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Quantum Scattering without Magic: Part 0

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1 An apology to the general public

So, this will be a bit of a departure from what I usually write. But I *am* a physicist, so I am going to write physics from time to time. This log entry assumes prior knowledge of quantum mechanics. So, if you have no idea what I'm talking about, don't worry. I'm not expecting you to. Feel free to skip to the next log entry.

However.

I actually do expect anybody to be able to understand this, after they have learned basic quantum mechanics. I'm not about to engage in wishy washy qualitative descriptions of the work that I do, aimed at the general public. I remember trying to understand quantum mechanics in high school from such descriptions alone. Even when reading the work of some of the greatest physics educators of all time, like Richard Feynman's Six Easy Pieces, I still had no idea what was going on. It certainly didn't help that Feynman also said "Nobody understands quantum mechanics.". Then, there was new age hippie garbage like Deepak Chopra and What the Bleep do We Know.

What was the problem? A lack of mathematics. Quantum mechanics is an inherently mathematical theory, requiring statistics, complex numbers, linear algebra, and differential equations[1]. This is why all verbal descriptions fall utterly short. I did not understand quantum mechanics until I stopped learning *about* quantum mechanics, and started learning quantum mechanics.

After I did, I found that quantum mechanics is actually a very simple and logical system with few rules and no exceptions. *Quantum mechanics is not magic!* Not only *can* the theory be understood; its rules are so simple and so few that they can be easily simulated on a computer with a small amount of code, though, admittedly, the simulation runs extremely slowly[2].

Besides being understandable, it is actually quite shocking and awesome to see first-hand how such a simple and very unusual theory gives rise to all of the complexity of the world as we know it[3]. In the intervening fifteen years since I first learned quantum mechanics, I have found anything less than the full mathematical theory to be a grave disservice to one of the most beautiful and objectively correct theories that humans have ever discovered.

[1] These are actually rather common subjects that all mathematicians and many scientists and engineers have to learn anyway.

[2] Except on a quantum computer.

[3] Except for gravity. Quantum mechanics does not explain gravity.

2 Scattering, from what I have read

I tried reading about scattering on my own. I've read Griffiths; Sakurai; Wikipedia. None of it makes any sense. They solve the Time-Independent Shrödinger Equation (TISE) with an incoming plane wave and an outgoing spherical wave. This solution is unnormaliseable, though. In other words, it has no concrete physical interpretation. But they interpret the solution anyway, using some highly dubious qualitative reasoning which might as well be magic, ending up with what they claim are scattering cross sections, without even defining what a scattering cross section is.

Frustrated with and confused by what I read, I decided to try to recover their results on my own, only without magic. I succeeded. Here is what I found. It is quite beautiful.

All this work probably exists already, spread out over a dozen different papers and textbooks. I've assembled it here because I think *this* is how scattering theory should be introduced, rather than how Griffiths or Sakurai do it.

3 The inhomogeneous Schrödinger equation

We start with the Schrödinger equation we all know and love.

$$\psi(0) = \psi_0 \tag{1}$$
$$\dot{\psi}(t) = -iH\psi(t)\,[4] \tag{2}$$

where $\psi \in \mathbb{R} \to \mathcal{V}$ and $\mathcal{V}$ is some complex Hilbert space. Now, I'm going to rearrange it a little.

$$(\partial + iH)\psi = 0 \tag{3}$$

I'm treating the entire time-dependent ψ function as a single vector in the larger vector space of $\mathbb{R} \to \mathcal{V}$. That $\partial + iH$ on the left is a *non-invertible* linear operator, whose null space is the set of all solutions. I'm going to add a decay of $\varepsilon > 0$ now. This may seem crazy, but trust me, it is a good idea.

$$(\varepsilon + \partial + iH)\psi = 0 \tag{4}$$

I am also going to insist that ψ has finite norm.

$$\int_t |\psi(t)|^2 \in \mathbb{R} \tag{5}$$

This and the ε actually make the linear operator *invertible*, i.e. the only solution to equation 4 is $\psi = 0$.[5] This invertibility property is extremely useful!

Now, I'll make one last adjustment. I'm going to add an arbitrary time-dependent inhomogeneous forcing term, f to the right hand side.

$$(\varepsilon + \partial + iH)\psi = f \tag{6}$$

This is the inhomogeneous Schrödinger equation.

[4] "Where is $\hbar$?", you might ask. My response: *what* $\hbar$, esteemed reader? There is no such constant. The kilogram is a myth and energy is frequency. There also is no such thing as kelvins, metres, Boltzmann's constant, or hats, and the speed of light is actually 1. All that will have to be the subject of about three different log entries, though. There is only one joke in this footnote.

[5] At least, the only solution we will allow. There are solutions, but they blow up as $t \to -\infty$. These solutions do not have finite norm.

I'm going to give these linear operators names, because I am going to be referring to them often.

$$C = \varepsilon + \partial + iH \tag{7}$$
$$G = C^{-1} \tag{8}$$

The label of G was chosen because this is equation 6's Green's operator. Unlike most Green's operators, though, this one is invertible.

It is easy to prove that

$$\psi(t) = (Gf)(t) = \int_{u>0} e^{-(\varepsilon+iH)u} f(t-u) \tag{9}$$

Note that $f(t)$ may only affect $\psi(t+h)$, where $h > 0$. That is, f may only affect ψ's future, and not its past. G is perfectly causal. If ε were < 0, this would also create an invertible operator, but it would be anti-causal. This causality is going to be very useful and very important.

After C is inverted, take the limit as ε approaches zero from the positive side.

$$\psi(t) = \int_{u>0} e^{-iHu} f(t-u) \tag{10}$$

This is the physical ψ, which oscillates forever without decay. If this ψ is used in an operation that requires it to have finite norm, the ε will need to remain.

3.1 Encoding initial conditions into the forcing term

When using this technique, our forcing function f is used to set the initial conditions for a time evolution happening after t_0. The idea is that f starts at zero in the infinite past, does some non-zero stuff in around $t = t_0$, then goes back down to zero and stays there out into the infinite future. The simplest way to do this is with the pulse response:

$$f(t) = \delta(t - t_0)\psi_0, \tag{11}$$

where δ is the Dirac delta "function". This gives the actual, normalised, physical $\psi(t)$:

$$\psi(t) = \Theta(t - t_0)e^{-iH(t-t_0)}\psi_0, \tag{12}$$

where Θ is the Heaviside function.

4 Unforeseen Consequences

At this point, some of you might be a little upset that I had taken a nice smooth e^{-iHt} and added this god-awful discontinuous Heaviside function to it. I know I certainly was not happy to find it there. But it was necessary to make C invertible. It's not just that though. The more I looked, the more I realised that ψ with the discontinuity is actually more correct than ψ without it.

These forcing terms aren't just useful for setting initial conditions. They can also be used to extract probability amplitudes from the resulting time evolution. Starting with the probability amplitude, π of a measurement ψ_1 occurring at t_1:

$$\pi = {\psi_1}^\dagger \psi(t_1) \tag{13}$$
$$\pi = \int_t (\delta(t - t_1)\psi_1)^\dagger \psi(t) \tag{14}$$
$$\pi = {f_1}^\dagger \psi, \text{ where} \tag{15}$$
$$f_1(t) = \delta(t - t_1)\psi_1 \tag{16}$$

Look familiar? Now, instead of using the usual ψ, let's substitute the ψ from the inhomogeneous Schrödinger equation (6).

$$\pi = {f_1}^\dagger G f_0 \tag{17}$$

This isn't exactly right, because of ε, but as $\varepsilon \to 0^+$, π will approach the original probability amplitude, with one critical difference. Suppose both fs are pulse responses. This would mean that in the limit as $\varepsilon \to 0^+$,

$$\pi = \Theta(t_1 - t_0){\psi_1}^\dagger e^{-iH(t_1-t_0)}\psi_0 \tag{18}$$

If $t_1 < t_0$, then $\pi = 0$. In other words, that Heaviside makes it impossible for the system to transition from the present into the past! The original expression for the probability amplitude (13) allows for this transition. Thus one can express probability amplitudes solely using the Green's operator and these forcing functions, and when one does, the results are more correct *with* the Heaviside function than without. [6]

5 Scattering using the inhomogeneous Schrödinger equation

Let $H = T + V$, where e^{-iHt} is difficult to calculate, but e^{-iTt} is easy. It is quite typical to use a particle with kinetic energy T moving mostly freely, but with a potential V localised around the origin. But I'll leave T and V general so that the result applies more generally. The important part is that T is easy and $T + V$ is hard.

We are going to use C's invertibility to systematically approximate $\psi(t)$, given a certain initial forcing term, f. Substitute this H into the inhomogeneous Schrödinger equation (6):

$$(\varepsilon + \partial + iT + iV)\psi = f \tag{20}$$

$(\varepsilon + \partial + iH)^{-1}$ is going to be hard, because e^{-iHt} is hard. But $(\varepsilon + \partial + iT)^{-1}$ is going to be easy. So, let's set G to that instead, and apply it to both sides:

$$(1 + iGV)\psi = Gf, \text{ where} \tag{21}$$
$$G = (\varepsilon + \partial + iT)^{-1} \tag{22}$$

Equation 21 is like the Lippmann-Schwinger equation, only time-dependent and, critically, normalised. Solving for ψ,

$$\psi = (1 + iGV)^{-1}Gf \tag{23}$$

This is interesting, but that $(1 + iGV)^{-1}$ operator isn't really a step forward in ease of calculation. Arguably, it is a step back. That GV inside of it, though, is easy enough. Might $(1 + iGV)^{-1}$ expand to a series of such operators?

If GV were just a real number, this would be a geometric series.

$$\sum_{n=0}^{\infty} a^n = \frac{1}{1-a}, \text{ where } |a| < 1 \tag{24}$$

That can work on linear operators?

[6] Another place where the Heaviside occurs naturally is in path integrals over a quantum field of non-interacting bosons, where each boson behaves according to the Schrödinger equation (2). The probability amplitude *with* a Heaviside just falls out of these integrals.

$$\int_{\psi \in \mathbb{R} \to \mathcal{V}} {f_1}^\dagger \psi \psi^\dagger f_0 = {f_1}^\dagger G f_0 \tag{19}$$

I will write a separate log entry about this.

Yes it can, though just like the geometric series, there are pretty severe convergence criteria. What are these criteria?

To answer this, it is easiest to start with the formula for the finite geometric series. It is easy to prove that for all linear operators A, where $1 - A$ is invertible,

$$\sum_{c=0}^{N-1} A^c = (1 - A)^{-1}(1 - A^N) \tag{25}$$

Now we can see that as long as A^N vanishes as $N \to \infty$, the geometric series converges. Let's apply this to equation 23.

$$\text{If } \lim_{N\to\infty} (GV)^N = 0, \text{ then} \tag{26}$$

$$\psi = \sum_{c=0}^{\infty} (-iGV)^c Gf \tag{27}$$

This is like the Born series, only again, it is time-dependent and *normalised*. Also like the Born series, this offers a very straight forward method of iteratively solving scattering problems. Intuitively, using the example from the beginning of the section, G propagates the particle and V scatters the particle. The final result of the calculation is a series of these alternating propagations and scatterings. Since it is normalised it has a very exact physical meaning, which, and I can't stress this enough, is *not magic*.

6 To be continued...

There is a lot more to say about this. I haven't even gotten into scattering cross sections or the time Fourier transforms.

You can do that?

Well, we can *now*, can't we? And it is awesome. This is another reason why I absolutely insist that ψ, as a vector in $\mathbb{R} \to \mathcal{V}$, has finite norm.

But it has taken me far too long to finish this log entry, so in the interest of keeping up a reasonable publishing cadence, this is going to have to be an N parter. I am sorry to keep you in suspense.

But hey, in the meantime, why don't you try doing the time Fourier transform of the inhomogeneous Schrödinger equation (6) for yourself? The results are particularly interesting when applied to the Born-like series of a particle in a 3D potential. In this case, after a Fourier transform, the Green's operator in the Born-like series (27) has a very simple form. If you do try this at home, remember that ψ must have finite norm, so be sure to leave in the ε, so that the Fourier transform remains well-defined.

Until next time...