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Sources in quantum mechanics and quantum field theory

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Tiivistelmä — Referat — Abstract

The Schrödinger equation is modified. A source term, or *source*, is added, making it non-homogeneous. A time-L^2 constraint $\int_{-\infty}^{\infty} dt\, |\psi(t)|^2 \in \mathbb{R}$ and an unphysical decay are also added. The result is called the *blue equation* because "non-homogeneous Schrödinger equation with unphysical decay" is too long. The source term is a way to set the initial condition of a system, thus a source term can be used to specify a time-dependent quantum state.

The ramifications of representing quantum states with sources are explored throughout. Measurement, in the form of probability amplitudes between sources, is used to normalise the sources.

Sources are used to simplify scattering theory. The "in" and "out" states of the Lippmann-Schwinger equation are normalised. The Neumann series is used to do time-dependent perturbation theory. A new kind of S-matrix, the red operator, is defined, which works the same way, only on sources. This red operator is used to interpret sources as physical quantities of their own.

Applications of sources to quantum field theory are considered. It is shown that a source is dual to a field operator, thus sources can be contracted directly with the field operators in a correlation function. The result is the probability amplitude between sources. In this way, one can avoid the use of the LSZ reduction formula. A path integral is defined and used to demonstrate that the duality between source and field operators exists in the context of path integrals as well.

The source reveals a causal nature which was hidden or absent before. There is a causal connection from a source to the generated quantum state. A naïve definition of causality based off of this connection is considered. This definition cannot be used, however, due to special relativity. Epstein and Glaser's definition of causality, as used in causal perturbation theory, is used instead. It is proven that a *time-local* system is causal, according to this definition.

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Contents

1 Introduction

The theory of quantum mechanics is one of the most massively successful theories of all of physics. It is a model consisting of a couple dozen remarkably simple rules. See, for example Griffiths[6] and Sakurai[12] for a good treatment of quantum mechanics. The model is not exact. It fails when the particles are moving too close to the speed of light. It also fails when light frequencies above that of gamma rays are involved. But it still explains all of the hundreds of rules of chemistry, down to the last rule, along with the endless litany of exceptions to those rules. It does all of this, while still reproducing the laws of classical mechanics. That is to say, it, along with Newtonian gravity, explains almost everything that happens on Earth's surface on a regular basis.

The model's inexact nature is not actually a problem for what the model is designed to describe, i.e. particle speeds well below the speed of light, and light frequencies well below gamma rays. It is only a model after all. It does not need to be exact. It *does* need to be mathematically well-defined, internally consistent, and usable to make meaningful predictions. Measurement and some other open issues notwithstanding, most of the model actually is well-defined and internally consistent. Most of the model, the Schrödinger equation, is just a linear partial differential equation with an initial condition.

The problems with the model are more practical in nature. Though the equations are simple to write and to understand at a mathematical level, they are impossible to solve at the scale of more than a hundred particles, even with a supercomputer. Scattering theory and statistical approximations are needed in order to, for example, predict heat transfer coefficients, viscosities, and rates of reaction. It is here where problems arise. Some intermediate steps between quantum and statistical mechanics are unknown. Along the way, some rules of quantum mechanics are ignored. In particular, it is common practice to use unnormalisable states in the Lippmann-Schwinger equation to derive differential cross sections to be used in the Boltzmann equation, even though one of the rules of quantum mechanics is that quantum states must be normalised. It is also in this transition from quantum to statistical that measurement happens, so solving these problems may solve outstanding issues with measurement, as well.

Quantum mechanics is a good model, but what about a complete model? If the objective is the more philosophical one of discovering a complete mathematical description of the

universe, of course special relativity must be considered. This means quantum field theory, the theory that combines special relativity with quantum mechanics. This theory is a mess. The standard mathematics are ill-defined and there is no wide agreement about even many basic ideas, like the path integral. Dimensional regularisation asserts the existence of vector spaces with a complex number of dimensions.[11] Approximations use series expansions which usually appear to converge after the first few terms, but then diverge in the higher order terms. Epstein and Glaser found better mathematics for describing the theory[5, 13], called causal perturbation theory, but the whole method is very difficult to read and understand.

There are other aesthetic issues. Some parts of the theory, like the Lagrangians, the Feynman propagators, and correlation functions, are Lorentz-invariant, with simple, straightforward Lorentz transforms, as one would expect. Other parts, like the S-matrix and the LSZ reduction formula, have an implied reference frame baked-in, massively complicating Lorentz transforms and scarring an otherwise beautiful framework. Causal perturbation theory relies heavily on the S-matrix, so this may be why it is so difficult to read.

A new technique has been found that may help solve some of these outstanding problems in quantum mechanics and quantum field theory. It is essentially a new method of setting the initial conditions of the Schrödinger equation. I will use an analogy from Maxwell's equations, which are also partial differential equations. The initial conditions of the electromagnetic field in a vacuum can be set by specifying the electric and magnetic fields over all space at a certain point in time. This is how it is normally done for the Schrödinger equation as well. In Maxwell's equations, though, there is another way to set the initial conditions. The system starts with an electric and magnetic field that is and has always been zero. Then, a pulse of charge and current happens over a finite time. That pulse then generates the desired electromagnetic field. Any electromagnetic field can be created with the right pulse. In mathematics, assuming the Lorentz gauge,

$$-\partial_\theta \partial^\theta A^\alpha = \mu_0 J^\alpha \tag{1.0.1}$$

In the language of partial differential equations, this equation with $J^\alpha = 0$ is a homogeneous differential equation. With the non-zero pulse, J^α, it is an *non-homogeneous* differential equation, and J^α is called the *source term*, or *source*.

The Schrödinger equation is a homogeneous differential equation. A source can also be added to it, making it an non-homogeneous Schrödinger equation. The consequences are very interesting and useful. Exploring these consequences and demonstrating the utility is the primary objective of this thesis.

Sources provide a method of removing unnormalisable states from the Lippmann-Schwinger equation, clarifying the transitional theory between quantum mechanics and statistical mechanics. It also provides an alternative to the S-matrix and the LSZ reduction formula, tidying up quantum field theory generally, and potentially making the method of causal perturbation theory more viable.

Sources in the Schrödinger equation also reveal interesting causal properties. In Maxwell's equations, there is a causal relationship between the charge-current pulse and the resulting radiation. The same thing happens in the Schrödinger equation. Causal perturbation theory, unsurprisingly, hinges on the concept of causality. The definition of causality used in causal perturbation theory relies on the S-matrix. The S-matrix in this definition can be replaced, though, with the source-based equivalent.

Other examples of a non-homogeneous Schrödinger equation have been found from the mathematics literature.[4, 1, 7] They only ever use positive time, though, which is unsuitable for real physical problems, and is especially unsuitable for special relativity. They also never offer a physical interpretation for their source term, or explore its physical ramifications.

There is an article[3], which does talk about the physics of these sources. These sources are used as models for particle creation and annihilation due to strong radiation fields[10, 2], and alpha decay[9, 8]. This article also finds an equivalent to the source derived in section 3.3. This source is the result of the interaction of an incident quantum state with a scattering potential.

In quantum field theory, there is already a concept of a source. An action can have a source term:[14]

$$S(\varphi) = S_0(\varphi) + \int_{x\in\mathbb{R}^{1,3}} \mathrm{d}^4x\, J(x)\varphi(x) \tag{1.0.2}$$

This source is added to the action and used to generate a partition function, which is used to generate correlation functions. The sources discussed in this thesis, however, are added to the Schrödinger equation, and are used to set the initial conditions of the time-dependent quantum state. They are not the same sources.

1.1 Standards

The constant τ is used instead of 2π.

$$\tau = \frac{\text{circumference}}{\text{radius}} \approx 6.28319 \tag{1.1.1}$$

Natural units are used, eliminating seconds and kilograms, leaving only metres.

$$\hbar = c = 1 \tag{1.1.2}$$

This time Fourier transform is used:

$$(\mathcal{F}\psi)(\omega) = \tilde{\psi}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, e^{i\omega t}\psi(t) \tag{1.1.3}$$

$$(\mathcal{F}^{-1}\tilde{\psi})(t) = \psi(t) = \frac{1}{\tau}\int_{-\infty}^{\infty} \mathrm{d}\omega\, e^{-i\omega t}\tilde{\psi}(\omega) \tag{1.1.4}$$

This space Fourier transform is used:

$$\varphi_k(k) = \int_{r\in\mathbb{R}^3} \mathrm{d}^3 r\, e^{-ik^T r}\varphi(r) \tag{1.1.5}$$

$$\varphi(r) = \frac{1}{\tau^3}\int_{k\in\mathbb{R}^3} \mathrm{d}^3 k\, e^{ik^T r}\varphi_k(k) \tag{1.1.6}$$

The $-,+,+,+$ metric signature is used for spacetime.

2 The blue equation

Consider the following quantum system:

The state space, $\mathcal{U}$, is a Hilbert space, with inner product $\beta^\dagger\alpha \in \mathbb{C}$, where $\alpha, \beta \in \mathcal{U}$. On its own, $\beta^\dagger \in \mathcal{U}^*$ is the mapping through the inner product of a vector to its corresponding covector in the dual space of $\mathcal{U}$. A quantum state, $\varphi \in \mathcal{U}, |\varphi|^2 = 1$, is a normalised vector in the state space. A time-dependent quantum state, $\Psi : \mathbb{R} \to \mathcal{U}$, is not a quantum state, but a function whose input is time, and whose output is a quantum state. A time-dependent quantum state evolves according to the Schrödinger equation,

$$\dot{\Psi}(t) = -iH_0\Psi(t), \text{ where} \tag{2.0.1}$$

$$\Psi(t_0)^\dagger\Psi(t_0) = 1 \tag{2.0.2}$$

H_0, the hamiltonian, is a *bounded, self-adjoint* linear operator. Ψ, of course, must be differentiable.

The quantum system is generic, though mathematically simplified. It is generic in that $\mathcal{U}$ could contain the states of two-state systems like qubits, systems of point particles, photons trapped in a cavity, the tensor product of any of these, etc. It is simplified because even in simple systems of point particles, H_0 is unbounded. The state of a system of point particles is representable, but not its hamiltonian. Dealing with unbounded operators would lead to technical complications, though, and would only distract from this thesis's focus. Note also that H_0 has been defined to be time-independent.

Now, we will modify this system. First, we will consider time-dependent quantum states not as functions, but as vectors in the larger vector space of functions $\mathbb{R} \to \mathcal{U}$. We will also only consider a subspace, $\mathcal{V}$, of this space:

$$\psi \in \mathcal{V} \iff \psi : \mathbb{R} \to \mathcal{U}, \tag{2.0.3}$$

$$\psi \text{ differentiable, and} \tag{2.0.4}$$

$$\psi^{\mathrm{B}}\psi \in \mathbb{R}, \text{ where} \tag{2.0.5}$$

$$u^{\mathrm{B}}v = \int_{-\infty}^{\infty} \mathrm{d}t\, u(t)^\dagger v(t) \tag{2.0.6}$$

An inner product on $\mathcal{V}$ is defined using the notation $u^{\mathrm{B}}v$ to make it completely clear that there is an extra time integral. Note that condition (2.0.5) means all ψ in $\mathcal{V}$ are

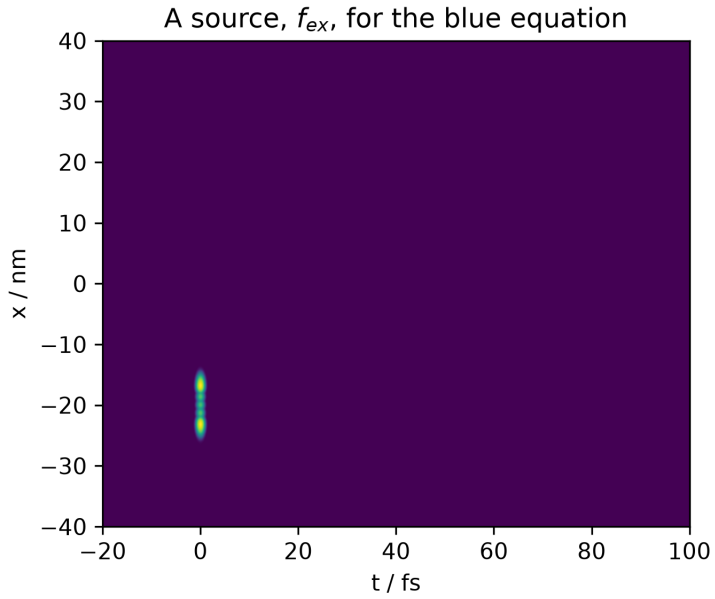

Figure 2.1: The modulus squared of an example source, $|f_{ex}(t,x)|^2$, is plotted in false colour, on a log scale.

finite in time. The Schrödinger equation preserves the norm of $\Psi(t)$ for all t, causing the time integral in the new inner product to diverge. This actually excludes *all* solutions to the Schrödinger equation. The states in this new space, $\mathcal{V}$, are so different from time-dependent quantum states that they will be called *blue states*. A blue state is given the symbol ψ insted of Ψ.

Now, we are ready to define the *blue equation*:

$$(\varepsilon + \partial_t + iH)\psi = f, \text{ where} \tag{2.0.7}$$

$$\varepsilon > 0 \tag{2.0.8}$$

$$(H\psi)(t) = H_0\psi(t) \tag{2.0.9}$$

$$\psi, f \in \mathcal{V} \tag{2.0.10}$$

This new f is called the *source term*, or just the source. (The H is there to make it completely clear that H operates on $\mathcal{V}$ vectors and H_0 operates on $\mathcal{U}$ vectors, that is H is the inclusion of H_0 into the set of linear operators on $\mathcal{V}$.) The idea behind this equation is that at $t = -\infty$, ψ and f start out at 0, then at some point, there is a pulse from f, causing a response in ψ. Then, f drops back down to zero, where it stays from then on, and ψ slowly decays at a rate determined by ε.

That is what is supposed to happen. There is also a possibility for ψ to grow exponentially

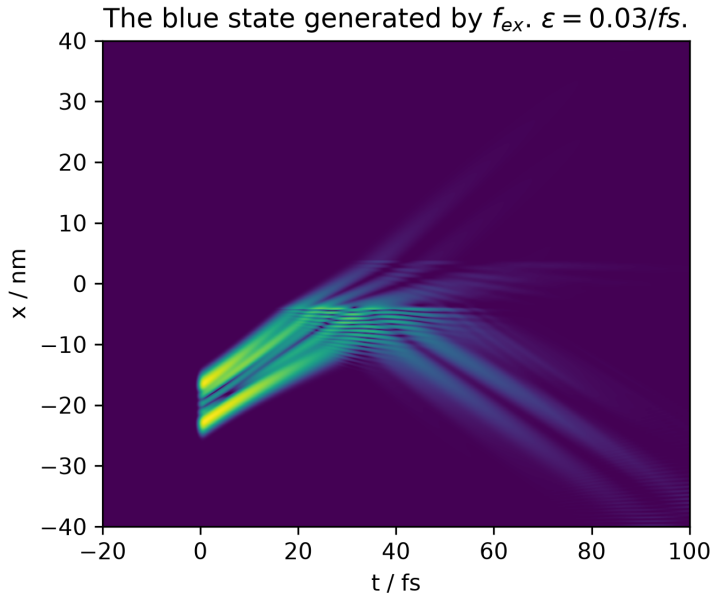

Figure 2.2: The modulus squared of the blue state generated by the example source, $|\psi(t,x)|^2$, is plotted in false colour, on a log scale. The blue state is zero before the source, then gets a kick from the source. The blue state then collides with the barrier at $[-4\text{ nm}, 4\text{ nm}]$. There is decay, making the whole blue state L^2 in space and time.

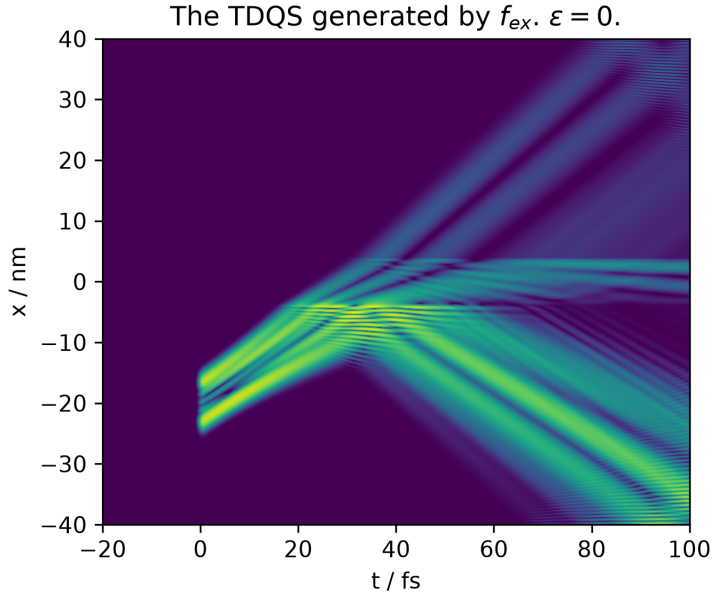

Figure 2.3: This is the same simulation as figure 2.2, but without decay. This makes the result a physical, time-dependent quantum state (TDQS), but only after the source's pulse is finished. It is L^2 in space, but not in time. The simulation has infinite-potential boundary conditions at $x = \pm 40$ nm, so that is why the state can be seen bouncing off of the boundaries.

without bound as $t \to -\infty$. This is why ψ must be L^2 in time (2.0.5)—to explicitly forbid this. This condition also allows for a time Fourier transform.

The $\varepsilon > 0$ constraint forces ψ to propagate *forward* in time from f. If $\varepsilon < 0$, then ψ propagates backward instead.

The blue equation will be illustrated with the following example:

$$\mathcal{U} = L^2(\mathbb{R} \to \mathbb{C}) \tag{2.0.11}$$

$$H_0 = -\frac{1}{2m}\partial_x^2 + V, \text{ where} \tag{2.0.12}$$

$$(V\varphi)(x) = V_0(x)\psi(x) \text{ and} \tag{2.0.13}$$

$$V_0(x) = \begin{cases} V_h & x \in [-x_0, x_0] \\ 0 \end{cases} \tag{2.0.14}$$

This describes a particle with mass m moving in one dimension, scattering off of a barrier at the origin. The barrier has a width $2x_0$ and a height $V_h > 0$. Even this system has an unbounded H_0, but everything still seems to work fine. This is demonstrated with a simple simulation of a source generating a blue state. The results are shown in Figures 2.1, 2.2, and 2.3.

As $\varepsilon \to 0$, and after the source goes to 0, the original Schrödinger equation is recovered. In this way, in the physical $\varepsilon \to 0$ limit, the source term, f, is used to set the initial condition of the time-dependent quantum state, Ψ. In fact, the left hand side of the blue equation is invertible, thus the blue state ψ is actually uniquely determined by f.

2.0.1 Proof of invertibility of the blue equation

To prove the left hand side of the blue equation (2.0.7) is invertible, a time Fourier transform of both sides can be used:

$$(\varepsilon - i\omega + iH_0)\tilde{\psi}(\omega) = \tilde{f}(\omega) \tag{2.0.15}$$

$$(H_0 - \omega - i\varepsilon)\tilde{\psi}(\omega) = -i\tilde{f}(\omega) \tag{2.0.16}$$

From spectral theory, an operator's spectrum is defined in terms of invertibility:

$$\sigma(A) = \{\lambda \in \mathbb{C} | (A - \lambda) \text{ is not invertible}\} \tag{2.0.17}$$

Also from spectral theory, a bounded self-adjoint operator, A, has a real spectrum.

$$A \text{ is bounded and self-adjoint } \implies \sigma(A) \subset \mathbb{R} \tag{2.0.18}$$

These two conditions can be combined. Suppose A is bounded and self-adjoint. Then,

$$(A - \lambda) \text{ is not invertible } \implies \lambda \in \mathbb{R} \tag{2.0.19}$$

This is equivalent to its contrapositive:

$$\lambda \notin \mathbb{R} \implies (A - \lambda) \text{ is invertible} \tag{2.0.20}$$

In our case, $A = H_0$ and $\lambda = \omega - i\varepsilon$. ω is real and $\varepsilon > 0$, therefore $\lambda \notin \mathbb{R}$. Thus $(H_0 - \omega - i\varepsilon)$ is invertible! Since the Fourier transform is also invertible, the same operator in the time domain, $(\varepsilon + \partial_t + iH)$, is also invertible. Call that operator's inverse the *propagator* and give it a symbol:

$$B = (\varepsilon + \partial_t + iH)^{-1} \tag{2.0.21}$$

The propagator can be expressed in terms of a time convolution:

$$\psi = Bf = G * f, \text{ where} \tag{2.0.22}$$

$$G(t) = \Theta(t) e^{-\varepsilon t} e^{-iH_0 t} \tag{2.0.23}$$

The $*$ operator has been extended to work on operator-valued and vector-valued functions of t, as follows:

$$(G * f)(t) = \int_{-\infty}^{\infty} \mathrm{d}u \, G(t - u) f(u) \tag{2.0.24}$$

In other words, $G * f$ is a convolution in time and an operator evaluation in $\mathcal{U}$.

Θ is the Heaviside function:

$$\Theta(t) = \begin{cases} 1 & t \geq 0 \\ 0 & \end{cases} \tag{2.0.25}$$

The Heaviside function is never evaluated at $t = 0$, so it doesn't actually matter what value is assigned there.

Note that the propagation kernel, G, is causal, that is f may affect the future of ψ, but not its past. If $f(t) = \delta(t)\varphi_0$, where $\varphi_0 \in \mathcal{U}$, then the original Schrödinger equation with initial condition φ_0 is almost recovered, as $\varepsilon \to 0$. In the Schrödinger equation, ψ propagates backward in time with unit norm, as well as forward in time, but in the blue equation, $\psi(t) = 0$ when $t < 0$.

It has already been proven that B is invertible, and therefore unique. So to prove that equation (2.0.22) yields the propagator, it suffices to prove that $\psi = G * f$ solves the blue equation. Start by expanding ψ:

$$\psi = G * f \tag{2.0.26}$$

$$\psi(t) = \int_{-\infty}^{\infty} \mathrm{d}u\, G(t-u) f(u) \tag{2.0.27}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}u\, \Theta(t-u) e^{(-\varepsilon - iH_0)(t-u)} f(u) \tag{2.0.28}$$

$$= e^{(-\varepsilon - iH_0)t} \int_{-\infty}^{t} \mathrm{d}u\, e^{(\varepsilon + iH_0)u} f(u) \tag{2.0.29}$$

(Using the boundedness of H_0 is the easy way to prove that the integral and operator exponentials can be reordered.) Now, differentiate with respect to t:

$$\partial_t \psi(t) = (-\varepsilon - iH_0)\psi(t) + e^{(-\varepsilon - iH_0)t} e^{(\varepsilon + iH_0)t} f(t) \tag{2.0.30}$$

$$\partial_t \psi(t) = (-\varepsilon - iH_0)\psi(t) + f(t) \tag{2.0.31}$$

$$(\varepsilon + \partial_t + iH_0)\psi(t) = f(t) \tag{2.0.32}$$

Thus $\psi = Bf$ solves the blue equation and B is indeed the propagator.

2.0.2 Mapping from a source to a time-dependent quantum state

As was mentioned before, in the $\varepsilon \to 0$ limit, the source can be used to specify the initial condition of a time-dependent quantum state. This means a source completely specifies a time-dependent quantum state. Just remember that t must be after the source is finished.

$$t > \text{supp } f \implies \Psi(t) = \lim_{\varepsilon \to 0} (B_\varepsilon f)(t) \tag{2.0.33}$$

Technically, the source needs compact support, but in practice, this works as long as t is "high enough". The integral $\int_t^\infty \mathrm{d}u\, |f(u)|^2$ must eventually approach zero as $t \to \infty$ anyway, since f is L^2 in time.

The $\varepsilon \to 0$ limit will be considered throughout this section, so define a new propagator with this limit already taken:

$$B_0 = \lim_{\varepsilon \to 0} B_\varepsilon \tag{2.0.34}$$

$$G_0 = \lim_{\varepsilon \to 0} G_\varepsilon \tag{2.0.35}$$

So, under these constraints, what is Ψ?

$$\Psi = B_0 f \tag{2.0.36}$$
$$= G_0 * f \tag{2.0.37}$$
$$\Psi(t) = \int_{-\infty}^{\infty} \mathrm{d}u\, G_0(t-u) f(u) \tag{2.0.38}$$
$$= \int_{-\infty}^{t} \mathrm{d}u\, e^{-iH(t-u)} f(u) \tag{2.0.39}$$

It is here where we can use $t > \text{supp } f$ to simplify things. $f(u) = 0$ for all u higher than t, so the upper limit of that integral might as well just go to infinity. The result does not change. Let's do that.

$$\Psi(t) = \int_{-\infty}^{\infty} \mathrm{d}u\, e^{-iH(t-u)} f(u) \tag{2.0.40}$$
$$\Psi(t) = U * f, \text{ where} \tag{2.0.41}$$
$$U(t) = e^{-iHt} \tag{2.0.42}$$

Effectively, the Heaviside in the kernel is gone.

Even though there is a bijection between sources and blue states, there are many equivalent sources producing the same time-dependent quantum state. To see this, imagine two blue states equal to each other after a certain time t_0, but that disagree before t_0. Maybe one was created by an earlier source than the other, for example. After t_0, and as $\varepsilon \to 0$, they represent the same physical state.

With this mapping established, in general, what would happen if we were to use sources instead of quantum states or time-dependent quantum states to describe quantum systems?

2.1 Probability, measurement, and normalisation

When sources instead of quantum states are used to specify quantum systems, what are the implications to measurement? To simplify matters, we will adopt the not-too-controversial stance that all measurement can be expressed using probability amplitudes between quantum states. Then, all we have to do is examine the behaviour of probability amplitudes.

So, what is the probability amplitude between two sources, f_0 and f_1? f_0 is the state being measured and f_1 is the measurement. Each generates blue states ψ_0 and ψ_1. Since these

are physical results, let $\varepsilon \to 0$, removing the unphysical decay. What is the probability amplitude, π, between the states? Starting from the usual formula,

$$\pi = \Psi_1(t)^\dagger \Psi_0(t) \tag{2.1.1}$$

This is for time-dependent quantum states, so require that $t >$ supp $f_0 \cup$ supp f_1, and use equation (2.0.41).

$$\pi = (U * f_1)(t)^\dagger (U * f_0)(t) \tag{2.1.2}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}u \int_{-\infty}^{\infty} \mathrm{d}v \, (U(t-u) f_1(u))^\dagger U(t-v) f_0(v) \tag{2.1.3}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}u \int_{-\infty}^{\infty} \mathrm{d}v \, f_1(u)^\dagger U(u-t) U(t-v) f_0(v) \tag{2.1.4}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}u \int_{-\infty}^{\infty} \mathrm{d}v \, f_1(u)^\dagger U(u-v) f_0(v) \tag{2.1.5}$$

$$\pi = f_1^{\mathrm{B}} U * f_0 \tag{2.1.6}$$

A relatively simple formula. Since $\pi = 1$ when $f_1 = f_0$, this also defines the normalisation for sources. Inconveniently, the source normalisation depends on the hamiltonian. At least if $V = 0$ where the source is located, the normalisation only depends on kinetic energy, which depends a lot less on the problem than the potential energy.

What would happen, though, if that $U*$ were replaced with B? The Heaviside comes back, causing π to vanish when f_1 is before f_0. In other words, the time of the occurrance of a source would actually matter, and a transition from a source in the present to a source in the past would be impossible. This sounds right, but only if particles are actually being created and destroyed.

Also, if B is used instead of $U*$, π could be expressed as $\pi = f_1^{\mathrm{B}} \psi_0$. This offers the first hint that blue states may be dual to sources.

3 Scattering

The consequences of using sources instead of quantum states in scattering theory get very interesting. The theory is easier to derive and reason about, and unnormalisable states are no longer necessary. We'll start by reproducing the time-independent theory. That means the Lippmann-Schwinger equation.

3.1 The Lippmann-Schwinger equation

Suppose $H_0 = T + V$, where T and V are bounded and self-adjoint. T and V can be anything, but the idea is that T is simple, but $T + V$ is complicated. The exact meanings of "simple" and "complicated" will soon be made clear. Often, T is the kinetic energy and V is the potential energy, hence the choice of symbols. H_0 was already defined to be time-independent, so T and V must also be time-independent. Using the example from the previous section, $T = -\frac{1}{2m}\partial_x^2$ and V is the same.

This is the Lippmann-Schwinger equation:

$$\varphi_{\text{out}}(\omega) = \varphi_{\text{in}}(\omega) + (\omega - T + i\varepsilon)^{-1} V \varphi_{\text{out}}(\omega) \tag{3.1.1}$$

Given $T\varphi_{\text{in}}(\omega) = \omega\varphi_{\text{in}}(\omega)$, $\varphi_{\text{out}}(\omega)$ solves the time-independent Schrödinger equation $H_0\varphi_{\text{out}}(\omega) = \omega\varphi_{\text{out}}(\omega)$ in the limit as $\varepsilon \to 0$. Typically, when T is some kind of kinetic energy, $\varphi_{\text{in}}(\omega)$ is a plane wave. In the example,

$$\varphi_{\text{in}}(\omega) = e^{ik_0(\omega)x}, \text{ where} \tag{3.1.2}$$

$$k_0(\omega) = \sqrt{2m\omega} \tag{3.1.3}$$

But if H_0 has a continuous spectrum, which it usually does for scattering problems, then $\varphi_{\text{in}}(\omega)$ and $\varphi_{\text{out}}(\omega)$ both are unnormalisable, that is they have infinite norm. Indeed, plane waves have infinite norm. In other words, they are not quantum states—not physically possible. But these states can still be used in scattering theory to calculate differential cross sections. How is this possible?

The blue equation will now be used to explain the Lippmann-Schwinger equation. Start from the time Fourier transform, equation (2.0.15).

$$(\varepsilon - i\omega + iT + iV)\tilde{\psi}(\omega) = \tilde{f}(\omega) \tag{3.1.4}$$

It was said that T is simple and $T+V$ is complicated. Specifically, suppose that $(\varepsilon - i\omega + iT + iV)^{-1}$ is difficult, but $(\varepsilon - i\omega + iT)^{-1}$ is easy, and apply just $(\varepsilon - i\omega + iT)^{-1}$ to both sides.

$$(1 + i(\varepsilon - i\omega + iT)^{-1}V)\tilde{\psi}(\omega) = (\varepsilon - i\omega + iT)^{-1}\tilde{f}(\omega) \tag{3.1.5}$$

Now, rearrange.

$$\tilde{\psi}(\omega) = (\varepsilon - i\omega + iT)^{-1}\tilde{f}(\omega) - i(\varepsilon - i\omega + iT)^{-1}V\tilde{\psi}(\omega) \tag{3.1.6}$$

This fits the form of the Lippmann-Schwinger equation! Now, we can see that

$$\varphi_{\text{in}}(\omega) = (\varepsilon - i\omega + iT)^{-1}\tilde{f}(\omega) \text{ and} \tag{3.1.7}$$

$$\varphi_{\text{out}}(\omega) = \tilde{\psi}(\omega) \tag{3.1.8}$$

That is what the states of the Lippmann-Schwinger equation actually are! φ_{out} is just the time Fourier transform of the blue state ψ. After an inverse Fourier transform, one can see that φ_{in} is the time Fourier transform of another blue state, with the same source as φ_{out}, but with $H_0 = T$.

One can see that the correct φs are actually normalisable, since ψ have finite norm over all t, and the time Fourier transform preserves norm. They are only unnormalisable as $\varepsilon \to 0$. Such φ are unnormalisable because they are not single quantum states, but an integration over the entire history of a blue state. This also means that since time Fourier transforms are involved, regular time-dependent quantum states cannot be used at all.

3.2 The Neumann series

The Lippmann-Schwinger equation assumes the potential is time-independent. Sources can be used, though, to develop a time-dependent theory of scattering. Return to the H defined on all of $\mathcal{V}$, and suppose H has the form

$$H = T + V, \text{ where} \tag{3.2.1}$$

$$(T\psi)(t) = T_0\psi(t) \text{ and} \tag{3.2.2}$$

$$T_0, V \text{ self-adjoint} \tag{3.2.3}$$

In other words, T is time-independent, but V can be any operator on the larger space $\mathcal{V}$. This includes time-dependent operators. In this case, there is a very nice way of systematically approximating ψ given a particular f, similar to the Dyson series.

To start, substitute this H into into blue equation (2.0.7):

$$(\varepsilon + \partial_t + iT + iV)\psi = f \tag{3.2.4}$$

We do not know how to invert the entire left-hand side, but since T is time-independent, we can still invert $\varepsilon + \partial_t + iT$. So, redefine the propagator (2.0.22) to include just T:

$$B = (\varepsilon + \partial_t + iT)^{-1} \tag{3.2.5}$$

Then, apply B to both sides of the blue equation:

$$(1 + iBV)\psi = Bf \tag{3.2.6}$$

This is similar to the derivation (3.1.5) of the Lippmann-Schwinger equation from the blue equation, only there is no time Fourier transform, so it allows for time-dependent V. Now, we can use a standard result from functional analysis called the Neumann series. It turns out, *at least sometimes*,

$$(1 - A)^{-1} = \sum_{n=0}^{\infty} A^n \tag{3.2.7}$$

In our case, $A = -iBV$:

$$\psi = (1 + iBV)^{-1} Bf \tag{3.2.8}$$

$$= \sum_{n=0}^{\infty} (-iBV)^n Bf \tag{3.2.9}$$

$$= Bf - iBVBf - BVBVBf + iBVBVBVBf + \dots \tag{3.2.10}$$

In general, the Neumann series converges if $\|A\| < 1$. In our case, $\|A\| = \|-iBV\| \leq \|B\| \, \|V\|$. It is easily proven that $\|B\| \leq \frac{1}{\varepsilon}$. Thus our series converges if

$$\frac{\|V\|}{\varepsilon} < 1 \tag{3.2.11}$$

So, *the Neumann series can always be made to converge, given a high enough* ε. But ε is supposed to approach zero in order to recover physical results, so this upper bound is not that useful physically. Here, more work or more assumptions are needed to prove convergence for the $\varepsilon \to 0$ case.

There *are* conditions which help with this, though. If V is *time-local* (5.1.3) and f is compactly supported, then the series always converges pointwise at a particular time, t_1, but it does not necessarily converge uniformly over all t. Intuitively, that means, basically,

that the first terms of the series create an erroneous lump in the approximation of the blue state ψ. When another term is added to the series, the lump is pushed into the future, but it also could get bigger. This is fine if you only need the series to converge before a certain final time, t_1. Just add as many terms as you need to, to push the lump past t_1. But if the series needs to converge for *all* time, you may be in trouble. See Subsection 3.2.1 for details about this convergence in the $\varepsilon \to 0$ case. See Chapter 5 for more about time-locality.

The difference between this Neumann series and the Dyson series is that the Neumann series operates on a source instead of an initial quantum state and the Neumann series uses a generic V which is not necessarily time-local. When V is time-local, $f(t) = \delta(t)\varphi_0$, and φ_0 is the initial quantum state, it is exactly the Dyson series. If V is time-independent, then its time Fourier transform results in the Born series.

This series has a straight forward, and rather interesting physical interpretation. Since B takes a source and turns it into a blue state, every expression that goes into B must be some kind of source. This includes VBf, $VBVBf$, $VBVBVBf$, etc. By the same logic, V must be accepting blue states as inputs and returning sources, which agrees with the logic of the blue equation.

Consider the example system (2.0.12) again, but this time, with a general time-dependent scatterer V:

$$(V\psi)(t,x) = V_0(t,x)\psi(t,x) \tag{3.2.12}$$

Furthermore, suppose that V_0 has compact support, that is, it is localised to a certain compact region of spacetime, $\operatorname{supp} V_0 \subset \mathbb{R}^2$. The effect of V is to filter ψ to just $\operatorname{supp} V_0$. You'll notice that V is always the last operator to be applied to each of the sources generated by the Neumann series. This means that all of these new sources are localised to V_0's support!

Physically, every B is a free propagation, and every V is a "bounce" off of the scatterer. Thus each term follows an alternating move, scatter pattern. If a certain process requires two scatters—maybe the incoming particle scatters off of one V, then scatters off of another V—then at least the $BVBVBf$ term is required to approximate the process.

Choice of the initial source, f, is somewhat arbitrary, since many sources represent the same time-dependent quantum state. The sources, $(VB)^n f$, generated by the Neumann series, however, happened on their own due to the physical constraints of the problem. These Neumann sources all create states that begin at the scatterer, V. This is the first

hint that these sources have some kind of physical interpretation, and it might actually matter when the source occurs, even when an earlier source and a later source specify the same time-dependent quantum state.

3.2.1 Convergence when $\varepsilon \to 0$

Suppose V is time-local (5.1.3) and f has compact support. Set ε to 0, so that B becomes B_0 (2.0.34). Rearrange the Neumann series, applying the extra B_0 at the end, instead of at the beginning:

$$\psi = \sum_{n=0}^{\infty} (-i)^n B_0 (V B_0)^n f \tag{3.2.13}$$

Each $(VB_0)^n f$ in the sum is a source. Give each source a label, and observe the following recursion relation:

$$f_0 = f \tag{3.2.14}$$

$$\forall n > 0, f_n = V B_0 f_{n-1} \tag{3.2.15}$$

That makes the series

$$\psi = \sum_{n=0}^{\infty} (-i)^n B_0 f_n \tag{3.2.16}$$

Since V is time-local, $(V\psi)(t) = V_0(t)\psi(t)$. Using this and evaluating both sides of equation (3.2.15) at t,

$$f_n(t) = V_0(t)(B_0 f_{n-1})(t) \tag{3.2.17}$$

Now, use (2.0.39) on $B_0 f_{n-1}$.

$$f_n(t) = V_0(t) \int_{-\infty}^{t} \mathrm{d}u \, e^{-iT_0 u} f_{n-1}(u) \tag{3.2.18}$$

Take the $\mathcal{U}$-norm of both sides. Then, use $\|V_0(t)\|_{\mathcal{U}} \leq \|V\|_{\mathcal{V}}$, $\left\| \int_a^b \mathrm{d}u \, v(u) \right\| \leq \int_a^b \mathrm{d}u \, \|v(u)\|$, and the unitarity of $e^{-iT_0 u}$ to get the following inequality:

$$\|f_n(t)\|_{\mathcal{U}} \leq \|V\|_{\mathcal{V}} \int_{-\infty}^{t} \mathrm{d}u \, \|f_{n-1}(u)\|_{\mathcal{U}} \tag{3.2.19}$$

As a base case, start with $n = 1$ instead of $n = 0$. This simplifies the bound.

$$\|f_1(t)\|_{\mathcal{U}} \leq \|V\|_{\mathcal{V}} \int_{-\infty}^{t} \mathrm{d}u \, \|f(u)\|_{\mathcal{U}} \tag{3.2.20}$$

Suppose $[t_0, t_1]$ is the smallest interval containing the support of f. When $t > t_1$,

$$\|f_1(t)\|_{\mathcal{U}} \leq \|V\|_{\mathcal{V}} \int_{t_0}^{t_1} \mathrm{d}u \; \|f(u)\|_{\mathcal{U}} \tag{3.2.21}$$

Using the Cauchy-Schwarz inequality,

$$\|f_1(t)\|_{\mathcal{U}} \leq \|V\|_{\mathcal{V}} \sqrt{t_1 - t_0} \, \|f\|_{\mathcal{V}} \tag{3.2.22}$$

That's for $t > t_1$. For $t < t_0$, the integral on the right hand side of (3.2.20) is just zero. What about when $t \in [t_0, t_1]$? Since the integrand in that same integral is always positive, it is bounded by the final value at $t = t_1$. Thus the left hand side is bounded by a multiple of the Heaviside function:

$$\|f_1(t)\|_{\mathcal{U}} \leq \|V\|_{\mathcal{V}} \sqrt{t_1 - t_0} \, \|f\|_{\mathcal{V}} \, \Theta(t - t_0) \tag{3.2.23}$$

Substituting this f_1 bound back into equation (3.2.19), the Heaviside just integrates, forming a ramp function:

$$\|f_2(t)\|_{\mathcal{U}} \leq \|V\|_{\mathcal{V}}^2 \sqrt{t_1 - t_0} \, \|f\|_{\mathcal{V}} \, \Theta(t - t_0)(t - t_0) \tag{3.2.24}$$

Repeating this process, one obtains the bound for the nth source:

$$\|f_n(t)\|_{\mathcal{U}} \leq \|V\|_{\mathcal{V}}^n \sqrt{t_1 - t_0} \, \|f\|_{\mathcal{V}} \, \Theta(t - t_0) \frac{(t - t_0)^{n-1}}{(n-1)!} \tag{3.2.25}$$

What happens when each source is propagated by the final B_0? Handling the special case $B_0 f_0 = B_0 f$ the same way as with f_1,

$$\|(B_0 f_0)(t)\|_{\mathcal{U}} \leq \sqrt{t_1 - t_0} \, \|f\|_{\mathcal{V}} \, \Theta(t - t_0) \tag{3.2.26}$$

The $n \geq 1$ cases are also handled using the same arguments as before:

$$\|(B_0 f_n)(t)\|_{\mathcal{U}} \leq \int_{t_0}^{t} \mathrm{d}u \; \|f_n(u)\|_{\mathcal{U}} \quad (n \geq 1) \tag{3.2.27}$$

Substituting (3.2.25) and integrating one last time,

$$\|(B_0 f_n)(t)\|_{\mathcal{U}} \leq \|V\|_{\mathcal{V}}^n \sqrt{t_1 - t_0} \, \|f\|_{\mathcal{V}} \, \Theta(t - t_0) \frac{(t - t_0)^n}{n!} \quad (n \geq 1) \tag{3.2.28}$$

Finally, $n = 0$ and $n \geq 1$ are united into the same formula:

$$\|(B_0 f_n)(t)\|_{\mathcal{U}} \leq \|V\|_{\mathcal{V}}^n \sqrt{t_1 - t_0} \, \|f\|_{\mathcal{V}} \, \Theta(t - t_0) \frac{(t - t_0)^n}{n!} \tag{3.2.29}$$

The $n!$ is making each term approach zero really fast. This is good. This can be used to prove that (3.2.16) converges absolutely:

$$\sum_{n=0}^{\infty} \|(B_0 f_n)(t)\|_{\mathcal{U}} \leq \sqrt{t_1 - t_0}\, \|f\|_{\mathcal{V}}\, \Theta(t - t_0) \sum_{n=0}^{\infty} \frac{(\|V\|_{\mathcal{V}}\,(t - t_0))^n}{n!} \tag{3.2.30}$$

That sum is just an exponential. Replace it with the exponential to get the bound:

$$\sum_{n=0}^{\infty} \|(B_0 f_n)(t)\|_{\mathcal{U}} \leq \sqrt{t_1 - t_0}\, \|f\|_{\mathcal{V}}\, \Theta(t - t_0) e^{\|V\|_{\mathcal{V}}(t - t_0)} \tag{3.2.31}$$

Thus the series converges absolutely. Since $\mathcal{U}$ is complete, the series also converges in the $\mathcal{U}$ norm.

3.3 The red operator

No treatment of scattering theory would be complete without considering the S-matrix, the quantity which, among other things, is used to calculate differential cross sections, determining the statistical behaviour of gases and rates of reaction. Something similar to the S-matrix exists in the context of sources and the blue equation as well.

First of all, let us review the S-matrix. This is regular quantum mechanics, so we are using Ψ and the Schrödinger equation, that is $f = 0$ and $\varepsilon = 0$. Suppose the hamiltonian has the form $H(t) = T + V(t)$. This means $\Psi(t) = U_H(t)\Psi(0)$, where the unitary evolution operator U_H is defined by

$$U_H(0) = \mathbb{1} \tag{3.3.1}$$

$$\partial_t U_H(t) = -iH(t)U_H(t) \tag{3.3.2}$$

Suppose also that V_0 is limited to an interval of time $I = [t_0, t_1]$, where $0 < t_0 < t_1$. Everywhere else, $V_0(t) = 0$ and $H(t) = T$. At $t = 0$, the system is initialised to state $\Psi(0) = \varphi_0$, and is "free", that is it moves according to just T. Then between t_0 and t_1, the scattering, V, happens. After that, Ψ is free again.

The idea of the S-matrix is that it summarises the effect of this scattering event. The input of the S-matrix is the initial quantum state φ_0 and the output $\varphi_1 = S\varphi_0$ is the initial quantum state required to reproduce the effect of V, only with free evolution, $U_T(t) = e^{-iTt}$, all the way through, *even in the interaction region, I*. That is, after the interaction, $\Psi(t)$ and $U_T(t)\varphi_1$ are the same:

$$U_T(t)\varphi_1 = U_H(t)\varphi_0 \quad (t > t_1) \tag{3.3.3}$$

Rearranging, one obtains the S-matrix:

$$S = U_T(t)^\dagger U_H(t) \quad (t > t_1) \tag{3.3.4}$$

Any t after t_1 will do. The expression is constant after that time. Note that if $V = 0$, i.e. there is no interaction, then $S = \mathbb{1}$ and $\varphi_1 = \varphi_0$. The stronger the scatterer, the bigger the difference between input state and output state. Note also that S is unitary, that is $|\varphi_1| = |\varphi_0|$. In this way, the scatterer is summarised as a unitary operator on the initial quantum state, φ_0.

Doing the same thing with sources is easy. Just as in the Neumann series, we are assuming the form (3.2.1). Note that V is more general in the Neumann series than in the example used to illustrate the S-matrix. In particular, V might not be time-local (5.1.3). We will be using the free and interacting propagators now, so we will give distinct labels to each:

$$B_H = (\varepsilon + \partial_t + iH)^{-1} \tag{3.3.5}$$

$$B = (\varepsilon + \partial_t + iT)^{-1} \tag{3.3.6}$$

Suppose we initialise the system with a source f_0. We are looking for an equivalent source, f_1, that, when propagated *freely* into a blue state with B, is equal to the propagation of f_0 *under interaction* with B_H. In math, this defines a new operator R such that if $f_1 = Rf_0$, then

$$Bf_1 = B_H f_0 \tag{3.3.7}$$

Substituting f_1 for Rf_0 and rearranging,

$$R = B^{-1}B_H \tag{3.3.8}$$

This is a different operator from the S-matrix, so we'll give it a name: the *red operator*. Note that when $V = 0$, $R = \mathbb{1}$, in analogy to S.

This operator has a Neumann series of its own. Rearranging,

$$R = B^{-1}B_H \tag{3.3.9}$$

$$= (B_H^{-1}B)^{-1} \tag{3.3.10}$$

$$= ((B^{-1} + iV)B)^{-1} \tag{3.3.11}$$

$$R = (\mathbb{1} + iVB)^{-1} \tag{3.3.12}$$

When convergence criteria are met,

$$Rf_0 = \sum_{n=0}^{\infty}(-iVB)^n f_0 \tag{3.3.13}$$

$$= f_0 - iVBf_0 - VBVBf_0 + iVBVBVBf_0 + \ldots \tag{3.3.14}$$

These terms are the same new sources that were identified in the Neumann series in section 3.2.

In scattering theory, it is common to consider an alternative S-matrix, $S' = S - \mathbb{1}$. Using this version, when there is no interaction, $S' = 0$. In this way, S' is "proportional" to the strength of the interaction. If we do the same thing with the red operator, and let $\varepsilon \to 0$, something interesting happens to our Neumann series:

$$R'f_0 = -iVB_0f_0 - VB_0VB_0f_0 + iVB_0VB_0VB_0f_0 + \ldots \tag{3.3.15}$$

There are many physically equivalent sources to f_0, and the choice of one over the other is somewhat arbitrary, but f_0, as a term on its own, is now gone from this series. All of the remaining f_0s are passed into B_0, which erases all of the physically irrelevant properties of f_0. Thus each term is determined solely by the physically meaningful properties of f_0 and the interaction, V. This $R'f_0$ is a new source whose properties are determined solely by physics, and not by arbitrary mathematics. Physically, *sources exist*. This first example of a physical source is the result of the interaction of an incoming free state with a scatterer. If the same example hamiltonian for a 1D position state is used as in section 3.2, then this new source is localised to the site of the scattering.

4 Quantum Field Theory

Sources are natural objects in quantum field theory. There is a lot to discuss here, especially when introducing real relativistic quantum systems, like the Klein-Gordon equation or the Dirac equation. There is no room for this, so instead, a toy model will be introduced. It is basically the same model that has already been discussed, only instead of just one quantum system, there are many identical quantum systems, combined together with boson statistics.

4.1 Particle creation and annihilation

Sources are particularly useful in the context of creation and annihilation operators.

Consider non-interacting bosons in the Heisenberg picture. Suppose that each boson moves according to the same time-independent single-particle hamiltonian, H. We will keep the space $\mathcal{U}$ generic, though, so these "particles" are not necessarily free particles moving in three dimensions. For example, they could be identical two-state systems. We'll use an orthonormal basis of $\mathcal{U}$ space, so that $\varphi_1^\dagger \varphi_0$ is written $\sum_n \varphi_{1n}^* \varphi_{0n}$, a linear operator applied to a $\mathcal{U}$ vector $A\varphi$ is written $\sum_c A_{nc}\varphi_c$, and the Schrödinger equation becomes

$$\dot{\Psi}_n(t) = -i \sum_c H_{nc} \Psi_c(t) \tag{4.1.1}$$

This clears the way for Fock space, the annihilation operator, $a_n(t)$, and its adjoint, the creation operator, $a_n(t)^\dagger$. (Now, $A^\dagger$ is the Fock space adjoint, rather than the $\mathcal{U}$ adjoint.) They are partly defined by the rules:

$$a_n(t) \left|0\right\rangle = 0 \tag{4.1.2}$$

$$\dot{a}_n(t) = -i \sum_c H_{nc} a_c(t) \tag{4.1.3}$$

The rest of the definition is in the statistics. Since these are boson statistics,

$$[a_m(t), a_n(t)] = 0 \tag{4.1.4}$$

$$[a_m(t), a_n(t)^\dagger] = \delta_{mn} \tag{4.1.5}$$

Rule (4.1.3) can be integrated from t to u:

$$a_n(u) = \sum_c U_{nc}(u-t)a_c(t), \text{ where} \tag{4.1.6}$$

$$U(t) = e^{-iHt} \tag{4.1.7}$$

Equation (4.1.6) is true for all t, making its right-hand side constant with respect to t. To prove it is right, first set u to t, proving the initial conditions agree. Then, differentiate both sides of equation (4.1.6) with respect to u, to recover equation (4.1.3).

Now, we are going to consider: *what happens when we contract the creation and annihilation operators with sources*—not a contraction over just $\mathcal{U}$, but over all of $\mathcal{V}$? In particular, one creates a new operator on Fock space:

$$X(f) = \int_{-\infty}^{\infty} \mathrm{d}t \sum_n f_n(t)^* a_n(t) \tag{4.1.8}$$

It is *some* kind of annihilation operator. Here is its Fock space adjoint:

$$X(f)^\dagger = \int_{-\infty}^{\infty} \mathrm{d}t \sum_n a_n(t)^\dagger f_n(t) \tag{4.1.9}$$

It is some kind of creation operator. We'll do this twice, for two different sources, f and g, then we are going to calculate this vacuum expectation value, and see what happens:

$$\langle 0| X(g)X(f)^\dagger |0\rangle \tag{4.1.10}$$

Expanding using (4.1.8):

$$\langle 0| X(g)X(f)^\dagger |0\rangle = \int_{-\infty}^{\infty} \mathrm{d}u \int_{-\infty}^{\infty} \mathrm{d}t \sum_{mn} g_n(u)^* f_m(t) \langle 0| a_n(u)a_m(t)^\dagger |0\rangle \tag{4.1.11}$$

Now, we can focus on just the $\langle 0| a_n(u)a_m(t)^\dagger |0\rangle$ in the right hand side. Use equation (4.1.6) on the annihilation operator, substituting the t in the creation operator into the t of equation (4.1.6):

$$\langle 0| a_n(u)a_m(t)^\dagger |0\rangle = \langle 0| \sum_c U_{nc}(u-t)a_c(t)a_m(t)^\dagger |0\rangle \tag{4.1.12}$$

Now, use the commutator (4.1.5):

$$\langle 0| a_n(u)a_m(t)^\dagger |0\rangle = \langle 0| \sum_c U_{nc}(u-t)(a_m(t)^\dagger a_c(t) + \delta_{mc}) |0\rangle \tag{4.1.13}$$

$$= \sum_c U_{nc}(u-t) \langle 0| a_m(t)^\dagger a_c(t) |0\rangle + U_{nm}(u-t) \tag{4.1.14}$$

Finally, use the definition of the vacuum state, (4.1.2):

$$\langle 0|\, a_n(u) a_m(t)^\dagger \,|0\rangle = U_{nm}(u-t) \tag{4.1.15}$$

Substitute this back into (4.1.11):

$$\langle 0|\, X(g)X(f)^\dagger \,|0\rangle = \int_{-\infty}^{\infty} \mathrm{d}t \int_{-\infty}^{\infty} \mathrm{d}u \sum_{mn} g_n(u)^* f_m(t) U_{nm}(u-t) \tag{4.1.16}$$

$$\langle 0|\, X(g)X(f)^\dagger \,|0\rangle = g^{\mathrm{B}} U * f = \pi \tag{4.1.17}$$

Hey, that's just the probability amplitude (2.1.6) from the section about probability! This implies sources are dual to creation and annihilation operators, and the inner product of a source and a creation operator results in a new creation operator that creates a particle in the same state that the source represents. This is a very clean and powerful result, which makes the source a natural mathematical object in the context of quantum field theory. There is one oddity, though: what if f and g represent the same quantum state, but g happens before f? This would mean that if $X(f)^\dagger$ creates a particle in the present, then $X(g)$ destroys a particle in the past. But we started with a vacuum. One would expect the probability amplitude of this to be zero. Instead, one gets $\pi = 1$. In other words, this allows a creation in the present to interact with an annihilation in the past. That does not seem right.

It turns out, there *is* something wrong with (4.1.17). The creation and annihilation operators have been ordered such that there are later operators to the right of earlier operators. In real quantum field theory problems, vacuum expectation values like this are actually almost always time-ordered. That is, regardless of the written order, the operators are ordered in increasing t, with the earliest operator on the right. Suppose $t < u < v$. When using time ordering,

$$\mathrm{TO}(a(t)a(u)^\dagger a(v)) = \mathrm{TO}(a(v)a(t)a(u)^\dagger) = \mathrm{TO}(a(u)^\dagger a(t)a(v)) = \cdots = a(v)a(u)^\dagger a(t) \tag{4.1.18}$$

What happens when we time-order our vacuum expectation value? Just what you would expect:

$$\langle 0|\, \mathrm{TO}(a_n(u)a_m(t)^\dagger) \,|0\rangle = G_{nm}(u-t) \tag{4.1.19}$$

$$\langle 0|\, \mathrm{TO}(X(g)X(f)^\dagger) \,|0\rangle = g^{\mathrm{B}} G * f = g^{\mathrm{B}} B f \tag{4.1.20}$$

Now, an annihilation in the past can no longer interact with a creation in the present. This makes more sense than without time ordering. Maybe this really should be the definition

of the probability amplitude. Repeat this with a *correlation function*, i.e. a time-ordered expectation value of N creation and N destruction operators, and you get Wick's theorem with B as the propagator.

4.2 Path integrals and sources

This is just a sketch of how one might develop a path integral-based quantum field theory with sources. Its main purpose is just to demonstrate how sources are a natural companion to path integrals.

The more quantum field theory one learns, the more it becomes apparent: *the only good ordering is time ordering.* When this idea is taken to its logical conclusion, where does that lead us?

In the Fock space, the only allowed operators are composed of different combinations of the identity operator and $a_m(t)$, added and multiplied together. The order of the operators in a product is supposed to matter, but in reality, the operators are just going to get time-ordered anyway. The entire non-commutative nature of the operator algebra is erased. This vacuum expectation value $\langle 0|\,\mathrm{TO}(a_n(u)a_m(t)^\dagger)\,|0\rangle$ does contain the Fock vector $\mathrm{TO}(a_n(u)a_m(t)^\dagger)\,|0\rangle$, but then it is just reduced to a complex number with the $\langle 0|$ on the left. No Fock space vector is ever treated in isolation. Is Fock space even needed any more?

This is the motivation behind the path integral approach to quantum field theory. Using it allows one to remove Fock space from the theory entirely. Every $a_n(t)$ in the time ordered vacuum expectation value is replaced by $a_n(t) \to e_n^\dagger \psi(t)$, where $\psi \in \mathcal{V}$, resulting in a function $W : \mathcal{V} \to \mathbb{C}$. Then, that function is integrated, over all $\mathcal{V}$. For example:

$$\langle 0|\,\mathrm{TO}\left(\int_{-\infty}^{\infty}\mathrm{d}u\,\sum_n g_n(u)^* a_n(u)\int_{-\infty}^{\infty}\mathrm{d}t\,\sum_m a_m(t)^\dagger f_m(t)\right)|0\rangle = \int_{\psi\in\mathcal{V}}\mathrm{d}???\; g^{\mathrm{B}}\psi\psi^{\mathrm{B}}f \tag{4.2.1}$$

Here, $W(\psi) = g^{\mathrm{B}}\psi\psi^{\mathrm{B}}f$. The trouble is that there is no consensus on what the definition of this integral over $\mathcal{V}$ should be. We will adopt the following definition. To make it clear that we mean this particular path integral, and not some other path integral, we'll call it the *blue integral*. First define:

$$\int_{z\in\mathbb{C}^N}\mathrm{d}^N z\, f(z) = \int_{x\in\mathbb{R}^N}\mathrm{d}^N x\int_{y\in\mathbb{R}^N}\mathrm{d}^N y\, f(x+iy) \tag{4.2.2}$$

Now, suppose $\mathcal{S}$ is an N-dimensional, complex vector space with basis $e : \mathbb{Z}_N \to \mathcal{S}$. Suppose $M, W \in \mathscr{C}(\mathcal{S} \to \mathbb{C})$. Define:

$$\int_{x\in\mathcal{S}} \mathrm{d}M\ W(x) = \frac{\int_{z\in\mathbb{C}^N} \mathrm{d}^N z\ M(\sum_a e_a z_a) W(\sum_a e_a z_a)}{\int_{z\in\mathbb{C}^N} \mathrm{d}^N z\ M(\sum_a e_a z_a)} \tag{4.2.3}$$

It is an integral of a function W with respect to another function M. It has been normalised such that if $W(x) = 1$, then $\int_{x\in\mathcal{S}} \mathrm{d}M\ W(x) = 1$. Note that this integral is basis-invariant. To see this, just do a basis transformation and use the Jacobian. The Jacobians are constant, and the top Jacobian just cancels with the bottom Jacobian.

Now, consider the full Hilbert space $\mathcal{H}$ containing the $\mathcal{V}$ defined by (2.0.3) etc. That is $\mathcal{H} = L^2(\mathbb{R} \to \mathcal{U})$. Suppose $e : \mathbb{N} \to \mathcal{V}$ is an orthonormal basis of $\mathcal{H}$. That is, e is an orthonormal basis of $\mathcal{H}$, but every basis vector e_n is still in the smaller space, $\mathcal{V}$. In particular, every e_n is still differentiable. Use the basis truncated to N vectors to define an expanding sequence of subspaces $\mathcal{V}_N \subset \mathcal{V}_{N+1} \subset \mathcal{V}$. Extend M and W to all of $\mathscr{C}(\mathcal{V} \to \mathbb{C})$. Define the blue integral:

$$\int_{\psi\in\mathcal{V}} \mathrm{d}M\ W(\psi) = \lim_{N\to\infty} \int_{\psi\in\mathcal{V}_N} dMW(\psi) \tag{4.2.4}$$

This is an integral over the entire space of blue states, $\mathcal{V}$. If this integral give the same result independent of the chosen basis of $\mathcal{H}$, then W is integrable with respect to M. Using this definition and a fair amount of work, it can be proven that when M is defined as

$$M(\psi) = e^{-\psi^{\mathrm{B}} B^{-1} \psi} \tag{4.2.5}$$

$$= e^{-\psi^{\mathrm{B}} (\varepsilon + \partial_t + iH)\psi} \tag{4.2.6}$$

the following partition function arises:

$$Z(f) = \int_{\psi\in\mathcal{V}} \mathrm{d}M\ e^{f^{\mathrm{B}}\psi + \psi^{\mathrm{B}} f} \tag{4.2.7}$$

$$= e^{f^{\mathrm{B}} B f} \tag{4.2.8}$$

Note that the ε in the blue integral now acts as a sort of cutoff, giving an overall decaying Gaussian factor of $e^{-\varepsilon\psi^{\mathrm{B}}\psi}$. Without it, the integral does not converge. Thus, the same ε that was used to allow time-L^2 blue states in the blue equation and to force causality is playing a totally different role in the blue integral. One might wonder whether this means the blue integral forbids anti-causal solutions, since that requires a negative ε.

Unfortunately, this is false, since one can just add the needed $-$ signs elsewhere: $\psi^{\mathrm{B}}(\varepsilon - \partial_t - iH)\psi$.

Derivatives of this partition function can then be used to prove

$$\int_{\psi\in\mathcal{V}} \mathrm{d}M\ g^{\mathrm{B}}\psi\psi^{\mathrm{B}} f = g^{\mathrm{B}} B f = \pi \tag{4.2.9}$$

In other words, sources can be used directly in a path integral, and the result is the probability amplitude between sources. No LSZ reduction formula is necessary to extract physical results from correlation functions. When there are N ψs and ψ^{B}s in the integral, the result is Wick's theorem with B as the propagator. In other words, this chosen M reproduces the system of non-interacting bosons from section 4.1. The same thing works with the Klein-Gordon equation, but there are some complications and there is no room for it in this thesis.

5 Causality

5.1 Non-relativistic causality

It was already proven (2.0.23) that when H is time-independent, there is a causal relationship between the source f and blue state ψ. That is, *f may affect the future of ψ, but not its past.* So, let's adopt this as our definition of causality and see what happens when H is more general.

Rearranging the blue equation (2.0.7),

$$\partial_t \psi = (-\varepsilon - iH)\psi + f \tag{5.1.1}$$

Consider the effect of just the $-iH\psi$ term on $\partial_t \psi$ when H looks like this:

$$(H\psi)(t) = \int_{-\infty}^{\infty} \mathrm{d}u\, K(t,u)\psi(u) \tag{5.1.2}$$

One can easily see how $\partial_t \psi$ in the present could depend on ψ in the future, thus depending on f in the future. Therefore, as a bounded self-adjoint operator on $\mathcal{V}$, H is not causal in general. An additional constraint is required.

One simple way to ensure causality is to require that H must be time-local:

$$(H\psi)(t) = H_0(t)\psi(t) \tag{5.1.3}$$

This demonstrates that causality puts non-trivial constraints on the system, and some definition of causality is required. This definition is useful in the non-relativistic setting, but when adding special relativity, our definition of causality is immediately ruined.

5.2 A relativistic blue equation

This is not meant to be a thorough exploration of relativity with sources. The point is just to demonstrate that the previous section's definition of causality is insufficient.

The idea of an non-homogeneous state equation with unphysical decay is useful in rela-

tivistic quantum mechanics as well. Here is a blue variant of the Klein-Gordon equation:

$$\psi, f : \mathbb{R}^{1,3} \to \mathbb{C} \tag{5.2.1}$$

$$(\varepsilon - i(\partial_\alpha \partial^\alpha - m^2))\psi = f \tag{5.2.2}$$

Now, the functions in $\mathcal{V}$ have time and space dependence, on equal footing. If the left hand side is inverted and $\varepsilon \to 0$, one gets the Feynman propagator, Δ:

$$\psi = \Delta * f \tag{5.2.3}$$

This time, the convolution is over all space and time. But the Feynman propagator is not causal! To see this, here is a representation of the Feynman propagator in k space, i.e. after a space Fourier transform:

$$\psi_k(t,k) = (\Delta_k *_t f_k)(t) = \int_{-\infty}^{\infty} \mathrm{d}u\, \Delta_k(t-u,k) f_k(u,k), \text{ where} \tag{5.2.4}$$

$$\Delta_k(t,k) = \frac{1}{2\omega_0(k)} e^{(-\varepsilon - i\omega_0(k))|t|} \text{ and} \tag{5.2.5}$$

$$\omega_0(k) = \sqrt{m^2 + |k|^2} \tag{5.2.6}$$

There is no Heaviside function anymore that could have shielded the past of ψ from the present behaviour of f. That is why this propagator is not causal.

There are causal propagators for the Klein-Gordon equation, but without getting into the details, they can't be used to do quantum field theory, because the correct propagator in Wick's theorem is the Feynman propagator—not a causal propagator. A new definition of causality is needed.

5.3 The red operator and causality

A definition of causality that works in special relativity comes from Epstein and Glaser's causal perturbation theory.[5] The version that is used here comes from Scharf's textbook on their approach.[13] They define causality using the S-matrix. It operates on quantum states, though, and we are using sources to characterise states, so we will use the red operator, (3.3.8), instead, but the idea is the same.

Suppose one has a hamiltonian with a free component, T, and an interaction V, as in equation (3.2.1). It is the same setup that is used to find the Neumann series and to

define the red operator. To localise the effect of the interaction, V can be screened with a compactly supported test function $\alpha \in \mathscr{C}_0^\infty(\mathbb{R} \to \mathbb{R})$:

$$V_\alpha \psi = V(\alpha\psi) \tag{5.3.1}$$

This *should* localise the effect of V to the support of α, but this will only work if V is causal. This is the angle of attack of the problem of defining causality.

Now, suppose there are two non-overlapping test functions, $\alpha, \beta \in \mathscr{C}_0^\infty(\mathbb{R} \to \mathbb{R})$. Define a combined V that includes the effects of the α and β parts:

$$V_{\alpha\beta} \psi = V((\alpha + \beta)\psi) \tag{5.3.2}$$

Each of V_α, V_β, and $V_{\alpha\beta}$ produces its own respective red operator, R_α, R_β, and $R_{\alpha\beta}$. Remember that the red operator summarises the effect of the interaction on the source. Suppose supp $\beta >$ supp α, that is β happens after α. When V is causal, R_α and R_β shouldn't have anything to do with each other, so applying the earlier one, then the later one, should have the same effect as applying the combined $R_{\alpha\beta}$. Thus, by definition, V *is causal* if and only if for all α and β, *the combined red operator always factors*:

$$\forall \alpha, \beta \in \mathscr{C}_0^\infty(\mathbb{R} \to \mathbb{R}),\ \text{supp}\ \beta > \text{supp}\ \alpha \implies R_{\alpha\beta} = R_\beta R_\alpha \tag{5.3.3}$$

As a first test of this new definition of causality, V really should be causal when it is time-local (5.1.3).

$$(V\psi)(t) = V_0(t)\psi(t) \implies V \text{ is causal} \tag{5.3.4}$$

To prove this, consider (3.3.12):

$$R = (\mathbb{1} + iVB)^{-1} \tag{5.3.5}$$

This means the red operator's inverse has a simpler form than the operator itself:

$$R^{-1} = \mathbb{1} + iVB \tag{5.3.6}$$

So, to prove causality, we can invert both sides of (5.3.3), obtaining the following equivalent condition:

$$R_{\alpha\beta}^{-1} = R_\alpha^{-1} R_\beta^{-1} \tag{5.3.7}$$

We will substitute (5.3.6) into the right side, and we'll see if we can recover the left side.

$$R_\alpha^{-1} R_\beta^{-1} = (\mathbb{1} + iV_\alpha B)(\mathbb{1} + iV_\beta B) \tag{5.3.8}$$

$$= \mathbb{1} + i(V_\alpha + V_\beta)B - V_\alpha B V_\beta B \tag{5.3.9}$$

Notice that a time-local $V_{\alpha\beta}$ separates as follows:

$$(V_{\alpha\beta}\psi)(t) = (V((\alpha+\beta)\psi)(t) \tag{5.3.10}$$
$$= V_0(t)(((\alpha(t)+\beta(t))\psi(t)) \tag{5.3.11}$$
$$= \alpha(t)V_0(t)\psi(t) + \beta(t)V_0(t)\psi(t) \tag{5.3.12}$$
$$= (V_\alpha\psi)(t) + (V_\beta\psi)(t) \tag{5.3.13}$$
$$V_{\alpha\beta} = V_\alpha + V_\beta \tag{5.3.14}$$

That takes care of $V_\alpha + V_\beta$. What about $V_\alpha B V_\beta B$? V_β filters its input state to the support of β, then B, being causal (2.0.23), propagates that strictly into the future. The result is zero in the support of α. But then V_α filters to just the support of α. That means $V_\alpha B V_\beta = 0$. This finishes the proof.

$$R_\alpha^{-1}R_\beta^{-1} = \mathbb{1} + i(V_\alpha + V_\beta)B - V_\alpha B V_\beta B \tag{5.3.15}$$
$$= \mathbb{1} + iV_{\alpha\beta}B \tag{5.3.16}$$
$$= R_{\alpha\beta}^{-1} \tag{5.3.17}$$

Therefore a time-local V is always causal, by this new definition of causality as well as the old one.

The point of this new definition of causality is that it can be applied to special relativity, that is quantum field theory, but there is no room in this thesis for that.

6 Conclusions

This investigation of sources and causality has raised more questions than answers, but there *are* some clear results.

The clearest immediate application is to scattering theory. A complicated, unnormalised theory is made simple and normalised. Time-dependent perturbation theory is immediately accessible using a standard mathematical tool, the Neumann series. The Neumann series even works on acausal interactions, though the convergence for time-local interactions is stronger. If the interaction potential is time-independent, i.e. $(V\psi)(t) = V_0\psi(t)$, then the time-independent theory, i.e. the Lippmann-Schwinger equation and the Born series, is just the time Fourier transform of the time-dependent theory. This time Fourier transform is made possible by the constraint that ψ must be L^2 in space *and* time.

The other clear result is that sources can set initial conditions, thus sources can specify quantum states. This applies to the blue equation and to quantum field theory. In the toy quantum field theory model of chapter 4, sources can be contracted with creation and annihilation operators in a correlation function to obtain probability amplitudes. The contraction is the inner product on the whole space of blue states, $\mathcal{V}$. That is, it is over the state space $\mathcal{U}$ *and* time. The LSZ reduction formula is no longer necessary.

Finally, there is causality. A causal structure is immediately apparent after discovering the Heaviside function in the formula for the propagator, (2.0.23). After demonstrating problems with applying a naïve definition of causality to special relativity, Epstein and Glaser's definition of causality is adopted instead. It is proven that as long as the interaction is time-local, it is causal.

6.1 Loose ends

There were many other ideas that were explored in this investigation, for which there was no room in this thesis. The most interesting continuation in the non-relativistic theory of scattering is a rigorous treatment of the cross section. The cross section applies to a particle moving in three dimensions and colliding with an immovable scatterer, but it also works on a pair of particles scattering off of each other. For the latter, one simply

adopts centre-of-mass coordinates, reducing the 6D space to a 3D space. Either way, the model is a single particle moving in a 3D position space, $\mathcal{U} = L^2(\mathbb{R}^3 \to \mathbb{C})$, scattering off of a time-independent potential, localised at the origin. The source is also assumed to be localised, but at a certain point in space far away from the scatterer. There is a very elegant far field approximation for the blue state generated by such a source, which works the same way as other far field approximations, like in classical electrodynamics. That is, when the blue state generated by the source reaches the origin, it is effectively the spacetime Fourier transform of the generating source. This far field approximation is applied to the original source and to the scattered source obtained by the red operator, (3.3.8). In an interesting, but rather lengthy calculation, the cross section is recovered from this process.

A common phenomenon in quantum mechanics and quantum field theory is called resonance. A resonant state is a nearly-bound state. An example of such a state is if a 1D particle starts trapped between two barriers. The particle does escape, but only very slowly. Another example of a resonant state is any kind of radioactive atom. The Neumann series does apply to resonant states, but it converges slowly. The behaviour is exactly analogous to the Taylor series expansion of the exponential function $F(t) = e^{-i\omega t} = \sum_{n=0}^{\infty} \frac{(-i\omega t)^n}{n!}$.

It was found, though, that the Neumann series can be done in steps. In the regular Neumann series, the same, free, propagator is applied on every step. Instead, a different propagator can be selected depending on the nature of the residual source left over from the previous step. In the example of the 1D particle, the adaptive Neumann series could switch between the free propagator and the infinite square well propagator. The result is an adaptive Neumann series.

Chapter 4 on quantum field theory works entirely with bosons. Fermions are never addressed. The blue integral (4.2.4), in particular, relies on boson statistics. A fermion version of the blue integral is easy to define, however, using an exterior algebra. The logic of a limit of a ratio of two finite integrals still applies.

In special relativity, i.e. quantum field theory, sources are helpful for a reason besides the field-source duality. Using the standard approach to quantum mechanics *and* quantum field theory, one sets the initial conditions of a system at a certain time. This forces a choice of reference frame. In non-relativistic quantum mechanics, this is fine, but when adding special relativity, due to relativity of simultaneity, different reference frames disagree on ordering of events. An initial condition that happens entirely at just one time in one frame gets spread out over an interval of time in another reference frame. This really complicates

the Lorentz transform of an initial condition from one reference frame to another. Setting an initial condition using a source avoids this whole mess. When extended to Minkowski space, a source is a function of space *and* time, and its Lorentz transform is the same as that of any other such function.

This was not included in detail because of the complications of using Feynman propagators, which, as the reader may recall, are *acausal*. In spite of this, it was found that if the whole space of sources is restricted to a certain subset, then the causal relationship from the source to the field, ψ, is restored. There is another subset, though, whose sources have an *anti-causal* relation to the field, i.e. they propagate the field *backward* in time. The physical interpretation of these backward-propagating sources is not clear. It is not possible to disregard them, however, as a particle annihilation is equivalent to an anti-causal particle creation.

6.2 Further directions

In chapter 2 introducing the blue equation, it was assumed that the hamiltonian is bounded when, in reality, it rarely is. As part of the research, though, the propagators of unbounded free hamiltonians were derived anyway. The results weren't rigorous, but they seemed to work. In fact, as long as $\varepsilon > 0$, the propagators were bounded, even when extending $\mathcal{V}$ to $L^2(\mathbb{R} \to \mathcal{U})$. Thus one possible solution to the boundedness problem is to simply *define* the propagators, then work with propagators only, never using the unbounded differential operators. This idea applies to non-relativistic quantum mechanics *and* to quantum field theory.

In section 2.1, concerning measurement, there is a huge hole. It is just assumed that the measurement, f_1, is an inherent parameter of the problem at hand, which can be determined as easily as the hamiltonian. But how does one actually determine f_1? It should be possible by modelling the measurement using a single scattering event. The 1D barrier example (2.0.12) could be used. There would be two outcomes: the particle is transmitted; and the particle is reflected. Such an example would refine the ideas of measurement using sources, which were introduced in this section.

The condition for absolute convergence of the Neumann series on an infinite time domain (3.2.11) is a little unsatisfying, but it may only apply to V which have infinite extent in space and time. What if we add the condition that V has compact support in time or space? This may actually be sufficient to guarantee uniform convergence, since there will

be a time limit to how long an incident wave can interact with the scatterer.

It was rather disappointing that an example of renormalisation using sources, red operators, and causal perturbation theory could not be completed. This was the original goal of the thesis. There is hope, however, that such a thing could be achieved. If so, it could make Epstein and Glaser's method much more concise and accessible.

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