cases} \dfrac{\delta(\tau^2)}{4\pi} - \dfrac{m}{8\pi\tau}H_1^{(1)}(m\tau) & \text{if } \tau^2\geq 0 \\ \dfrac{-im}{4\pi^2\sqrt{-\tau^2}}\,K_1(m\sqrt{-\tau^2}) & \text{if } \tau^2<0 \end{cases}
\end{aligned}
\tag{7.24}
$$

These are the retarded, advanced, Feynman and Dyson[99] Green's functions respectively. All four are Lorentz invariant[100] distribution solutions of (7.18).

If the source function $j(x)$ can be altered in any way by an external observer, we can now see that the only Green's function that can be used in

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[98]The Hankel functions of the first and second kind (or order ν) are defined by

$$H_\nu^{(1)}(x) \equiv J_\nu(x) + iY_\nu(x),$$

$$H_\nu^{(2)}(x) \equiv J_\nu(m\tau) - iY_\nu(x).$$

J_ν and Y_ν here are the Bessel functions of first and second kind respectively. Some authors, *e.g.* [79], refer to the latter as N_ν, the Neumann function. The expression for $\Delta_F(x)$ given in Huang [71, p.29] employs the wrong Hankel function.

The modified Bessel function of the second kind, $K_\nu(x)$, also known as the Basset function or Macdonald function [80], is related to the Hankel functions by [57, §9.6] [81, §10.27.8]

$$K_\nu(x) \equiv \begin{cases} (i)^{\nu+1}\dfrac{\pi}{2}H_\nu^{(1)}(ix) & \text{if } -\pi < \arg(x) \leq \pi/2, \\ (-i)^{\nu+1}\dfrac{\pi}{2}H_\nu^{(2)}(-ix) & \text{if } -\pi/2 < \arg(x) \leq \pi. \end{cases}$$

[99]These four are named (as propagators) for example in [82, §4]. The form of G_D was derived using the contour integrals given in [79, §App. II]. In terms of the quantities presented by Boguliobov and Shirkov, $G_D(x) = \theta(x^0)D^+(x) - \theta(x^0)D^-(x)$, taking the opposite poles in each case to $G_F(x) = \theta(x^0)D^-(x) - \theta(x^0)D^+(x)$. This implies $G_D - G_F = D^+ - D^-$. The authors provide an expression for $D^1 \equiv i(D^+ - D^-)$, which then yields the expression given here for G_D.

[100]G_R and G_A are invariant under orthochronous Lorentz transformations, and $G_R(-x) = G_A(x)$. G_F, G_D and the sum $G_R + G_A$ are invariant under all Lorentz transformations.

(7.17) is indeed the retarded Green's function $G_R(x-y)$. A brief argument runs as follows. Let us take x in equation (7.20) to be a point in the timelike past of the whole of the source region $\mathcal{R}_j$. The term $\hat{\phi}_0(x)$ on the left hand side is, by definition, independent of $j(x)$. But we know the source affects the field $\hat{\phi}(y)$ where $y \in \mathcal{R}_j$, so if we choose a surface ∂R that cuts through $\mathcal{R}_j$, the expression on the right hand side also depends on $j(x)$ unless $G(x-y) = 0$ in that region. As $x \prec y$, this requires G to be the retarded Green's function.

This assertion is proved using a causal argument in the box below.

The classical source is determined independently from the system that the action (7.15) describes. Let us suppose that it is possible for an external observer to (a) exert some control over the source function $j(x)$, and (b) make local measurements of some observable $\hat{B}$ in a spacetime region $\mathcal{R}_B$.[101] We are free to select any propagator for our problem, provided we evaluate Φ correctly in (7.23). Let us select $G_R(x-y)$, so that

$$\hat{\phi}(x) \;=\; \hat{\phi}_0(x) + \int_{\mathcal{R}_j} d^4y \left[G_R(x-y) + \Phi(x-y)\right] j(y)\hat{1}. \qquad (7.25)$$

For the purpose of this proof, let us consider $\mathcal{R}_B$ to be entirely in the past light cone of all points in $\mathcal{R}_j$. Any j-dependence in the outcomes of measurements made there would constitute a signal from the observer to him or herself in the past, which he or she could then act upon to make the signal contradict itself. This is rejected as absurd, implying[102]

$$\int_{\mathcal{R}_j} d^4y\, \Phi(x-y)j(y) = -\int_{\mathcal{R}_j} d^4y\, G_R(x-y)j(y) \quad \forall x \in \mathcal{R}_B. \qquad (7.26)$$

The right-hand side of this equation is zero by (7.24). As the function $j(x)$ can be varied, it follows that $\Phi(x-y) = 0$ for all $x \in \mathcal{R}_B$ and $y \in \mathcal{R}_j$. If a solution Φ of the homogeneous Klein–Gordon equation

[101] This is a minimal requirement for causal structure, in the sense of giving meaning to the question of what observable effect the source can have. Following Section 7.1.2, we assume that the observables to hand are functions $\hat{B}(\{\hat{\phi}(x) : x \in \mathcal{R}_B\})$ of the field operators in region $\mathcal{R}_B$.

[102] An alternative means of ensuring the observer cannot signal to the past is by placing j-dependent restrictions on observables. This seems sufficiently contrived as to not warrant further consideration.

is zero over a finite range, it is zero everywhere. Hence,

$$\hat{\phi}(x) \;=\; \hat{\phi}_0(x) + \int_{\mathcal{R}_j} d^4y\, G_R(x-y) j(y) \hat{1}. \tag{7.27}$$

G_R is zero outside the forward light cone. Therefore, from the existence of one region $\mathcal{R}_B$ in the past light cone of the source within which observations cannot be influenced by altering $j(x)$, it follows that **the influence of the source on the outcomes of any measurements is necessarily restricted to the forward light cone** of points in $\mathcal{R}_j$.

The outcomes of any general observable $\hat{B}$ of the form (7.8) cannot be affected by $j(x)$ if all of the field operators in region $\mathcal{R}_B$ are independent of $j(x)$. Therefore there can be no correlations between a classical source and a detector of this type if they are spacelike separated. **Scalar field theory is relativistically causal with respect to classical sources.**

A different approach to investigating causality in the presence of classical sources can be found in a paper by Buscemi and Compagno [83]. The authors begin with the same scalar field action (7.15) expressed in terms of the Hamiltonian, which is split into a free field part[103] and an interaction part

$$H_{\text{int}}(t) \;=\; g \int d^3\mathbf{x}\; \hat{\phi}(t,\mathbf{x}) j(t,\mathbf{x}). \tag{7.28}$$

Note that, since $L_{\text{int}} = -H_{\text{int}}$, this is equivalent to (7.15) if we set $g = -1$. This is used to calculate the time evolved state $|\Psi(t)\rangle = \hat{U}(t,0)\,|0\rangle$ on the basis that at $t = 0$ the system is in the vacuum state and $j(0,\mathbf{x}) = 0$, from which it is possible to derive expressions for *expectation values* of general observables of the form (7.15). Because it is straightforward to generalise, we focus on the limit in which both source and detector are pointlike (at x_A and x_B respectively), and take $\hat{B}$ to be a single term from a Taylor expansion of a general function of the field operators and their derivatives at that point:

$$\begin{aligned} j(x) \;&=\; J\,\delta^4(x-x_A) \\ \hat{B} \;&=\; \hat{\phi}^j (\partial_0\hat{\phi})^k (\nabla\hat{\phi})^l \big|_{x=x_B} \end{aligned} \tag{7.29}$$

[103] Their equation (19). The free field Hamiltonian has the form (7.40), although the authors use a different normalisation (on which see footnote[109]).

The result is[104]

$$\langle\Psi(t)|\,\hat{B}\,|\Psi(t)\rangle \;=\; \langle 0|\left\{\left[\hat{\phi}(x)+J\,G_R(x-x_A)\right]^j\left[\partial_0\hat{\phi}(x)+J\,\partial_0 G_R(x-x_A)\right]^k \times\;\left[\nabla\hat{\phi}(x)+J\,\nabla G_R(x-x_A)\right]^l\right\}|0\rangle_{x=x_B} \quad (7.30)$$

$$=\; \langle 0|\,\hat{B}\,|0\rangle \qquad \text{if } (x_B-x_A)^2<0 \quad (7.31)$$

The expectation value of this operator for spacelike separations has no dependence on the strength of the source g: all source-dependent terms are proportional to the retarded Green's function or its derivatives. This result generalises to any source function $j(x)$ that is non-zero outside a region $\mathcal{R}_j$, and to any operator that can be expressed as an integral over point-like functions of field operators and their first derivatives $\hat{B}=\int_{\mathcal{R}_B} d^4x\, f\big(\hat{\phi}(x),\partial_0\hat{\phi}(x),\nabla\hat{\phi}(x)\big)$. Operators of this type are referred to by the authors as 'good operators'.

It may be seen that this result is far more easily derived from (7.27). Putting $j(x)=J\,\delta^4(x-x_A)$, we obtain

$$\hat{\phi}(x) \;=\; \hat{\phi}_0(x)+J\,G_R(x-x_A)\hat{1}. \quad (7.32)$$

In the Heisenberg picture, a system initially in the vacuum state at $t=0$ has state $|\Psi\rangle=|0\rangle$ for all t. We can calculate the expectation value of $\hat{B}$ directly:

$$\langle\Psi|\hat{B}|\Psi\rangle \;=\; \langle 0|\Big\{\hat{\phi}^j(\partial_0\hat{\phi})^k(\nabla\hat{\phi})^l\Big\}_{x=x_B}|0\rangle$$

$$=\; \langle 0|\left\{\left[\hat{\phi}_0(x_B)+JG_R(x_B-x_A)\right]^j\left[\partial_0\hat{\phi}_0(x)+J\,\partial_0 G_R(x-x_A)\right]^k \times\;\left[\nabla\hat{\phi}_0(x)+J\,\nabla G_R(x-x_A)\right]^l\right\}|0\rangle_{x=x_B} \quad (7.33)$$

For spacelike x_B-x_A, this is simply $\langle 0|\hat{B}_0|0\rangle$, where $\hat{B}_0$ is identical to $\hat{B}$ with $\hat{\phi}$ replaced with $\hat{\phi}_0$. It is the expectation value that the operator would have if $J=0$, and therefore identical to (7.31).

Indeed, (7.33) is equivalent to (7.30). The causality result proved in the box on page 110-11 is more general than Buscemi and Compagno's result on

[104]Equation (51), [83]. I have used $|\Psi(t)\rangle$ rather than the authors' $|t\rangle$ to emphasise that $|0\rangle$ refers to the vacuum state and not a general state at $t=0$. Their $\tilde{\Delta}_R(x-y)$ is defined in their equation (37); taking the $j(\mathbf{x}',t')$ in that expression to be $J\,\delta^4(x'-y)$, and referring also to their equation (6), we have $\tilde{\Delta}_R(x-y)=J\,\Delta_{\rm ret}(x-y)\equiv J\,\theta(x^0-y^0)\Delta(x-y)\equiv -iJ\,\theta(x^0-y^0)\langle 0|[\hat{\phi}(x),\hat{\phi}(y)]|0\rangle=-J\,G_R(x-y)$ as defined in (7.24). Thus, from their (51), when we put $g=-1$ (see (7.28)) we obtain (7.30).

three counts: it does not depend on the field initially being in the vacuum state, it does not depend on the operators being 'good operators', and it is valid not only for expectation values but for the probability of any individual measurement outcome. Their method of calculation, however, does reveal some interesting properties of the state vector itself.

They calculate the single-particle component of $|\Psi(t)\rangle$ in a Newton–Wigner basis (we will discuss such a basis in Section 7.4.1). Their result, for general $j(x)$, is[105]

$$\psi(t,\mathbf{x}) \equiv \langle \mathbf{x}|\psi(t)\rangle = e^{if(t)}\, g \int_0^t dt' \int d^3\mathbf{x}\; j(x)\Delta^+(x-x') \tag{7.34}$$

where $e^{if(t)}$ is some phase factor and $\Delta^+(x-x') = -G_F(x-x') + G_A(x-x')$ in terms of the Green's functions of (7.24). At a point that does not lie in the causal past of any part of $\mathcal{R}_j$, the G_A term vanishes.

In the limit $j(x) = J\,\delta^4(x-x_A)$, with $g=-1$ again, we have

$$\psi(t_B, \mathbf{x_B}) = J\, e^{if(t)}\, \theta(t_B - t_A)\, G_F(x_B - x_A). \tag{7.35}$$

The fact that this is non-zero for spacelike $x_B - x_A$, even though there are no measurable effects, reaffirms the finding of Section 6.4.5 (and also Section 7.4.1) that it is the single-particle Newton–Wigner basis that does not respect causality, rather than the field theory.

7.3 Location-specific information in Hilbert space

In Section 4.3 it was noted that a continuous basis element $|x\rangle$ is associated with every point in space, and that therefore, in quantum mechanics, space could be said to emerge as a topological arrangement of the subspaces of the Hilbert space of states of a single particle.

In a quantum field theory, an *operator* (or a set of operators, $\hat{\phi}_a(\mathbf{x})$) in the Schrödinger picture is associated with every point in space. If we attempt to relate space to a representation of the Hilbert space $\mathcal{H}$ of states of the field, it quickly becomes complicated. When quantum field theory is developed from Postulate 3 (via the Hamiltonian, by analogy with quantum mechanics) as it was in Section 7.1.2, the continuous basis $\{|\phi\rangle\}$ defined by (7.6) again provides a topological arrangement of the subspaces of $\mathcal{H}$ but, instead of being three-

[105] Their equation (32). The basis is defined in their (14), the RHS of which is missing a factor $e^{i\mathbf{k}.\mathbf{x}}$. It is equivalent to that of Section 7.4.2, allowing for the difference in normalisation.

dimensional and labelled by $i \in \{1, 2, 3\}$, this topology is infinite-dimensional and labeled by $\mathbf{x} \in \mathbb{R}^3$.

Although *field operators* can be conveniently labeled with spacetime points, the relationship between the *state vectors* and spacetime has become far more complicated in field theory than it is in single-particle quantum mechanics.

The following theorems illustrate how far removed the state vector is from having any straightforward relationship to spacetime. The first theorem below is particularly dramatic – it shows that if an observer were confined to a tiny region of empty space for a short period of time, and they had access to any combination of field operators in that region, **there is no quantum state (of the Universe) that they could not reproduce using only those local operators.**

Reeh–Schlieder (1961) Given any spacetime region $\mathcal{R}$, no matter how small, and a field theory with causal commutation relations,[106] there is no state in the Hilbert space that cannot be constructed to arbitrary precision from the action of local field operators $\hat{\phi}(x)$ $(x \in \mathcal{R})$ acting on the vacuum state $|0\rangle$ [84] [85, §II.5.3].

$$\left(\sum_n \int_{\mathcal{R}^n} \mathrm{d}^4 x_1 ... \mathrm{d}^4 x_n f_n(x_1, ..., x_n) \hat{\phi}(x_1) ... \hat{\phi}(x_n) \right) |0\rangle$$

To reproduce a state with features at great distance would entail extremely fine tuning, exploiting the unlimited range of non-zero correlations within the vacuum state. The result is not special to the vacuum state – any state with finite energy has this property.

This result appears to go against relativistic causality in an extreme sense. Yet it is derived *from* relativistic causality: the commutator of operators in spacelike separated regions is axiomatically zero. There is no question of any signalling across spacelike regions.

Many attempts to identify a relation between spacetime and state vectors have focused on three-dimensional spatial regions, motivated by single particle theory. As a result, a number of very general no-go theorems have arisen [86], some of the more relevant of which are listed below.

[106] Relations such as (7.4) and (7.11) which give rise to microcausality.

Hegerfeldt (1998) If it were possible to create a state localised in a spatial region R in a theory that does not allow instantaneous wavepacket spreading, then the unitary evolution of that state would keep it localised in R forever [87] [86, §2].[107]

Conversely, if the evolution of a localised state didn't confine it to remain within its local region for all time, there would be superluminal spreading.

Malament (1996) In a relativistically causal theory, there are no sets of non-zero operators P_R that could act as projection operators with respect to spatial regions R in the sense that $P_{R_A} P_{R_B} = 0$ for any pair of disjoint regions R_A and R_B. [88] [86, §3].

For the case of a single particle, this means there *cannot* be a map between regions of Euclidean space and subspaces of Hilbert space (as described above and in Section 4.3) without violating relativistic causality. This is indeed what we have found in Sections 5 and 6: every propagator was found to be non-zero for spacelike separations, implying a violation of causality if measurements involving projection operators onto spatial regions exist (Section 5.1).

Halvorson–Clifton (2001) Developed from a theorem by Busch [89]. In a relativistically causal theory, there are no sets of non-zero operators A_R for which $0 \leq \langle\Psi|A_R|\Psi\rangle \leq 1 \; \forall \, |\Psi\rangle \in \mathcal{H}$ and $A_{R_A \bigcup R_B} = A_{R_A} + A_{R_B}$ for any pair of disjoint regions R_A and R_B [86, §5].

This supplements the Malament theorem above by supposing that general quantum measurements (in the general sense of a POVM – see Section 3.2.3) might exist even if strict projection operators do not. For example, let us say a particle exists, but it can never (because of Malament) be located exclusively within any region, yet *a probability distribution over space exists* such that the probability associated with the union of two spatial regions was equal to the sum of the probabilities associated with each region. Is it possible to have a measurement whose outcomes have such a distribution over space? The answer is no.

These theorems above rule out any relativistic quantum theory of single particles, and they underline the difficulty of making any straightforward association between a state and a location.

However, **the quantum state *must* carry spatial information in this**

[107] This conclusion is similar to that of the toy example given in the introduction to Section 7, but far more general.

theory, for the following reason. The evolution of this system between times t_A and t_B is governed by Postulate 3, the time evolution *of a state vector* $|\Psi\rangle$. If a disturbance takes place at $x_A \equiv (t_A, \mathbf{x_A})$, whether that disturbance is represented by a classical source (7.15) or a local observable (7.8) or (7.14), we have seen that any detectable effects at a time $t_B > t_A$ are absolutely spatially restricted to a ball of radius $c\,(t_B - t_A)$.

A state in a quantum field theory can be very highly localised, even if it cannot be completely localised [70, §5.2]. In the following section we will see how a simple example of localisation – the Newton–Wigner representation of single-particle theory – emerges as an approximation within a free scalar field.

7.4 Particles in quantum field theory

7.4.1 The Fock representation

The $\{|\phi\rangle\}$ basis for quantum field theory was introduced in Section 7.1 is extremely large. A basis element exists for every point on the continuous spectrum of the unbounded operator $\hat{\phi}(x)$ at every $x \in \mathbb{R}^{1,3}$. Its cardinality is therefore $2^{(2^{\aleph_0})}$, where $\aleph_0$ is the cardinality of a countably infinite set. We might ask whether such an enormous basis is justified.

First, let us note that a *separable* Hilbert space must have a basis that is no more than countably infinite, and that separability is often suggested as a fundamental requirement of a working quantum theory [8, §7.1]. Quantum mechanics freely makes use of uncountable bases such as $\{|x\rangle\}$, but this is not a true basis (its elements are not members of the space of states – see Section 3.4) and the space of wavefunctions $\psi(x) = \langle x|\psi\rangle$ that differ by a set of non-zero measure and are square-integrable ($\int d\mathbf{x}\,|\psi(\mathbf{x})|^2 \in \mathbb{R}$) is a separable Hilbert space. The appearance of such a huge basis in constructing quantum field theory needn't necessarily cause concern, but it is reasonable to seek one that is less redundant.

A more practical basis is provided by the **Fock representation**, which in the free field theory reveals a direct correspondence with N-particle quantum mechanics.

A single real free scalar field, following (7.15) and (7.16) with $j = 0$, has a Lagrangian density and resulting field equation:

$$\hat{\mathcal{L}} = -\tfrac{1}{2}(\partial_\mu \hat{\phi})(\partial^\mu \hat{\phi}) - \tfrac{1}{2} m^2 \hat{\phi}^2 \tag{7.36}$$

$$(\partial_\mu \partial^\mu + m^2)\hat{\phi} = 0. \tag{7.37}$$

The most general self-adjoint operator solution to (7.37) is

$$\hat{\phi}(x) \;=\; \int \frac{d^3\mathbf{p}}{(2\pi)^{3/2}} \frac{1}{(2E_p)^{1/2}} \Big(\hat{a}_{\mathbf{p}}\, e^{-i(E_p t - \mathbf{p}.\mathbf{x})} + \hat{a}^\dagger_{\mathbf{p}}\, e^{i(E_p t - \mathbf{p}.\mathbf{x})} \Big). \tag{7.38}$$

where $a_{\mathbf{p}}$ is some operator that may vary with a parameter $\mathbf{p}$ that we shall come to identify with momentum, and $E_p \equiv \mathbf{p}^2 + m^2$.

Since $\hat{\pi}(x) \equiv \partial\mathcal{L}/\partial(\partial_0\hat{\phi}) = \partial^0\hat{\phi}$, the canonical commutation relations (7.4) require

$$\begin{aligned} \big[\hat{a}_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{q}}\big] \;&=\; \delta^3(\mathbf{p}-\mathbf{q}) \\ \big[\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{q}}\big] \;=\; \big[\hat{a}^\dagger_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{q}}\big] \;&=\; 0, \end{aligned} \tag{7.39}$$

whereupon, with normal ordering,[108]

$$:\hat{H}: \;=\; \int d^3\mathbf{p}\, E_p\, \hat{a}^\dagger_{\mathbf{p}}\, \hat{a}_{\mathbf{p}}. \tag{7.40}$$

We first note that if a state $|0\rangle$ exists such that $\hat{a}_{\mathbf{p}}|0\rangle = 0\ \forall\mathbf{p}$, then it is an eigenstate of $\hat{H}$. We call this the **vacuum**, and we assume that it is unique.

Secondly, we note that $[\hat{H}, \hat{a}^\dagger_{\mathbf{p}}] = E_p\, \hat{a}^\dagger_{\mathbf{p}}$, which means the state[109]

$$|\mathbf{p}\rangle \equiv \hat{a}^\dagger_{\mathbf{p}}|0\rangle \tag{7.41}$$

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[108] The Hamiltonian calculated directly for this theory is $\hat{H} = \int d^3\mathbf{p}\, E_p\, \hat{a}^\dagger_{\mathbf{p}}\, \hat{a}_{\mathbf{p}} + E_V$. The constant energy term E_V is infinite if the theory is taken to be valid for unlimited energies and measured over infinite space. More realistically, a field theory should be considered to be *effective*, meaning that it is a low-energy approximation to a theory that remains unspecified for higher energies, but satisfies the conditions for a field theory subject to renormalisation group equations [74, §12]. In an effective field theory, E_V becomes a finite energy per unit volume. In neither case does this term have any physical consequence (general relativistic complications aside). A normal ordered operator $:\hat{A}: = \hat{A} - \langle 0|\hat{A}|0\rangle\hat{1}$ measures a quantity relative to its expectation value in state $|0\rangle$.

[109] As they are elements of a continuous basis, they are not true states in the sense of elements of a Hilbert space (or a Fock space), but the term 'state' is in common use for them. I have normalised these elements such that $\langle\mathbf{p}|\mathbf{q}\rangle = \delta^3(\mathbf{p}-\mathbf{q})$ to maintain continuity with results of earlier Sections, for example the derivations of propagators in which $\int d\mathbf{p}\, |p\rangle\langle p| = \hat{1}$ is employed. For a Lorentz invariant normalisation, a prefactor proportional to E_p is required, for example $\langle\mathbf{p}|\mathbf{q}\rangle = (E_p/m)\,\delta^3(\mathbf{p}-\mathbf{q})$. This may be achieved by redefinition of the state in terms of the creation operator, *e.g.* $|\mathbf{p}\rangle \equiv (E_p/m)^{1/2}\hat{a}^\dagger_{\mathbf{p}}|0\rangle$, retaining (7.39). Alternatively, $a_{\mathbf{p}}$ and $a^\dagger_{\mathbf{p}}$ may be defined so that, for example, $[\hat{a}_{\mathbf{p}}, \hat{a}^\dagger_{\mathbf{q}}] = (2\pi)^3(2E_p)\,\delta^3(\mathbf{p}-\mathbf{q})$, which results in a particularly simple field expansion when (7.4) is applied:

$$\hat{\phi}(x) \;=\; \int \frac{d^3\mathbf{p}}{2E_p} \Big(\hat{a}_{\mathbf{p}}\, e^{-i(E_p t - \mathbf{p}.\mathbf{x})} + \hat{a}^\dagger_{\mathbf{p}}\, e^{i(E_p t - \mathbf{p}.\mathbf{x})} \Big).$$

Conventions among quantum field theory texts vary.

is an eigenstate of $\hat{H}$ with eigenvalue E_p. As $\langle \mathbf{p}|\mathbf{q}\rangle = \delta^3(\mathbf{p}-\mathbf{q})$, these states form a continuous basis for a single-particle Hilbert space $\mathcal{H}_1$. For this reason, $\hat{a}^\dagger_{\mathbf{p}}$ is referred to as the *creation operator* for a particle of momentum $\mathbf{p}$.

Finally, it follows that any state $|\{\mathbf{p}_i\}\rangle \equiv \Big(\prod_{i=1}^N \hat{a}^\dagger_{\mathbf{p}_i}\Big)|0\rangle$, for *any set* of N momenta $\{\mathbf{p}_i \in \mathbb{R}^3\}$, is an eigenstate of $\hat{H}$ with eigenvalue $\sum_i E_{p_i}$ above the vacuum, and may be referred to as an N-particle state (see Section 7.4.2). The direct product of any two such states is zero unless they involve identical sets of creation operators *regardless of order*, in which case it is an N-fold product of delta functions. The space of states $\mathcal{H}_N$ is therefore a *symmetrised*[110] direct product of N Hilbert spaces:

$$\mathcal{H}_N \;\equiv\; S\,\mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_1. \tag{7.42}$$

The direct sum of these spaces $\mathcal{H}_N$, which are themselves mutually orthogonal, is known as a symmetrised Fock space:

$$\mathcal{F}_S = \bigoplus_{N=0}^{\infty} \mathcal{H}_N. \tag{7.43}$$

The Fock representation allows any state in the field theory to be expressed as a superposition of these basis elements $|\{\mathbf{p}_i\}\rangle$. As is appropriate for any continuous basis, each basis element must appear in an N-fold integral over momenta in order to give a state in $\mathcal{F}_S$.

The representation can be generalised to include complex fields:

$$\hat{\mathcal{L}} \;=\; -(\partial_\mu \hat{\phi}^\dagger)(\partial^\mu \hat{\phi}) - m^2 \hat{\phi}^\dagger \hat{\phi} \tag{7.44}$$

$$(\partial_\mu \partial^\mu + m^2)\hat{\phi} \;=\; 0 \tag{7.45}$$

$$\hat{\phi}(x) \;=\; \int \frac{d^3\mathbf{p}}{(2\pi)^{3/2}} \frac{1}{(2E_p)^{1/2}} \Big(\hat{a}_{\mathbf{p}}\, e^{-i(E_p t - \mathbf{p}.\mathbf{x})} + \hat{b}^\dagger_{\mathbf{p}}\, e^{i(E_p t - \mathbf{p}.\mathbf{x})}\Big), \tag{7.46}$$

in which the $\hat{a}^\dagger_{\mathbf{p}}$ and $\hat{b}^\dagger_{\mathbf{p}}$ operators act as creation operators for particles and their anitparticles, with equal mass and opposite charge. The resulting Fock space is the direct product of two of the Fock spaces defined above – one for particle states and one for antiparticle states.

[110] The symmetrising operator S maps all equivalent states corresponding to the same unordered set of momenta to a single state in $\mathcal{H}_N$.

Where there are multiple fields, the space of states will be a direct product of multiple Fock spaces.

Fermion fields can be accommodated by replacing the symmetrisation operator in (7.42) with an antisymmetrisation operator.

To follow up on the note at the start of this Section, we should ask whether the Fock space is separable, since a large number of the theorems that are used in quantum theory apply only to separable Hilbert spaces. A great deal of the power of the theory would be lost if the space of states were non-separable.

It may be shown that any countable direct sum of finite direct products of separable Hilbert spaces is itself separable. The definition (7.43) of a Fock space, however, makes clear that there is no finite limit to the number direct products (7.42). It is still possible to work with a separable Hilbert space by restricting the theory to finite numbers of particles, but this is a difficult constraint to apply to a field theory.

Alternatively, one may take advantage of physical restrictions on the types of operators that can act between the states. This constrains the time evolution operators and observables of the theory to a subset of operators on $\mathcal{F}$ (known as a 'superselection sector'), and isolates a separable subspace in which all the dynamics takes place. This subspace is the full space of states accessible to the system, so the theorems of separable Hilbert spaces remain valid for the field theory that describes it [77, §§1.1, 2.6].

7.4.2 The correspondence between quantum field theory and quantum mechanics

The claim that states in the $\mathcal{H}_N$ subspace of Fock space represent systems of N physical *particles* can be verified in several ways.

We may identify quantities such as energy and momentum of the field, and compare them to the properties of particles. These quantities emerge naturally in the field theory as conserved Noether charges arising from the invariance of the action under space and time translations [74, §2.2]:

$$\begin{aligned} \hat{P}^\mu &\equiv \int d^3\mathbf{x} \; :\hat{\mathcal{T}}^{0\mu}: \equiv \int d^3\mathbf{x} \; :\left(\hat{\pi}\,\partial^\mu\hat{\phi} - \eta^{0\mu}\hat{\mathcal{L}}\right): \\ &= \int d^3\mathbf{p}\,(E_p,\mathbf{p})\left(\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} + \hat{b}^\dagger_{\mathbf{p}}\hat{b}_{\mathbf{p}}\right) \end{aligned} \tag{7.47}$$

Applying (7.46) yields $\hat{P}^\mu\,|\{\mathbf{p}_i\}\rangle = \sum_i (E_{p_i},\mathbf{p}_i)\,|\{\mathbf{p}_i\}\rangle$. The field momentum of a Fock eigenstate is equal to the sum of the momenta in its set of creation

operators, whether particle or antiparticle.

A charge operator also emerges as a conserved quantity due to the invariance of the action under a global phase change:

$$\hat{Q} \equiv \int d^3\mathbf{x}\; i\; :(\hat{\phi}^\dagger\hat{\pi}^\dagger - \hat{\pi}\hat{\phi}): = \int d^3\mathbf{p}\,\big(\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} - \hat{b}^\dagger_{\mathbf{p}}\hat{b}_{\mathbf{p}}\big), \tag{7.48}$$

and this yields $\hat{Q}\,|\{\mathbf{p}_i\}\rangle = (N_a - N_b)|\{\mathbf{p}_i\}\rangle$, where N_a and N_b are the numbers of particle and antiparticle creation operators involved in the state $|\{\mathbf{p}_i\}\rangle$, again in agreement with the particle claim.

Let us consider the space of single particle and antiparticle states, $\mathcal{H}_1 \oplus \overline{\mathcal{H}}_1$. A general state can be expressed in terms of particle basis states $|\mathbf{p}\rangle \equiv \hat{a}^\dagger_p|0\rangle$ and antiparticle basis states $|\bar{\mathbf{p}}\rangle \equiv \hat{b}^\dagger_p|0\rangle$ using two functions $\psi(\mathbf{p})$ and $\bar{\psi}(\mathbf{p})$ as follows:

$$|\psi\rangle = \int d^3\mathbf{p}\,\Big(\psi(\mathbf{p})\,|\mathbf{p}\rangle + \bar{\psi}(\mathbf{p})\,|\bar{\mathbf{p}}\rangle\Big). \tag{7.49}$$

We already have a reliable momentum operator on this space:

$$\hat{P}_i = \int d^3\mathbf{p}\; p_i\,\big(\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} + \hat{b}^\dagger_{\mathbf{p}}\hat{b}_{\mathbf{p}}\big), \tag{7.50}$$

so we may construct a position operator in the standard way (4.13), summing over both sets of basis states:[111]

$$\hat{x}^{(1)}_i \equiv \int d^3\mathbf{p}\,\Big(|\mathbf{p}\rangle\, i\frac{\partial}{\partial p_i}\langle\mathbf{p}| + |\bar{\mathbf{p}}\rangle\, i\frac{\partial}{\partial p_i}\langle\bar{\mathbf{p}}|\Big) \tag{7.51}$$

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[111] This position operator may be written in terms of field operators and the vacuum projection operator $|0\rangle\langle 0|$, but it isn't very revealing. From (7.46), we can obtain an expression for the particle annihilation operator

$$\hat{a}_{\mathbf{p}} = \frac{1}{(2E_p)^{1/2}}\int\frac{d^3\mathbf{x}}{(2\pi)^{3/2}}\,\Big(E_p\hat{\phi}(x) + i\hat{\pi}^\dagger(x)\Big)\,e^{i(E_pt - \mathbf{p}.\mathbf{x})}.$$

The antiparticle operator $\hat{b}_{\mathbf{p}}$ has the same form with $\hat{\phi} \leftrightarrow \hat{\phi}^\dagger$ and $\hat{\pi} \leftrightarrow \hat{\pi}^\dagger$. From this,

$$\frac{\partial}{\partial p_i}\langle\mathbf{p}| = \frac{1}{(2E_p)^{1/2}}\int\frac{d^3\mathbf{x}}{(2\pi)^{3/2}}\,\Big[\big(i\frac{p_i}{E_p}t - ix_i\big)\big(E_p\hat{\phi} + i\hat{\pi}^\dagger\big) + \frac{p_i}{2E_p^2}\big(E_p\hat{\phi} - i\hat{\pi}^\dagger\big)\Big]\,e^{i(E_pt - \mathbf{p}.\mathbf{x})}$$

and so, with $\hat{\phi} \equiv \hat{\phi}(x)$ and $\hat{\phi}' \equiv \hat{\phi}(x')$ and similarly for $\hat{\pi}$,

$$\begin{aligned}\hat{x}^{(1)}_i \;=\; \int\frac{d^3\mathbf{p}}{2E_p}\int\frac{d^3\mathbf{x}'d^3\mathbf{x}}{(2\pi)^3}\,\Big\{&\Big(E_p\hat{\phi}'^\dagger - i\hat{\pi}'\Big)\,|0\rangle\langle 0|\,\Big[\big(x_i - \frac{p_i}{E_p}t\big)\big(E_p\hat{\phi} + i\hat{\pi}^\dagger\big) + i\frac{p_i}{2E_p^2}\big(E_p\hat{\phi} - i\hat{\pi}^\dagger\big)\Big]\\ +\;&\Big(E_p\hat{\phi}' - i\hat{\pi}'^\dagger\Big)\,|0\rangle\langle 0|\,\Big[\big(x_i - \frac{p_i}{E_p}t\big)\big(E_p\hat{\phi}^\dagger + i\hat{\pi}\big) + i\frac{p_i}{2E_p^2}\big(E_p\hat{\phi}^\dagger - i\hat{\pi}\big)\Big]\Big\}\,e^{i\mathbf{p}.(\mathbf{x}'-\mathbf{x})}.\end{aligned}$$

The momentum operator has two sets of eigenstates, $|\mathbf{p}\rangle$ and $|\bar{\mathbf{p}}\rangle$, with identical eigenvalue spectra. There are also two sets of eigenstates for the position operator, and we can express them and define the associated creation operators as follows:[112]

$$\begin{aligned} |x\rangle &\equiv \int \frac{d^3\mathbf{p}}{(2\pi)^{3/2}}\, e^{-i\mathbf{p}.\mathbf{x}}\, \hat{a}^\dagger_{\mathbf{p}}\, |0\rangle \;\equiv\; \hat{a}^\dagger_{\mathbf{x}}|0\rangle \\ |\bar{x}\rangle &\equiv \int \frac{d^3\mathbf{p}}{(2\pi)^{3/2}}\, e^{-i\mathbf{p}.\mathbf{x}}\, \hat{b}^\dagger_{\mathbf{p}}\, |0\rangle \;\equiv\; \hat{b}^\dagger_{\mathbf{x}}|0\rangle. \end{aligned} \tag{7.52}$$

These results then follow straightforwardly:

$$\begin{aligned} \hat{x}^{(1)}_i|x\rangle &= x_i|x\rangle \\ \hat{x}^{(1)}_i|\bar{x}\rangle &= x_i|\bar{x}\rangle \\ \langle x|p\rangle = \langle \bar{x}|\bar{p}\rangle &= (2\pi)^{-3/2}\, e^{i\mathbf{p}.\mathbf{x}} \\ \langle \bar{x}|p\rangle = \langle x|\bar{p}\rangle &= 0 \qquad (7.53) \\ \big[\hat{x}^{(1)}_i, \hat{P}_j\big] &= i\,\delta_{ij} \int d^3\mathbf{p}\, \Big(|\mathbf{p}\rangle\langle\mathbf{p}| + |\bar{\mathbf{p}}\rangle\langle\bar{\mathbf{p}}|\Big) \;=\; i\,\delta_{ij}\,\hat{1}^{(1)} \qquad (7.54) \\ \big[\hat{P}_i, \hat{H}\big] &= 0 \\ \big[\hat{x}^{(1)}_i, \hat{H}\big] &= i \int d^3\mathbf{p}\, \Big(|\mathbf{p}\rangle \frac{p_i}{E_p}\langle\mathbf{p}| + |\bar{\mathbf{p}}\rangle \frac{p_i}{E_p}\langle\bar{\mathbf{p}}|\Big) = i\,\hat{v}^{(1)}_i. \qquad (7.55) \end{aligned}$$

Here, $\hat{1}^{(1)}$ refers to the unit operator on $\mathcal{H}_1 \oplus \overline{\mathcal{H}}_1$, and $\hat{v}^{(1)}_i$ is a one-particle operator with eigenvalues equal to the velocity of a classical particle for states of well-defined momentum. All of these correspond directly with Postulate 3 and reproduce the principles of quantum mechanics of a single particle or antiparticle – the two are treated on equal footing. With reference to the discussion of position operators in Section 6, the fact that $\hat{x}_i$ preserves a particle as a particle (not mixing it with antiparticle states) makes it a **Newton–Wigner operator**.

The Hamiltonian may be decomposed into one-particle and many-particle operators, $:\hat{H}: \;= \hat{H}^{(1)} + \hat{H}^{(N>1)}$, where $\hat{H}^{(N>1)}$ annihilates any one-particle

[112] A similar construction is suggested in [74, §2.3]. In [72, §2.8.1], it is noted that in the Schrödinger picture,

$$\hat{\phi}^\dagger_S(\mathbf{x})|0\rangle \equiv e^{-iHt}\,\hat{\phi}^\dagger(x)\,e^{iHt}|0\rangle = \int \frac{d^3\mathbf{p}}{(2\pi)^{3/2}} \frac{1}{(2E_p)^{1/2}}\,\hat{a}^\dagger_{\mathbf{p}}\,e^{i\mathbf{p}.\mathbf{x}}|0\rangle,$$

which means $(2m)^{1/2}\hat{\phi}^\dagger_S(\mathbf{x})|0\rangle$ would make a good position eigenstate in a *non-relativistic* theory, in which $(2m)^{1/2}/(2E_p)^{1/2}$ is essentially constant – compare (7.52).

state and

$$\hat{H}^{(1)} = \hat{1}^{(1)} \hat{P}^0 \, \hat{1}^{(1)} = \int d^3\mathbf{p} \left(|\mathbf{p}\rangle E_p \langle \mathbf{p}| + |\bar{\mathbf{p}}\rangle E_p \langle \bar{\mathbf{p}}| \right). \tag{7.56}$$

If we also define a momentum operator exclusive to one-particle states $\hat{\mathbf{p}}^{(1)} \equiv \hat{1}^{(1)} \hat{\mathbf{P}} \, \hat{1}^{(1)}$, then this Hamiltonian satisfies the Klein–Gordon relation $\left(\hat{H}^{(1)}\right)^2 = (\hat{\mathbf{p}}^{(1)})^2 + m^2 \, \hat{1}^{(1)}$. It is now possible, as per Postulate 3, to express the Hamiltonian directly in terms of the one-particle canonical operators, which brings us back to the relativistic particle mechanics discussed in Section 6.

If we bring the operator $\hat{x}_i^{(1)}$ to the full Fock space, it projects all states onto the one-particle subspace $\mathcal{H}_1 \oplus \overline{\mathcal{H}}_1$. The momentum operator $\hat{P}_i$ of (7.47) does not. With care, the position operator can be extended over the whole of the Fock space.

Let us denote a general basis state by $|A, B\rangle = \prod_{a=1}^{N_A} \hat{a}^\dagger_{\mathbf{p_a}} \prod_{b=1}^{N_B} \hat{b}^\dagger_{\mathbf{p_b}} |0\rangle$ where $A = \{\mathbf{p}_a\}$ is a set of N_A particle momenta and $B = \{\bar{\mathbf{p}}_b\}$ is a set of N_B antiparticle momenta. The position operator proposed below involves a sum over all basis states, with combinatorial factors to ensure states are not counted more than once given the symmetry of the Fock space. For multi-particle states, symmetry suggests that the single $i\partial/\partial p_i$ operator be replaced by the mean of all such operators for that state. The resulting operator $\hat{X}_i$ is

$$\sum_{N_A=0}^{\infty} \frac{1}{N_A!} \sum_{N_B=0}^{\infty} \frac{1}{N_B!} \int \prod_{a=1}^{N_A} d^3\mathbf{p_a} \int \prod_{b=1}^{N_B} d^3\mathbf{p_b} \, |A, B\rangle \frac{\left(\sum_{a=1}^{N_A} i \frac{\partial}{\partial p_{a,i}} + \sum_{b=1}^{N_A} i \frac{\partial}{\partial p_{b,i}} \right)}{N_A + N_b} \langle A, B| \tag{7.57}$$

One may verify that its eigenvalues correspond to the position of the centre of mass of a set of localised particles and/or antiparticles of equal mass: for example,

$$\hat{X}_i \, \hat{a}^\dagger_{\mathbf{x_1}} \hat{a}^\dagger_{\mathbf{x_2}} \hat{b}^\dagger_{\mathbf{x_3}} |0\rangle = \frac{1}{3}(x_{1i} + x_{2i} + x_{3i}) \, \hat{a}^\dagger_{\mathbf{x_1}} \hat{a}^\dagger_{\mathbf{x_2}} \hat{b}^\dagger_{\mathbf{x_3}} |0\rangle.$$

This adds weight to the suggestion that $\hat{a}^\dagger_{\mathbf{x}}$ and $\hat{b}^\dagger_{\mathbf{x}}$ as defined in (7.52) are creation operators for particles and antiparticles at position $\mathbf{x}$ in this free field theory.

The relation for conjugate operators now holds throughout the Fock space:

$$\left[\hat{X}_i \, , \, \hat{P}_j \right] \; = \; i \, \delta_{ij}. \tag{7.58}$$

7.4.3 Particle creation

In Section 5.1, two equivalences were established for a quantum theory in which that the spatial representation in which measurements can be localised is the same as the spatial representation of a position operator $\hat{\mathbf{x}}$.

1. The probability of a measurement localised in a spatial region $\mathcal{R}_B$ made at time t_B giving a particular outcome will in general depend on the region $\mathcal{R}_A$ in which an earlier measurement was made at time t_A unless the propagator vanishes:

   $$\langle x_B|\hat{U}(t_B,t_A)|x_A\rangle = 0 \;\text{ for all } \mathbf{x_A}\in\mathcal{R}_A,\ \mathbf{x_B}\in\mathcal{R}_B \quad\Rightarrow\quad \text{no causal link.}$$

   In particular, if the propagator is non-zero for any $(\mathbf{x_B},t_B)$ outside the future light cone of any $(\mathbf{x_A},t_A)$, this would mean that we do not have a relativistically causal theory in which one-particle operators of the form

   $$\hat{A}^{(1)} = \int_{\mathcal{R}_A} d\mathbf{x}\, d\mathbf{x}'\ |x'\rangle \hat{A}^{(x,x')}\langle x|,$$

   defined with respect to a spatial region $\mathcal{R}_A$, can represent physical measurements.

2. There is no causal link between Alice and Bob if and only if every possible position measurement $\hat{A}$ available to Alice at time t_A, subject to an appropriate forwards time evolution, *commutes* with the operator of every possible position measurement $\hat{B}$ available to Bob at a later time t_B:

   $$\Big[\hat{U}(t_B,t_A)\,\hat{A}\,\hat{U}^\dagger(t_B,t_A)\ ,\ \hat{B}\Big] = 0 \quad\Leftrightarrow\quad \text{no causal link.}$$

In Section 7.4.2, a Newton–Wigner position representation was found for the one-particle subspace of a free scalar field. Since the single-particle Hamiltonian satisfies the Klein–Gordon relation, we know that the relevant propagator for the first of these statements is the single-particle relativistic propagator $K_+(\mathbf{x_B},t_B;\mathbf{x_A},t_A)$ of (6.8), and we know that it does not vanish outside the future light cone.[113]

---

[113] If we were to use the approximate position eigenstates defined in footnote[112], the propagator for $t_B > t_A$ would be

$$\langle x_B|\,\hat{U}(t_B,t_A)\,|x_A\rangle = 2m\,\langle 0|\,\hat{\phi}_S(\mathbf{x_B})\,e^{i\hat{H}(t_B-t_A)}\,\hat{\phi}_S^\dagger(\mathbf{x_A})\,|0\rangle = 2m\,\langle 0|\,\hat{\phi}(x_B)\,\hat{\phi}^\dagger(x_A)\,|0\rangle.$$

This quantity is $2m$ times the *Feynman* propagator, $i\,G_F(x_B{-}x_A)$. However, as noted there, this is not a suitable position eigenstate for a relativistic theory.

It follows that one-particle operators of the form $\hat{A}^{(1)}$ cannot represent observables in a relativistically causal quantum field theory. We can extend this to a wider class of observables: any operator $\hat{A}$ that acts in an identical way to $\hat{A}^{(1)}$ on the one-particle space: *i.e.* any $\hat{A}$ for which $\hat{1}^{(1)}\hat{A}\,\hat{1}^{(1)} = \hat{A}^{(1)}$.[114]

A measurement on a free scalar field that (a) takes place in a finite spatial region and (b) does not mix one-particle states with $n \neq 1$-particle states would allow signalling that violated relativistic causality. To put it another way, in a causal theory, **if a measurement is to take place in a finite spatial region, that measurement must have the capacity for particle creation.**

In contrast, with regard to the statement 2 on the previous page, if our observables are functions of the field operators within bounded *spacetime* regions as prescribed in Section 7.1, we have seen that the no-signalling condition does hold between pairs of measurements when the regions are spacelike separated.

We may conclude that the violation of the first condition but not of the second is informative not so much about the nature of particles as about the nature of *observables* in quantum field theory.

7.5 The return of relativistic causality violations

7.5.1 Signalling using more than two measurements

We have seen that no signalling is possible using a pair of observables $\hat{A}$ and $\hat{B}$ constructed from the field operators in spacetime regions $\mathcal{R}_A$ and $\mathcal{R}_B$ that are entirely spacelike separated from each other. If more than two field observables are involved, however, the spectre of superluminal signalling re-emerges.

In [90], Sorkin outlines a scheme for generalising from two to any number of observables defined on non-overlapping spacetime regions, whereby the postulates of quantum mechanics can be applied to the measurements in a well-defined way. He then presents a simple case in which three measurements can be used to signal across a spacelike interval.

An example of the kind of arrangement of three spacetime regions $\mathcal{R}_A$, $\mathcal{R}_B$ and $\mathcal{R}_C$ that allows superluminal signalling is shown in Figure 3.

Regions $\mathcal{R}_A$ and $\mathcal{R}_C$ are entirely spacelike separated from each other, but neither of them is entirely spacelike separated from $\mathcal{R}_B$. The choice of mea-

[114] To make a reliable single-particle measurement, the measurement must be able to distinguish a one-particle state from a $n \neq 1$-particle state, but proof of signalling only requires that the probabilities of measurement B be affected by the choice of measurement A.

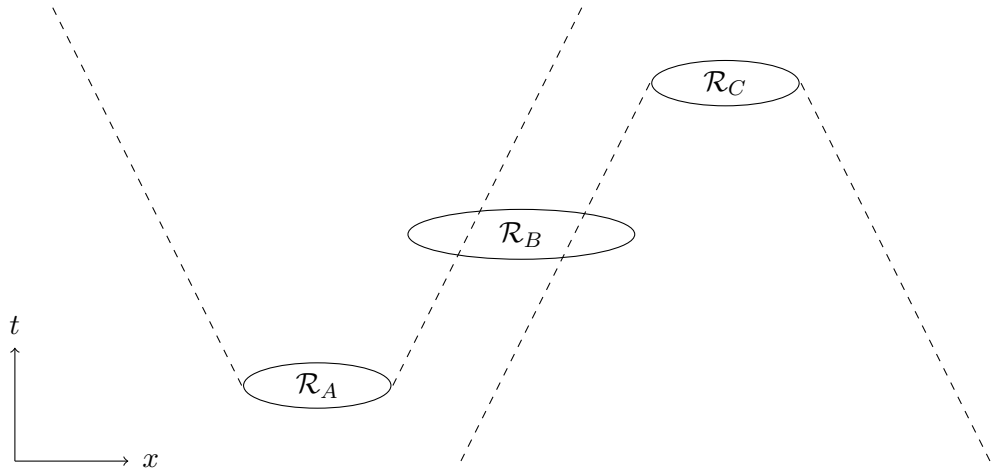

Figure 3: An arrangement of three spacetime regions. The future light cone of $\mathcal{R}_A$ and the past light cone of $\mathcal{R}_C$ are indicated by the dashed lines.

surement A in $\mathcal{R}_A$ affects both the outcomes and the updated state after measurement B in $\mathcal{R}_B$, and this in turn affects the outcomes of measurement C in $\mathcal{R}_C$. If a pre-arranged measurement takes place at B, it is argued that signalling from $\mathcal{R}_A$ to $\mathcal{R}_C$ can occur.

A simple idealisation – employed by Sorkin – is to reduce $\mathcal{R}_A$ to a spacetime point $x_A = (t_A, \mathbf{x_A})$, and likewise $\mathcal{R}_C$ to point $x_C = (t_C, \mathbf{x_C})$, while extending $\mathcal{R}_B$ to the entire spacelike hypersurface $x^0 = t_B$, with $t_A < t_B < t_C$. We consider a real scalar quantum field $\hat{\phi}(x)$.

The density operator (Section 3.2.1) of the state at $t < t_A$ is taken to be $\hat{\rho}_0$. The explicit form of the observable $\hat{A}$ is not required: the overall effect of the measurement on $\hat{\rho}_0$ is necessarily that of a unitary operator constructed from the fields in $\mathcal{R}_A$, resulting in an updated state $\hat{\rho}_A = \hat{U}_A\,\hat{\rho}_0\,\hat{U}_A$. Following Sorkin, we take $\hat{U}_A = e^{i\lambda\hat{\phi}_A}$, where $\hat{\phi}_A \equiv \hat{\phi}(x_A)$; λ is an adjustable parameter that we propose to use to transmit information.

For measurement B, we use $\hat{B} = |1\rangle\langle 1|$, where $|1\rangle$ is some one-particle state.[115] This simplifies the calculation, since it doubles as both the projection operator onto state $|1\rangle$ and the observable itself. The measurement gives an outcome of 1 with probability $p(1_B|\lambda) = \mathrm{Tr}(\hat{\rho}_A\hat{B})$ and an outcome of 0 with probability $p(0_B|\lambda) = \mathrm{Tr}\big(\hat{\rho}_A(\hat{1}-\hat{B})\big)$. After the measurement, the updated state is $\hat{\rho}_{B1}$ if the outcome is 1, $\hat{\rho}_{B0}$ if the outcome is 0. With the outcome

[115] Sorkin uses $\hat{B} = |b\rangle\langle b|$ with $|b\rangle = \alpha|0\rangle + \beta|1\rangle$, but notes that the case $\alpha = 0$ is sufficient.

unknown, the mixed state after measurement B is

$$\begin{aligned}\hat{\rho}_B &= p(1_B|\lambda)\,\hat{\rho}_{B1} + p(0_B|\lambda)\,\hat{\rho}_{B0} \\ &= \mathrm{Tr}(\hat{\rho}_A\hat{B})\frac{\hat{B}\hat{\rho}_A\hat{B}}{\mathrm{Tr}(\hat{\rho}_A\hat{B})} + \mathrm{Tr}(\hat{\rho}_A(\hat{1}-\hat{B}))\frac{(\hat{1}-\hat{B})\hat{\rho}_A(\hat{1}-\hat{B})}{\mathrm{Tr}(\hat{\rho}_A(\hat{1}-\hat{B}))} \\ &= \hat{B}\hat{\rho}_A\hat{B} + (\hat{1}-\hat{B})\hat{\rho}_A(\hat{1}-\hat{B}) \qquad (7.59)\end{aligned}$$

For measurement C we take $\hat{C} = \hat{\phi}_C \equiv \hat{\phi}(x_C)$, and simply ask whether the expectation value $\langle\hat{C}\rangle$ of this measurement varies with λ. The derivative of $\langle\hat{C}\rangle$ at $\lambda=0$ is a measure of the sensitivity of the reception of the signal from A. Taking the vacuum as the initial state, $\hat{\rho}_0 = |0\rangle\langle 0|$,[116]

$$\begin{aligned}\frac{d}{d\lambda}\langle\hat{C}\rangle &= \frac{d}{d\lambda}\Big|_{\lambda=0}\mathrm{Tr}(\hat{\rho}_B\hat{C}) \\ &= -i\mathrm{Tr}(\hat{B}\hat{\rho}_0\hat{\phi}_A\hat{B}\hat{\phi}_C) + i\mathrm{Tr}(\hat{B}\hat{\phi}_A\hat{\rho}_0\hat{B}\hat{\phi}_C) \\ &\qquad - i\mathrm{Tr}((\hat{1}-\hat{B})\hat{\rho}_0\hat{\phi}_A(\hat{1}-\hat{B})\hat{\phi}_C) + i\mathrm{Tr}((\hat{1}-\hat{B})\hat{\phi}_A\hat{\rho}_0(\hat{1}-\hat{B})\hat{\phi}_C) \\ &= 2\,\Im\Big[\mathrm{Tr}(|0\rangle\langle 0|\hat{\phi}_A\hat{\phi}_C) + 2\mathrm{Tr}(|0\rangle\langle 0|\hat{\phi}_A|1\rangle\langle 1|\hat{\phi}_C|1\rangle\langle 1|) \\ &\qquad - \mathrm{Tr}(|0\rangle\langle 0|\hat{\phi}_A|1\rangle\langle 1|\hat{\phi}_C) - \mathrm{Tr}(|0\rangle\langle 0|\hat{\phi}_A\hat{\phi}_C|1\rangle\langle 1|)\Big] \\ &= -2\,\Im\big[\Psi(x_A)\Psi^*(x_C)\big], \qquad (7.60)\end{aligned}$$

where $\Psi(x) \equiv \langle 0|\hat{\phi}(x)|1\rangle$. The sensitivity of C as a receiver of a superluminal signal from A is then non-zero unless $\Psi(x_A) = 0$ or $\Psi(x_C) = 0$ or the phase difference $\Delta\theta_{AC}$ between them satisfies $\sin\Delta\theta_{AC} = 0$.

As $|1\rangle \in \mathcal{H}_1$, we may use (7.49) to write $|1\rangle = \int d^3\mathbf{p}\,\psi_1(\mathbf{p})\,\hat{a}^\dagger_{\mathbf{p}}|0\rangle$. If $\hat{\phi}(x)$ is a free field (7.38), then

$$\begin{aligned}\Psi(t,\mathbf{x}) &= \langle 0|\int\frac{d\mathbf{p}'}{(2\pi)^{3/2}}\frac{1}{(2E_{p'})^{1/2}}\hat{a}_{\mathbf{p}'}e^{-i(E_{p'}t-\mathbf{p}'.\mathbf{x})}\int d\mathbf{p}\,\psi_1(\mathbf{p})\hat{a}^\dagger_{\mathbf{p}}\,|0\rangle \\ &= \int\frac{d\mathbf{p}}{(2\pi)^{3/2}}\frac{1}{(2E_p)^{1/2}}\,\psi_1(\mathbf{p})\,e^{-i(E_pt-\mathbf{p}.\mathbf{x})} \qquad (7.61)\end{aligned}$$

This cannot be zero for all x unless $\psi_1(\mathbf{p}) = 0\ \ \forall\,\mathbf{p}$, which contradicts $|1\rangle \in \mathcal{H}_1$.We may choose a point x_A so that $\Psi(x_A) \neq 0$, whereupon $|\Psi(x_C)\sin\Delta\theta_{AC}|$ becomes a relative measure of the signal strength.

If the one-particle state $|1\rangle$ has well-defined momentum $\mathbf{p}'$, measurement B

[116]The identity $[\mathrm{Tr}(\hat{A}\hat{B}\hat{C})]^* \equiv \mathrm{Tr}(\hat{C}\hat{B}\hat{A})$ for self-adjoint $\hat{A}$, $\hat{B}$ and $\hat{C}$ has been used to obtain (7.60), along with the cyclic property of the trace. This property also tells us that $\Im[\mathrm{Tr}(\hat{\rho}_0\hat{\phi}_A\hat{\phi}_C)] = -\Im[\mathrm{Tr}(\hat{\rho}_0\hat{\phi}_C\hat{\phi}_A)] = 0$, because $\hat{\phi}_A$ and $\hat{\phi}_C$ commute at spacelike separation. The other two terms that vanish in the final step do so simply because $\langle 1|0\rangle = 0$.

corresponds to an ideal detector that responds only to particles of exactly this momentum. In this case, (7.61) shows that the signal strength is independent of the interval x_C–x_A in both time and space, aside from the rapidly oscillating factor $\sin[E_{p'}(t_C-x_A)-\mathbf{p'}.(\mathbf{x_C}-\mathbf{x_A})]$.

A less extreme situation is explored in [91]. The state $|1\rangle$ is taken to be a massless particle with a Gaussian function in momentum space with peak at $(k_0, 0, 0, k_0)$ and width σ. Region $\mathcal{R}_B$ is thickened to give measurement B a duration t_C-t_A, but the form of the measurement is essentially the same: it is a projection operator onto a one-particle state. Taking $x_A = (0, 0, 0, 0)$ and $x_C = (t, 0, 0, t+\delta)$ where $t \gg k_0/\sigma^2$ and $0<\delta<1/\sigma$, they find a superluminal signal whose strength is proportional to $\sqrt{k_0/\sigma}\,\cos(k_0\delta)\,t^{-1}$. As δ (the spatial distance by which x_C is outside the future light cone of x_A) increases, the signal strength is modulated by a function $e^{-\sigma^2\delta^2/4}D_{-3/2}(-i\sigma\delta-k_0/\sigma)$, which drops off as $e^{-\sigma^2\delta^2/2}\sqrt{\delta}$ as $\delta \to \infty$.

Rejecting superluminal signalling, the conclusion of the authors is that either the unitary transformation at x_A, the ideal measurement $\hat{B} = |1\rangle\langle 1|$ or the final measurement at x_C is impossible, and that this represents a fundamental failing of the Hamiltonian approach to quantum mechanics (the three postulates of Sections 3.1 and 4.1), underlining the need, as they see it, to set the foundations of quantum mechanics firmly in a path integral approach.

7.5.2 The limits of canonical quantum theory?

The results outlined in Section 7.5.1 have much in common with those of Section 7.4.3: they involve a measurement that is a projection operator onto a subset of one-particle states leading to a violation of relativistic causality. It may be that measurements projecting onto the one-particle subspace simply cannot occur in quantum field theory. Alternatively, our three basic postulates may merely be conveniences that emerge as approximations from a very different and more solid foundation, and we may now have arrived at the place at which they finally break down.

The case against the 'Hamiltonian approach' has been running for a long time. The primary motivation is the clear absence of manifest relativistic invariance in the postulates – the evolution of the state vector with respect to time is generated by a spatially-global Hamiltonian. The action and the Lagrangian density, by contrast, are relativistic scalars. This was noted by Dirac in 1933 [92] and led Feynman to develop the path integral formulation of quantum mechanics [56] in terms of the action (which is demonstrably equivalent to the Hamiltonian approach in some circumstances, as is noted in Section

5.2.1). It may be thought unseemly for a relativistic theory to be developed in a manner that has such disregard for relativistic invariance; yet the Hamiltonian approach has persisted long into the development of quantum field theory as a practical tool. The majority of texts and courses give it precedence because of its relative simplicity and its compatibility with elementary quantum mechanics, and also because it is known to generate a relativistic theory in practice, in spite of its roots.

There is still room to defend the three basic postulates against challenges such as those described by the results of Section 7.5.1. In particular, a significant class of the observables proposed in Section 7.1.2 for a scalar field do not exhibit these superluminal signal facilitating properties. These observables are sums of infinitesimal *local* operators, each defined by the field at a point – that is, operators of the form

$$\hat{B} = \int_{R_B} d^3\mathbf{x}\, F(\hat{\phi}(x), \partial_\mu \hat{\phi}(x), \partial_\mu \partial_\nu \hat{\phi}(x), \ldots). \tag{7.62}$$

where R_B is a spacelike hypersurface [90, §4] [91, §III].[117]

For operators to conform to the requirements of a measurement in a causal theory, therefore, they should be both local and instantaneous. (These would be considered natural conditions in quantum mechanics, the context in which these postulates arose.)

As was noted in Section 3.1, measurements may in fact be an emergent process: the unitary local evolution of an open system in a particular kind of complex environment, one that approximates to a set of projection operators under certain conditions. If this is the case, it may be that the kinds of causality-violating measurements described in Section 7.5.1 cease to arise, but the question of how and to what extent physical phenomena are located in spacetime would remain to be addressed.

[117] In the latter reference, this class of well-behaved observables is restricted further to *"field operators smeared with real functions over subsets of spacelike hypersurfaces."*

8 Conclusions

The study of causal relations in quantum theory requires us to pay close attention to the assumptions we make and the definitions we choose to work with. A class of **causal relationships** of interest was proposed in the Introduction, and defined quantitatively using the concept of **signalling** in Section 2.3. The information-theoretic context of that Section also helped us begin setting out an **operational definition** of quantum theory suitable for the scope of this work.

Three simple quantum postulates, introduced in Sections 3.1 and 4.1, were found to be sufficient to cover a vast amount of ground:

Postulate 1 *Any physical state can be represented by a vector in a vector space such that the probabilities for the outcomes of any measurement are given by the square of the norm of a projection of this vector onto some subspace that is characteristic of the measurement being made.*

Postulate 2 *Every measurement updates the state by projecting it onto the subspace associated with the outcome of the measurement.*

Postulate 3 *The generator of time evolution can be expressed as a function of a set of continuous operators that commute with each other, a set of operators canonically conjugate to them, and a set of discrete operators that commute with them.*

Individual quantum theories within this scheme can then be defined by (a) the function specified in Postulate 3 and (b) any restrictions placed on the subspaces of a measurement outcome in Postulates 1 and 2.

With regard to Postulate 3, we saw in Section 4 that if we include a **finite number of conjugate pairs** of continuous operators $\{\hat{x}_i, \hat{p}_i\}$ and no discrete operators, the result is a theory in which the expectation values of any operator obey the laws of classical Hamiltonian mechanics. Awareness of relativistic causality (revisited more quantitatively in Section 6.1.3) meant that it was necessary to be clear about how **location in space and time** is treated in the theory. By defining the coordinates of a spatial location as *the Hamiltonian coordinates of a classical single particle system in which the particle is at that location*, we generate a map $R \mapsto \mathcal{H}_R$ between spatial regions and subspaces of the vector space $\mathcal{H}$ of Postulate 1. For the purposes of quantum mechanics (Sections 4 to 6), this map is sufficient for the evaluation of causal relationships between different locations.

Two key results with regard to **signalling** and **relativistic causality** in single particle theories were established in Section 5.1. First, a proof was presented that if operators exist of the form (5.9):

$$\hat{A} = \int_{R_A} d\mathbf{x} \int_{R_A} d\mathbf{x}' \; |x'\rangle \hat{A}^{(x,x')} \langle x| \tag{8.1}$$

they can be used for superluminal signalling – that is, a transfer of information that violates relativistic causality – if and only if the **propagator** is non-zero for spacelike separated intervals:

$$K(\mathbf{x_B}, t_B; \mathbf{x_A}, t_A) \neq 0 \;\; \text{with } (\mathbf{x_B} - \mathbf{x_A})^2 > c^2 (t_B - t_A)^2 \tag{8.2}$$

Second, we have the more general result that two measurements represented by *any* operators $\hat{A}$ and $\hat{B}$ and made at times t_A and t_B can be used to transmit information if and only if their **commutator** in the Heisenberg picture is non-zero: $[\hat{A}(t_A), \hat{B}(t_B)] \neq 0$.

While it is a familiar idea in quantum physics that a non-zero propagator indicates the potential for influence between a pair of spacetime points, and a non-zero commutator indicates an interaction between a pair of measurements, to my knowledge, the causal implications and assumptions are not explicitly set out in any single text. It has been my intention to bring these details together here.

Through the rest of Section 5 and Section 6, a number of single particle propagators were calculated; it is clear that they all satisfy (8.2), implying a violation of relativistic causality. It was noted in the Introduction that *any* amount of signalling over spacelike separated distances, no matter how minuscule the associated probabilities, points to a logical contradiction in the theory. It follows that (notwithstanding the caveats in Sections 5.1 and 6.1.3) no operators of the form (8.1) can exist: **there can be no operators exclusively associated with a finite spatial region in a single particle theory**. (This result mirrors a general theorem by Malament, described in Section 7.3.)

Nevertheless, single particle theories are unarguably of value and can yield results agreeing with observation to a high degree of accuracy – most notably the success of the Dirac theory of the electron in calculating the energy levels of hydrogen[118] – results that must be reproduced and explained by whatever

[118] Although even this is somewhat suspect, since *"we have to replace the electron mass by the reduced mass, a concept which has no room in special relativity"* – H. Bacry [93].

theory is to replace them. With this in mind, relativistic single particle theories were the focus of Section 6.

In Section 6.3 it was established that, aside from attempting to take a simple 'square root', there are essentially only two Hamiltonians satisfying the relativistic single particle equation $\hat{H}^2 = \hat{\mathbf{p}}^2 + m^2\hat{1}$: the **Feshbach–Villars Hamiltonian** and the **Dirac Hamiltonian**. Both require a multi-component wavefunction, which is equivalent to admitting discrete operators in Postulate 3. We saw that each of the resulting theories has an ambiguous relationship to spatial location, having one position representation (the **'canonical' representation**) in which the *time evolution* of the state takes place point by point throughout space; and a second position representation (the **'Newton–Wigner' representation**) in which *location-specific measurements* may be defined. The propagators in both Feshbach–Villars theory and Dirac theory can be made Lorentz invariant, but only in the 'canonical' representation (6.75) and (6.88), and even then only by imposing a prescription on the propagator that identifies antiparticles as particles propagating backwards in time. The propagators that result from this prescription are found to be closely related to the Feynman propagators of quantum field theory.

One topic that is rarely approached in the literature is the form of the 'square root' operators $\hat{H} = \pm\sqrt{\hat{\mathbf{p}}^2 + m^2}$ acting on a one-component wavefunction in a position representation. Derivations of the propagators were presented in Section 6.1 and a **convolution expression for a 'square root Hamiltonian'** operator in the position representation was presented in Section 6.2. (The derivation can be found in Appendix A.2). In equation (6.63) this can be seen to be equivalent to the Feshbach–Villars Hamiltonian in the Newton–Wigner representation. A comparison of equations (6.52) and (6.85) is sufficient to see that this equivalence also holds in the Dirac theory.

In Section 7 we saw that a **quantum field theory** can be defined using the same three postulates, if no limit is placed on the number of continuous operators involved in Postulate 3. The operators are considered to be distributed over space[119] with the additional requirement that the generator of time evolution be **derived from a Lorentz invariant action** by the methods of classical Hamiltonian field theory. The radical change in going from the quantum theories of Sections 4–6 to the field theories of Section 7 is not in the formalism but in **the relationship between the space of states**

[119] In other words, the set is made Cauchy continuous and a three-dimensional Euclidean topology is imposed upon it. The description here refers to the Schrödinger picture (Section 7.1.2).

$\mathcal{H}$ **and spatial location**. Rather than a map $R \mapsto \mathcal{H}_R$ from spatial regions to subspaces of $\mathcal{H}$, we have a set of maps[120] $R \mapsto \int_R d^3\mathbf{x}\, \hat{\phi}_a(\mathbf{x})$ from spatial regions to **operators** on $\mathcal{H}$. The connection between individual *states* in $\mathcal{H}$ and spatial location is far more complicated (Section 7.3).

Despite the very different definitions of location, the relativistic single particle theory – along with a Newton–Wigner representation – emerges naturally from a free scalar field theory (Section 7.4.2). The observation that 'there can be no operators exclusively associated with a finite spatial region in a single particle theory' then gives rise to the implication '**if a measurement is to take place in a finite spatial region, that measurement must have the capacity for particle creation**' (Section 7.4.3).

Because of the map between location and operators, causal relations between pairs of localised **measurements** in quantum field theory are considerably simpler than in a single-particle theory. Measurements defined from the operators in finite regions of spacetime $\mathcal{R}_A$ and $\mathcal{R}_B$ **always commute if the regions are entirely spacelike separated from each other** (Section 7.1), in accordance with relativistic causality. In Section 7.2 we saw that if an influence on a free quantum field is represented by a **classical source**, this influence is also strictly relativistically causal.

In practice, however, applications of quantum field theory do not involve local measurements. No satisfactory model exists for a physical detector strictly confined to a finite region of spacetime, whether in terms of projection operators (per Postulate 1) or field operators (per Section 7.1). And while it may be reassuring that two measurements confined to finite spacetime regions would necessarily obey relativistic causality, we would still be left with the question of how we would physically determine exactly where the boundaries of those regions were.

Further, if we define a quantum field theory using these postulates and place no restrictions on measurements in spacetime regions, causality violations re-emerge (Section 7.5.1). This result suggests that a quantum field theory based on a projection postulate is only causally consistent in relation to measurements that are both local[121] and instantaneous.

To reiterate a point made in the Introduction: when we consider a measurement outcome, we implicitly take it to be something that can be made to

[120] One map for each field label a.

[121] A local operator is one that can be expressed as a sum of operators defined at each point in a region.

give rise to a lasting and discernible trace of its having happened. There is a great deal of idealisation in this requirement, suggesting that the reduction of the measurement process to Postulates 1 and 2 only approximates a deeper dynamical process. A review of what this kind of process might involve can be found in [36].

We know that the canonical approach to quantum field theory is equivalent to a coordinate space path integral formalism that is manifestly Lorentz invariant.[122] It may be that the measurement process within field theory can be clarified by appealing to foundational models[123] that generate path integrals without appealing to Hilbert space.

In the meantime, to the extent that we make use of quantum theories that are in accord with the postulates listed above, issues of location and causality such as those presented here remain relevant. It is hoped that this work on elementary theories will be of interest to those concerned with these issues, whether their motivation is to ensure such theories are causally consistent or to try to prove them false.

[122]This is shown to be the case in Section 5.2.1 for theories in which the Hamiltonian is quadratic in $\hat{p}$; the same principle applies to field theories that are quadratic in $\partial_\mu \hat{\phi}_a$ [74, §9].

[123]Such as causal sets [46].

A Appendix

A.1 Causal relation between observables in quantum mechanics

In Section 5.1, it was shown that a pair of idealised measurements giving simple yes/no answers as to whether a particle is in a particular spatial region at a given time (5.1) can in principle be used to send signals if and only if there are non-vanishing propagators between the regions and times of the two measurements (5.8).

Here, the result is generalised to any normal operator of the following type:

$$\hat{A} = \int_{R_A} d\mathbf{x} \int_{R_A} d\mathbf{x}' \; |x'\rangle \hat{A}^{(x,x')} \langle x|, \tag{A.1}$$

again defined strictly over a region R_A. The operator $\hat{A}^{(x,x')}$ may be a function of $\mathbf{x}$ and $\mathbf{x}'$, or any series of finite order differential operators with respect to $\mathbf{x}$ and $\mathbf{x}'$ with coefficients that are functions. This allows the operator to be any function of position and momentum – provided it is confined to the specified spatial region in this way. If $\hat{A}^{(x,x')} = \hat{A}^{(x)}\delta(\mathbf{x}-\mathbf{x}')$, the operator is a 'local' operator in the coordinate representation.

Let $\hat{A}$ have eigenvalues a_i, each with an eigenspace spanned by an orthonormal set $|A_{i,q}\rangle$, and let $A_{i,q}(\mathbf{x}) \equiv \langle x|A_{i,q}\rangle$. Then

$$\begin{aligned} \hat{A}|A_{i,q}\rangle &= a_i|A_{i,q}\rangle \\ \Rightarrow \quad \int d\mathbf{x} \; \hat{A}|x\rangle\langle x|A_{i,q}\rangle &= \int d\mathbf{x} \; |x\rangle a_i \langle x|A_{i,q}\rangle \\ \Rightarrow \quad \int d\mathbf{x} \; \langle y|\hat{A}|x\rangle A_{i,q}(\mathbf{x}) &= a_i A_{i,q}(\mathbf{y}) \end{aligned} \tag{A.2}$$

From (A.1), $\langle y|\hat{A}|x\rangle = 0$ if either $\mathbf{x}$ or $\mathbf{y}$ is not in R_A, therefore every function $A_{i,q}(\mathbf{y})$ must have support[124] R_A except for the case $a_0 = 0$.

The projection operator for outcome a_i is $\hat{P}_i^{(A)} = \sum_q |A_{i,q}\rangle\langle A_{i,q}|$. If the system is initially in state $\hat{\rho}$ at time t_A when the measurement is made, the probability, using (3.3), is

$$p(i|A) = Tr(\hat{P}_i^{(A)}\hat{\rho}) = \sum_n \int_{R_A} d\mathbf{x} \langle x|A_{i,q}\rangle\langle A_{i,q}|\hat{\rho}|x\rangle \tag{A.3}$$

[124] The support of a function is the smallest closed subset of its domain consisting of all arguments for which the function returns a non-zero value.

and the state immediately after the measurement, using (3.10), is

$$\hat{\rho} \;\rightarrow\; \hat{\rho}_i = \frac{\hat{P}_i^{(A)}\hat{\rho}\hat{P}_i^{(A)}}{Tr(\hat{P}_i^{(A)}\hat{\rho})} = \frac{\sum_{rs}|A_{i,r}\rangle\langle A_{i,r}|\hat{\rho}|A_{i,s}\rangle\langle A_{i,s}|}{\sum_q \int_{R_A} d\mathbf{x}\,\langle x|A_{i,q}\rangle\langle A_{i,q}|\hat{\rho}|x\rangle} \tag{A.4}$$

As in Section 5.1, we consider the case where Alice is able to choose from a selection of possible measurements of this type, to be carried out at time t_A in spatial region R_A. At a later time t_B and in region R_B, Bob makes a measurement B.

By this time, the system has evolved to state $U_{BA}\,\hat{\rho}_i\,\hat{U}_{BA}^\dagger$, where $\hat{U}_{BA} \equiv \hat{U}(t_B, t_A)$ is the time evolution operator between times t_A and t_B. The probability of outcome b_j in a subsequent measurement by operator $\hat{B}$ defined similarly over region R_B is then

$$\begin{aligned} p(j|A,B) &= \sum_i p(j|A,B,i)p(i|A) \\ &= \sum_i Tr(\hat{P}_j^{(B)}\,\hat{U}_{BA}\,\hat{\rho}_i\,\hat{U}_{BA}^\dagger)\sum_q \int_{R_A} d\mathbf{x}\,\langle x|A_{i,q}\rangle\langle A_{i,q}|\hat{\rho}|x\rangle \\ &= \sum_i\sum_t \int d\mathbf{y}\langle y|B_{j,t}\rangle\langle B_{j,t}|\,\hat{U}_{BA}\sum_{rs}|A_{i,r}\rangle\langle A_{i,r}|\hat{\rho}|A_{i,s}\rangle\langle A_{i,s}|\,\hat{U}_{BA}^\dagger|y\rangle \end{aligned} \tag{A.5}$$

If the sum over i were replaced by a double sum over i_1 and i_2, we would be able to use the completeness relation $\sum_i \hat{P}_i^{(A)} = \sum_{i,r}|A_{i,r}\rangle\langle A_{i,r}| = I$ to simplify the expression considerably. The original single sum is equivalent to the condition $i_1 = i_2$, which we can enforce by subtracting the terms where it does not hold:

$$\begin{aligned} p(j|AB) = &\sum_t \int d\mathbf{y}\langle y|B_{j,t}\rangle\langle B_{j,t}|\,\hat{U}_{BA}\,\hat{\rho}\,\hat{U}_{BA}^\dagger|y\rangle \;- \\ &\sum_{i_1\neq i_2}\sum_{rst}\int d\mathbf{y}\langle y|B_{j,t}\rangle\langle B_{j,t}|\hat{U}_{BA}|A_{i_1,r}\rangle\langle A_{i_1,r}|\hat{\rho}|A_{i_2,s}\rangle\langle A_{i_2,s}|\hat{U}_{BA}^\dagger|y\rangle \\ = \;& Tr(\hat{P}_i^{(B)}\hat{U}_{BA}\,\hat{\rho}\,\hat{U}_{BA}^\dagger) \;- \\ &\sum_{i_1\neq i_2}\sum_{rst}\int d\mathbf{y_1}d\mathbf{y_2}\int d\mathbf{x_1}d\mathbf{x_2}d\mathbf{x_3}d\mathbf{x_4}\,B_{j,t}(\mathbf{y_1})B_{j,t}^*(\mathbf{y_2})K_{BA}(\mathbf{y_2},\mathbf{x_1}) \\ &\qquad \times A_{i_1,r}(\mathbf{x_1})A_{i_1,r}(\mathbf{x_2})\langle x_2|\hat{\rho}|x_3\rangle A_{i_2,s}(\mathbf{x_3})A_{i_2,s}^*(\mathbf{x_4})K_{BA}^*(\mathbf{y_1},\mathbf{x_4}) \end{aligned} \tag{A.6}$$

where $K_{BA}(\mathbf{x},\mathbf{y}) \equiv \langle x|\hat{U}(t_B,t_A)|y\rangle$ is the propagator.

The first term is simply the probability of outcome b_j from B alone. For

any probability $p(j|A,B)$ of outcome b_j to have any dependence on the choice of measurement A, the second term must be non-zero.

If $j\neq 0$, we know that $B_{j,t}(\mathbf{y})$ has support R_B. In the second term, i_1 and i_2 are never both zero, so at least one of $A_{i_1,r}(\mathbf{x_1})$ and $A_{i_2,s}(\mathbf{x_4})$ must have support R_A. This immediately means that if $K_{BA}(\mathbf{y},\mathbf{x}) = 0$ for all $\mathbf{x} \in R_A$ and all $\mathbf{y} \in R_B$, the whole of the second term vanishes. This means $p(j)$ is independent of the choice of A when $j\neq 0$; and since $p(0) = 1-\sum_{j\neq 0} p(j)$, this holds for all j.

If $K_{BA}(\mathbf{y},\mathbf{x}) \neq 0$ for some $\mathbf{x} \in R_A$ and some $\mathbf{y} \in R_B$, then it would be possible, by selecting a different measurement (A.1) in region R_A, to alter the probabilities of the outcomes of B and therefore enable signalling.

A.2 The square root of the Klein–Gordon Hamiltonian as a convolution operation

Here we are concerned with the square root Hamiltonian in its Taylor-expanded form (6.31)

$$\hat{H}^{(x)}_{\surd} = m\sum_{n=0}^{\infty} \frac{-1}{2n-1}\frac{(2n)!}{(2^n n!)^2}\left(\frac{1}{m^2}\nabla^2\right)^n \tag{A.7}$$

and the derivation of the dependence of $\hat{H}^{(x)}_{\surd}\psi(\mathbf{x})$ at any given point $\mathbf{x}$ on the wavefunction at every point in space.

In one dimension, the convolution of an analytic function $\psi(x)$ with a function $f(x)$ over $x \in \mathbb{R}$ can be expanded as

$$f * \psi(x) \equiv \int_{-\infty}^{\infty} dr\, f(r)\psi(x+r) = \sum_{n=0}^{\infty}\int_{-\infty}^{\infty} dr\, f(r)\,\frac{r^n}{n!}\frac{d^n}{dx^n}\psi(x). \tag{A.8}$$

Comparing coefficients with those of (A.7), it follows that if we can find a function $f(r)$ that has the following definite integrals for $n \in \mathbb{N}$

$$\int_{-\infty}^{\infty} dr\, f(r)\, r^n = \begin{cases} m\dfrac{-1}{n-1}\dfrac{1}{2^n}\left(\dfrac{n!}{\frac{n}{2}!}\right)^2\dfrac{1}{m^n} & \text{if } n \text{ is even} \\ 0 & \text{if } n \text{ is odd,} \end{cases} \tag{A.9}$$

then we can infer that

$$f * \psi(x) = \hat{H}^{(x)}_{\surd}\psi(x) \tag{A.10}$$

for every analytic function $\psi(x)$ for which $\hat{H}^{(x)}_{\surd}\psi(x)$ is defined.

A general method for finding functions such as $f(r)$ is to use an inverse Mellin transform.[125] For our case, however, it suffices to note that the modified Bessel function of the second kind $K_\nu(x)$ has the following definite integrals:

$$\int_0^\infty dr\, K_\nu(r) r^{n-1} = 2^{n-2}\,\Gamma(\tfrac{n-\nu}{2})\Gamma(\tfrac{n+\nu}{2}) \qquad \text{if } \Re(n) > |\Re(\nu)|. \tag{A.11}$$

Since $\Gamma(s+\frac{1}{2}) = \sqrt{\pi}(2s)!/(2^{2s}s!)\ \forall s \in \mathbb{N}$, for even $n > 0$ this implies

$$\int_0^\infty dr\, \frac{K_1(r)}{r} r^n = \frac{\pi}{2}\frac{1}{n-1}\frac{1}{2^n}\left(\frac{n!}{\frac{n}{2}!}\right)^2. \tag{A.12}$$

whereupon, for $n > 0$,

$$\int_{-\infty}^\infty dr\, \frac{K_1(m|r|)}{|r|} r^n = \begin{cases} \pi\dfrac{1}{n-1}\dfrac{1}{2^n}\left(\dfrac{n!}{\frac{n}{2}!}\right)^2\dfrac{1}{m^n} & \text{if } n \text{ is even} \\ 0 & \text{if } n \text{ is odd.} \end{cases} \tag{A.13}$$

Therefore, the function

$$f_K(r) = -\frac{m}{\pi}\frac{K_1(m|r|)}{|r|} \tag{A.14}$$

satisfies (A.9) for $n > 0$. The Bessel K function doesn't quite work in the convolution function, however, because in the case $n = 0$, its integral diverges.

This can be remedied by adjusting the $n = 0$ term by hand, giving

$$\begin{aligned} \hat{H}^{(x)}_\vee \psi(x) &= m\psi(x) + \sum_{n=1}^\infty \int_{-\infty}^\infty dr\, f_K(r)\, \frac{r^n}{n!}\frac{d^n}{dx^n}\psi(x) \\ &= m\psi(x) - \frac{m}{\pi}\int_{-\infty}^\infty dr\, \frac{K_1(m|r|)}{|r|}\left[\psi(x+r) - \psi(x)\right]. \end{aligned} \tag{A.15}$$

In three spatial dimensions, a Taylor expansion of the convolution formula gives

---

[125] The Mellin transform $\phi(s)$ of $f(r)$ is defined for all $s \in \mathbb{C}$ by

$$\phi(s) \equiv \int_0^\infty dr\, f(r)\, r^{s-1}$$

and can be inverted using an integral along any line parallel to the imaginary axis in the complex s plane, provided $\phi(s)$ is analytic in the neighbourhood of every point on the line [81, §1.14(iv)].

$$f * \psi(\mathbf{x}) \equiv \int d\mathbf{r}\, f(\mathbf{r})\psi(\mathbf{x}+\mathbf{r}) = \sum_{n=0}^{\infty} \int d\mathbf{r}\, f(\mathbf{r})\, \frac{1}{n!}(\mathbf{r}.\nabla)^n \psi(\mathbf{x}). \qquad \text{(A.16)}$$

Focusing on the coefficient of the Cartesian coordinate r_3^n, we see that if we wish to generate the square root Hamiltonian (A.7) we require

$$\int d\mathbf{r}\, f(\mathbf{r})\, r_3^n \;=\; m\frac{-1}{n-1}\frac{1}{2^n}\left(\frac{n!}{\frac{n}{2}!}\right)^2\left(\frac{1}{m}\right)^n \;=\; -\frac{2m}{\pi}\int_0^\infty dr\, K(mr)\, r^{n-1}. \qquad \text{(A.17)}$$

If we integrate $K_1(m|\mathbf{r}|)r_3^n$ over three dimensions (using spherical polar coordinates), we find

$$\begin{aligned}\int d\mathbf{r}\, K_1(|\mathbf{r}|)\, r_3^n \;&=\; \int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi \int_0^\infty r^2 dr\; K_1(r)\, r^n \cos^n\theta \\ &=\; \frac{4\pi}{n+1}\int_0^\infty dr\, K_1(r)\, r^{n+2}. \qquad \text{(A.18)}\end{aligned}$$

The presence of n in the prefactor suggests that we use first derivatives of the Bessel K functions to construct a trial solution for $f(\mathbf{r})$. Let

$$f_{K3}(\mathbf{r}) = A\,\frac{\mathbf{r}.\nabla(K_1(m|\mathbf{r}|)) + b\,K_1(m|\mathbf{r}|)}{|\mathbf{r}|^\alpha} \qquad \text{(A.19)}$$

where A, b and α are undetermined. Then

$$\begin{aligned}\int d\mathbf{r}\, f_{K3}(\mathbf{r})\, r_3^n \;&=\; \frac{4\pi A}{n+1}\left\{\int_0^\infty dr\,\frac{\partial}{\partial r}K_1(mr)\, r^{n+3-\alpha} + b\int_0^\infty dr\, K_1(mr)\, r^{n+2-\alpha}\right\} \\ &=\; \frac{4\pi A}{n+1}\Bigg\{\left[K_1(mr)\, r^{n+3-\alpha}\right]_0^\infty \\ &\qquad +\; [b-(n+2-\alpha)]\int_0^\infty dr\, K_1(mr)\, r^{n+2-\alpha}\Bigg\}. \qquad \text{(A.20)}\end{aligned}$$

The boundary term vanishes for positive integer n; equation (A.17) is then satisfied if we take $\alpha = 3$, $b = -2$ and $A = m/2\pi^2$, giving:

$$\begin{aligned} f_{K3}(\mathbf{r}) \;&=\; \frac{m}{2\pi^2}\frac{\mathbf{r}.\nabla(K_1(m|\mathbf{r}|)) - 2\,K_1(m|\mathbf{r}|)}{|\mathbf{r}|^3} \\ &=\; \frac{mr}{2\pi^2}\,\frac{\partial}{\partial r}\left(\frac{K_1(mr)}{r^2}\right) \\ &=\; \frac{m}{2\pi^2}\,\frac{-\frac{1}{2}mr[K_0(mr)+K_2(mr)] - 2K_1(mr)}{r^2}. \qquad \text{(A.21)}\end{aligned}$$

To see if this can generate the full square root Hamiltonian, we need to check the terms in the expansion of $f_{K3} * \psi(\mathbf{x})$ from (A.16) against the equivalent terms in the expansion of $\hat{H}_{\surd}^{(x)}$ from (A.7). The powers n_i of each derivative $\partial/\partial x_i$ in (A.16) can be made explicit using a trinomial expansion of $(\mathbf{r}.\nabla)^n$. We avoid complications due to non-commuting differential operators by expanding in a Cartesian basis. The result is

$$\sum_{\{n_i\}}^{\infty} \int d\mathbf{r}\, f_{K3}(\mathbf{r})\, \frac{1}{n!} \frac{n!}{n_1! n_2! n_3!} \left(r_1 \frac{\partial}{\partial x_1}\right)^{n_1} \left(r_2 \frac{\partial}{\partial x_2}\right)^{n_2} \left(r_3 \frac{\partial}{\partial x_3}\right)^{n_3} \psi(\mathbf{x}), \qquad \text{(A.22)}$$

with $n \equiv n_1 + n_2 + n_3,\ n_i \in \{0, 1, 2, ...\}$. The integrals over $\mathbf{r}$ can be broken down as follows:

$$\begin{aligned} \int d\mathbf{r}\, f_{K3}(\mathbf{r})\, r_1^{n_1} r_2^{n_2} r_3^{n_3} \;=\; & \frac{m}{2\pi^2} \int_0^{\pi} d\theta\, \cos^{n_3}\theta \sin^{n-n_3+1}\theta \int_0^{2\pi} d\phi\, \sin^{n_2}\phi \cos^{n_1}\phi \\ & \times \int_0^{\infty} dr\, r^{n+3} \frac{\partial}{\partial r}\left(\frac{K_1(mr)}{r^2}\right). \end{aligned} \qquad \text{(A.23)}$$

When n_1, n_2 and n_3 are all even, the θ and ϕ integrals give

$$\left(\frac{2^{n-n_3+1}}{n+1} \frac{n_3! \frac{n-n_3}{2}! \frac{n}{2}!}{n! \frac{n_3}{2}!}\right)\left(\frac{2\pi}{2^{n_1+n_2}} \frac{n_1! n_2!}{\frac{n_1}{2}! \frac{n_2}{2}! \frac{n_1+n_2}{2}!}\right) = \frac{4\pi}{n+1} \frac{\frac{n}{2}!}{\frac{n_1}{2}! \frac{n_2}{2}! \frac{n_3}{2}!} \frac{n_1! n_2! n_3!}{n!}; \qquad \text{(A.24)}$$

otherwise they vanish. Therefore, in (A.16), the $n>0$ terms of $f_{K3} * \psi(\mathbf{x})$ are

$$\begin{aligned} & \sum_{\{n_i \text{ even}\,:\, n>0\}} \frac{1}{n_1! n_2! n_3!} \frac{m}{2\pi^2} \left(\frac{4\pi}{n+1} \frac{\frac{n}{2}!}{\frac{n_1}{2}! \frac{n_2}{2}! \frac{n_3}{2}!} \frac{n_1! n_2! n_3!}{n!}\right)(-n-1) \\ & \qquad \times \left(\frac{\pi}{2} \frac{1}{n-1} \frac{1}{2^n} \left(\frac{n!}{\frac{n}{2}!}\right)^2 \frac{1}{m^n}\right) \frac{\partial^{n_1}}{\partial x_1^{n_1}} \frac{\partial^{n_2}}{\partial x_2^{n_2}} \frac{\partial^{n_3}}{\partial x_3^{n_3}} \psi(\mathbf{x}) \\ = \; & m \sum_{\{n_i\,:\, n>0\}} \frac{-1}{2n-1} \frac{1}{2^{2n}} \frac{1}{m^{2n}} \frac{(2n)!}{(n!)^2} \left(\frac{n!}{n_1! n_2! n_3!}\right)\left(\frac{\partial^2}{\partial x_1^2}\right)^{n_1}\left(\frac{\partial^2}{\partial x_2^2}\right)^{n_2}\left(\frac{\partial^2}{\partial x_3^2}\right)^{n_3} \psi(\mathbf{x}), \end{aligned} \qquad \text{(A.25)}$$

while the $n=0$ term, again, is divergent.[126]

The sum of partial derivatives in the expansion of the square root Hamil-

[126]The sum over even n_i has been converted to a sum over all n_i in the final line of (A.25) by the replacement $n_i \to 2n_i$ within the sum.

tonian (A.7) is

$$
\begin{aligned}
& m\sum_{n=0}^{\infty}\frac{-1}{2n-1}\frac{(2n)!}{(2^n n!)^2}\frac{1}{m^{2n}}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial x_3^2}\right)^n\psi(\mathbf{x}) \\
= \; & m\sum_{\{n_i\}}\frac{-1}{2n-1}\frac{1}{2^{2n}}\frac{1}{m^{2n}}\frac{(2n)!}{(n!)^2}\left(\frac{n!}{n_1!n_2!n_3!}\right)\left(\frac{\partial^2}{\partial x_1^2}\right)^{n_1}\left(\frac{\partial^2}{\partial x_2^2}\right)^{n_2}\left(\frac{\partial^2}{\partial x_3^2}\right)^{n_3}\psi(\mathbf{x}).
\end{aligned}
\tag{A.26}
$$

The expressions are fully equivalent for $n>0$. Adding the $n=0$ term by hand, we obtain (in a selection of equivalent forms),

$$
\begin{aligned}
\hat{H}_{\vee}^{(x)}\psi(\mathbf{x}) &= m\psi(\mathbf{x})+\sum_{n=1}^{\infty}\int d\mathbf{r}\, f_{K3}(\mathbf{r})\,\frac{1}{n!}(\mathbf{r}.\nabla_{\mathbf{x}})^n\psi(\mathbf{x}) \\
&= m\psi(\mathbf{x})+\frac{m}{2\pi^2}\int d\mathbf{r}\;\frac{-\frac{1}{2}mr[K_0(mr)+K_2(mr)]-2K_1(mr)}{r^2} \\
&\qquad\qquad \times\;\; [\psi(\mathbf{x}+\mathbf{r})-\psi(\mathbf{x})] \\
&= m\psi(\mathbf{x})+\frac{m}{2\pi^2}\int d\mathbf{r}\; r\frac{\partial}{\partial r}\left(\frac{K_1(mr)}{r^2}\right)[\psi(\mathbf{x}+\mathbf{r})-\psi(\mathbf{x})] \qquad \text{(A.27)} \\
&= m\psi(\mathbf{x})-\frac{m}{2\pi^2}\int d\mathbf{r}\;\frac{K_1(mr)}{r^2}\left[3\,[\psi(\mathbf{x}+\mathbf{r})-\psi(\mathbf{x})]+r\frac{\partial}{\partial r}\psi(\mathbf{x}+\mathbf{r})\right].
\end{aligned}
$$

A.3 Note on the structure of the Feshbach–Villars space of states and the particle interpretation

The full space of states $\mathcal{H}_{FV}$ may be divided into three sets: those $|\psi\rangle$ for which $\langle\psi|\psi\rangle>0$, those for which $\langle\psi|\psi\rangle<0$ and those for which $\langle\psi|\psi\rangle=0$. The first two of these can be considered as extensions of the vector spaces $\mathcal{H}_{FV}^{(\pm)}$.

Any state in $\mathcal{H}_{FV}$ may be written as a superposition $|\psi\rangle=\alpha|\psi^{(+)}\rangle+\beta|\psi^{(-)}\rangle$ of two normalised states $|\psi^{(+)}\rangle\in\mathcal{H}_{FV}^{(+)}$ and $|\psi^{(-)}\rangle\in\mathcal{H}_{FV}^{(-)}$. Its norm-squared, using (6.46), is $\langle\psi|\psi\rangle=|\alpha|^2-|\beta|^2$. If we assert that this mixed state can be generated from a normalised state in $\mathcal{H}_{FV}^{(+)}$ by means of a pseudo-unitary operator $\hat{U}$, we find that such a $\hat{U}$ exists provided $|\alpha|^2-|\beta|^2=1$. Similarly, any state generated by pseudo-unitary transformation from a state in $\mathcal{H}_{FV}^{(-)}$ retains a norm-squared of -1. These operators preserve the norm, *i.e.* $\langle\hat{U}\psi|\hat{U}\psi\rangle=\langle\psi|\psi\rangle$, just as a unitary operator would preserve the norm of states in a Hilbert space.

Thus, *any* state $|\psi\rangle\in\mathcal{H}_{FV}$ having $\langle\psi|\psi\rangle>0$ is related by pseudo-unitary transformation to a state in $\mathcal{H}_{FV}^{(+)}$; and any state having $\langle\psi|\psi\rangle<0$ is related by a pseudo-unitary transformation to a state in $\mathcal{H}_{FV}^{(-)}$.

These extended sets of vectors are not vector spaces, since a superposition

of states with positive norm-squared may itself have negative norm-squared.[127]

Any set $\hat{U}\mathcal{H}_{FV}^{(+)}$ for a given pseudo-unitary $\hat{U}$, however, is a Hilbert space. With this in mind we may picture the $\langle\psi|\psi\rangle>0$ half of $\mathcal{H}_{FV}$ as a set of leaves, each one being a Hilbert space, related to each other by pseudo-unitary rotations. The $\langle\psi|\psi\rangle<0$ half is similarly arrayed. The $\langle\psi|\psi\rangle=0$ subset, whose members do not belong to either half, is their common disjoint boundary.[128]

Given a general self-adjoint operator $\hat{B}:\mathcal{H}_{FV}\to\mathcal{H}_{FV}$, there must exist an operator $\hat{A}$ related to it by a pseudo-unitary transformation $\hat{A}=\hat{U}_B^{-1}\hat{B}\hat{U}_B$ for which $\hat{A}^{(p\Phi)}$ is diagonal. Note that this $\hat{A}$ is a different operator on the space, not merely a different representation of $\hat{B}$. While operator $\hat{B}$ in general mixes states from $\mathcal{H}_{FV}^{(+)}$ and $\mathcal{H}_{FV}^{(-)}$, operator $\hat{A}$ does not. (The operator $\hat{U}_B$ is not unique, since there are pseudo-unitary operators that preserve the Φ-diagonal status of $\hat{A}$.)

Each of the eigenstates of $\hat{A}$ necessarily belong to one of the spaces $\mathcal{H}_{FV}^{(\pm)}$. Let us label them $|A_i^{(\pm)}\rangle$, with $\hat{A}|A_i^{(\pm)}\rangle = a_i^{(\pm)}|A_i^{(\pm)}\rangle$. Any such operator (in the discrete case) can therefore be expressed in the form

$$\hat{A}=\sum_{\pm}\sum_i a_i^{(\pm)}\hat{P}_i^{A^{(\pm)}}\equiv\sum_i\left(a_i^{(+)}|A_i^{(+)}\rangle\langle A_i^{(+)}|-a_i^{(-)}|A_i^{(-)}\rangle\langle A_i^{(-)}|\right), \tag{A.28}$$

where the projection operators $\hat{P}_i^{A^{(\pm)}}$ satisfy the completeness relation

$$\sum_{\pm}\sum_i\hat{P}_i^{A^{(\pm)}}\equiv\sum_i\left(|A_i^{(+)}\rangle\langle A_i^{(+)}|-|A_i^{(-)}\rangle\langle A_i^{(-)}|\right)=I. \tag{A.29}$$

This expression (or its continuous analogue) applies throughout the full space of states $\mathcal{H}_{FV}$ for any Φ-diagonal $\hat{A}$.

For our *general* self-adjoint operator $\hat{B}$, we may express it in terms of projection operators in an analogous way, with the same eigenvalues $a_i^{(\pm)}$ and

$$\hat{P}_i^{B^{(\pm)}}\equiv\pm\hat{U}_B|A_i^{(\pm)}\rangle\langle A_i^{(\pm)}|\hat{U}_B^{-1}. \tag{A.30}$$

The positive and negative norm-squared eigenstates $|B_i^{(\pm)}\rangle=\hat{U}_B|A_i^{(\pm)}\rangle$ now lie in the pair of vector spaces $\hat{U}_B\mathcal{H}_{FV}^{(\pm)}$, which are leaves of the full space $\mathcal{H}_{FV}$

[127] An example is $\hat{U}|\psi^{(+)}\rangle-\alpha|\psi^{(+)}\rangle$, where $\hat{U}$ is the pseudo-unitary operator that transforms $|\psi^{(+)}\rangle$ into $\alpha|\psi^{(+)}\rangle+\beta|\psi^{(-)}\rangle$.

[128] In [64, §4B], Feshbach and Villars describe *neutral* particles using wavefunctions for which $\sigma_1\Psi^*=\pm\Psi$. This would appear to imply that $\langle\psi|\psi\rangle=0$, yet they employ a normalisation of 1.

that in general lie askew from $\mathcal{H}_{FV}^{(\pm)}$.

If we are concerned with states in $\mathcal{H}_{FV}^{(\pm)}$ and we find ourselves with an operator $\hat{B}$ that is *not* Φ-diagonal, one way of welcoming it into the theory is by adopting the operator $\hat{B}_E \equiv \frac{1}{2}(\hat{B} + \hat{Q}\hat{B}\hat{Q})$ in its stead. This operator[129] is Φ-diagonal, and it has the same matrix elements to $\hat{B}$ throughout both of the positive and negative energy spaces, *i.e.* $\langle \psi_1^{(\pm)} | \hat{B}_E \, \psi_2^{(\pm)} \rangle = \langle \psi_1^{(\pm)} | \hat{B} \, \psi_2^{(\pm)} \rangle$ for any pair of states in the same space $\mathcal{H}_{FV}^{(\pm)}$. This equivalence extends to products of $\hat{B}$ with other diagonal operators: $\langle \psi_1^{(\pm)} | \hat{A}\hat{B}_E \, \psi_2^{(\pm)} \rangle = \langle \psi_1^{(\pm)} | \hat{A}\hat{B} \, \psi_2^{(\pm)} \rangle$, but not to products with other non-diagonal operators: $\langle \psi_1^{(\pm)} | \hat{B}_E^2 \, \psi_2^{(\pm)} \rangle \neq \langle \psi_1^{(\pm)} | \hat{B}^2 \, \psi_2^{(\pm)} \rangle$.

The failure of this prescription to cope with any non-linear function of non-diagonal operators suggests that it is not an appropriate way to motivate the introduction of a position operator for this theory (as Greiner does [63, §1.12]). The derivation of a position operator for the Feshbach–Villars theory in Section 6.4.5 flows instead from the implications of the quantum postulates outlined in Section 4.

A.4 Interaction of a Feshbach–Villars particle with an electromagnetic field

A.4.1 Minimal coupling in the canonical position space

In the Feshbach–Villars theory, the interaction of a charged particle with an electromagnetic field $(\mathbf{A}(\mathbf{x}), \phi(\mathbf{x}))$ is represented in the minimum coupling prescription[130] by the replacements $\hat{H}_{FV} \to \hat{H}_{FV} - q\,\phi(\hat{\mathbf{x}}_c)$ and $\hat{\mathbf{p}} \to \hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{x}}_c)$.

It is assumed that the *canonical* position operator should be employed here, in order that the Hamiltonian remains canonically local. With regard to the discussion in Section 6.4.6, we may say that the electromagnetic field enters the theory in the context of the unitary evolution of the system rather than in the context of a measurement, and therefore acts pointwise in the canonical representation.

In the Coulomb gauge, the vector potential shares a continuous basis with

[129] This is a generalisation of what is referred to as the 'even part' of an operator in [64, §1G].

[130] This is a semi-classical representation of the field, as is usual for quantum mechanics (as opposed to quantum field theory), in which the classical field as a function of position is replaced by an identical function of position operators. The minimum coupling prescription, in common with the classical mechanics of point particles, ignores any dynamical contribution from electric or magnetic multipoles beyond order 1. In other words, only the charge q is involved in the Hamiltonian.

the momentum operator because $[\mathbf{A}(\hat{\mathbf{x}}_c), \hat{\mathbf{p}}] = i(\nabla.\mathbf{A})(\hat{\mathbf{x}}_c) = 0$.

Using $\mathbf{A}(\hat{\mathbf{x}}_c)|p^\alpha\rangle = \mathbf{A}_\mathbf{p}|p^\alpha\rangle$, we can write

$$\hat{H}^{(p)}_{FV} \;=\; (\sigma_3 + i\sigma_2)\frac{(\mathbf{p}-q\mathbf{A}_\mathbf{p})^2}{2m} + \sigma_3 m \;+\; q\,\phi(\hat{\mathbf{x}}^{(p)}_c). \tag{A.31}$$

If this Hamiltonian is diagonalised in momentum space, it becomes a convolution integral over momenta [64, §2E], which obscures the basis vectors for physical states. Let us focus on the straightforward case of a static magnetic field, with $\phi(\hat{\mathbf{x}}_c) = 0$. By replacing $\mathbf{p}$ with $\mathbf{p} - \mathbf{A}_\mathbf{p}$ in the diagonalising matrix (6.50), we obtain

$$\hat{H}^{(p\Phi)} \equiv U_{|\mathbf{p}-q\mathbf{A}_\mathbf{p}|}\hat{H}^{(p)}_{FV}U^{-1}_{|\mathbf{p}-q\mathbf{A}_\mathbf{p}|} \;=\; E_A\sigma_3\,, \tag{A.32}$$

where $E_A = E_{|\mathbf{p}-q\mathbf{A}_\mathbf{p}|} \equiv \sqrt{(\mathbf{p}-q\mathbf{A}_\mathbf{p})^2 + m^2}$. The momentum basis vectors from which pure particle or antiparticle states are constructed are now

$$|p^{(\pm)}\rangle \;\equiv\; \frac{(m \pm E_A)}{\sqrt{4mE_A}}|p^1\rangle + \frac{(m \mp E_A)}{\sqrt{4mE_A}}|p^2\rangle, \tag{A.33}$$

in contrast to (6.47).

The electromagnetic potential has shifted the space of physical states from $\mathcal{H}^{(\pm)}_{FV}$ to a different pair of spaces of the form $\hat{U}_\mathbf{A}\mathcal{H}^{(\pm)}_{FV}$. This is a pseudo-unitary rotation given in the momentum representation by $\hat{U}^{(p)}_\mathbf{A} = U^{-1}_{|\mathbf{p}-q\mathbf{A}_\mathbf{p}|}U_p$. If an external electromagnetic field is suddenly turned on, a system in a particle state will find itself in a superposition of particle and antiparticle states with respect to the new Hamiltonian. These will proceed to evolve independently, with frequencies $\pm E_A$ for each momentum mode, and the expectation values of the position operator will oscillate in response. This suggests that Zitterbewegung – apparent oscillations in position due to interference between positive and negative energy states, which are not a feature of the Newton–Wigner representation of a free particle – are nevertheless inevitable when time-dependent perturbation theory is employed.

A.4.2 The non-relativistic limit

The momentum space Feshbach–Villars equation for a charged particle in a static magnetic field, then, is

$$\left[(\sigma_3 + i\sigma_2)\frac{(\mathbf{p}-q\mathbf{A}_\mathbf{p})^2}{2m} + \sigma_3 m\right]\Psi(\mathbf{p},t) = i\frac{\partial}{\partial t}\Psi(\mathbf{p},t). \tag{A.34}$$

The solutions – cf. (6.45) – are

$$\Psi^{(\pm)}(\mathbf{p},t) = \frac{1}{\sqrt{4mE_A}} \begin{pmatrix} m \pm E_A \\ m \mp E_A \end{pmatrix} \phi^{(\pm)}(\mathbf{p})\, e^{\mp iE_A t}. \tag{A.35}$$

They have the following $\mathbf{p}^2 \ll m^2$ approximation:

$$\begin{aligned} \Psi^{(+)}(\mathbf{p},t) &\approx \begin{pmatrix} 1 \\ -\frac{(\mathbf{p}-\mathbf{A}_\mathbf{p})^2}{2m^2} \end{pmatrix} \phi^{(+)}(\mathbf{p})\, e^{-i(m+\frac{(\mathbf{p}-\mathbf{A}_\mathbf{p})^2}{2m})t} \\ \Psi^{(-)}(\mathbf{p},t) &\approx \begin{pmatrix} -\frac{(\mathbf{p}-\mathbf{A}_\mathbf{p})^2}{2m^2} \\ 1 \end{pmatrix} \phi^{(-)}(\mathbf{p})\, e^{i(m+\frac{(\mathbf{p}-\mathbf{A}_\mathbf{p})^2}{2m})t}. \end{aligned} \tag{A.36}$$

In the non-relativistic limit, both $e^{imt}\Psi^{(+)}(\mathbf{p},t)$ and $e^{imt}\hat{C}\Psi^{(-)}(\mathbf{p},t)$ become solutions of the Schrödinger equation with $\hat{H}_S = (\hat{\mathbf{p}} \pm q\mathbf{A}(\hat{\mathbf{x}}))^2/2m$.

As each solution has only one non-zero component to first order, the Feshbach–Villars Hamiltonian effectively becomes $\hat{H}_{FV} \approx (m\hat{1} + \hat{H}_S) \otimes \sigma_3$. It follows from the Schrödinger equation that $e^{imt}\hat{H}_S e^{-imt}\psi = (m\hat{1} + \hat{H}_S)\psi$, so with $\psi = e^{imt}\Psi^{(+)}$ the two dynamical equations become fully equivalent in the limit.

In addition, the scale over which the position eigenstates are delocalised is effectively made inaccessible in the theory by the requirement that $\mathbf{p}^2 \ll m^2$. The non-relativistic theory is therefore recovered for physical states in this limit, with particle and antiparticle states displaying equal masses and opposite charges.

A.5 Observables in a spinor field

The following is a calculation of the commutator of two of the general (not necessarily self-adjoint) operators from which observables may be constructed, as outlined in Section 7.1.3. For clarity, the differential operators are taken to act to the right only: the proof generalises trivially to operators acting in both directions.

Consider a pair of operators

$$\begin{aligned} \hat{A} &= \int_{\mathcal{R}_A} d^4x\; \bar{\psi}_a(x)\, \hat{A}^{(x)}_{ab}\, \psi_b(x) \\ \hat{B} &= \int_{\mathcal{R}_B} d^4x\; \bar{\psi}_a(x)\, \hat{B}^{(x)}_{ab}\, \psi_b(x). \end{aligned}$$

where $\hat{A}^{(x)}_{ab}$ and $\hat{B}^{(x)}_{ab}$ are differential operators of (finite) order N_A and N_B respectively with respect to the spacetime coordinates x. Provided the fields

are N_A- and N_B-times differentiable, we may express the effects of these differential operators as (quadruple) sums of infinitesimal spacetime translations:

$$\begin{aligned}\hat{A}^{(x)}_{ab}\, f(x^\mu) &= \lim_{\delta x\to 0}\sum_{r^\mu=0}^{N_A^4} A^r_{ab}(x^\mu) f(x^\mu + r^\mu\delta x)\\ \hat{B}^{(x)}_{ab}\, f(x^\mu) &= \lim_{\delta x\to 0}\sum_{s^\mu=0}^{N_B^4} B^s_{ab}(x^\mu) f(x^\mu + s^\mu\delta x).\end{aligned}$$

The functions $A^r_{ab}(x)$ and $B^s_{ab}(x)$ are now c-numbers – they commute with the fields and with each other. In full, the commutator of the two operators is

$$\begin{aligned}\big[\,\hat{A}\,,\,\hat{B}\,\big] &= \lim_{\delta x\to 0}\int_{\mathcal{R}_A} d^4x \int_{\mathcal{R}_B} d^4y \sum_{rs} A^r_{ab}(x)\, B^s_{cd}(y)\\ &\qquad\times\ \Big[\,\bar\psi_a(x)\,\psi_b(x+r\delta x)\ ,\ \bar\psi_c(y)\,\psi_d(y+s\delta x)\Big]. \quad \text{(A.37)}\end{aligned}$$

The commutator on the right can be expressed in terms of the field anticommutators

$$\begin{aligned}S^1_{ab}(x-y) &\equiv \{\psi_a(x),\psi_b(y)\}\\ S^2_{ab}(x-y) &\equiv \{\psi_a(x),\,\bar\psi_b(y)\},\end{aligned}$$

all of which we know to be zero when $x-y$ is spacelike. This gives

$$\begin{aligned}&\bar\psi_a(x)\Big(S^2_{bc}(x+r\delta x-y) - \bar\psi_c(y)\,\psi_b(x+r\delta x)\Big)\psi_d(y+s\delta x)\\ &\quad - \bar\psi_c(y)\Big(S^2_{da}(y+s\delta x-x) - \bar\psi_a(x)\,\psi_d(y+s\delta x)\Big)\psi_b(x+r\delta x)\\ =\ &\bar\psi_a(x)\,S^2_{bc}(x+r\delta x-y)\,\psi_d(y+s\delta x) - \bar\psi_c(y)\,S^2_{da}(y+s\delta x-x)\,\psi_b(x+r\delta x)\\ &\quad - \bar\psi_a(x)\,\bar\psi_c(y)\,S^1_{db}(y+s\delta x-x-r\delta x) + \bar S^1_{ca}(y-x)\,\psi_d(y+s\delta x)\,\psi_b(x+r\delta x).\end{aligned}$$

Restoring the differential operators,

$$\begin{aligned}\big[\,\hat{A}\,,\,\hat{B}\,\big] &= \lim_{\delta x\to 0}\int_{\mathcal{R}_A} d^4x \int_{\mathcal{R}_B} d^4y \Big(\,\bar\psi_a(x)\,\hat{A}^{(x)}_{ab}\,S^2_{bc}(x-y)\,\hat{B}^{(y)}_{cd}\,\psi_d(y)\\ &\qquad - \bar\psi_c(y)\,\hat{B}^{(y)}_{cd}\,S^2_{da}(y-x)\,\hat{A}^{(x)}_{ab}\,\psi_b(x)\\ &\qquad - \bar\psi_a(x)\,\hat{A}^{(x)}_{ab}\,\bar\psi_c(y)\,\hat{B}^{(y)}_{cd}\,S^1_{db}(y-x)\\ &\qquad + \bar S^1_{ca}(y-x)\,\hat{B}^{(y)}_{cd}\,\psi_d(y)\,\hat{A}^{(x)}_{ab}\,\psi_b(x)\Big).\end{aligned}$$

This is zero if regions $\mathcal{R}_A$ and $\mathcal{R}_B$ are entirely spacelike separated.

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