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Quantum scattering using the inhomogeneous Schrödinger equation: Part 0

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1 Intro

I believe I have found a different way to do quantum mechanics. It is particularly useful for solving scattering problems with perturbation theory, but it is completely general, and does not rely on any of the assumptions that are usually made when solving scattering problems.

2 The inhomogeneous Schrödinger equation

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

$$\psi(0) = \psi_0 \tag{1}$$

$$\dot{\psi}(t) = -iH\psi(t)^{1} \tag{2}$$

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 $\psi = 0$.[2] This invertibility property is extremely useful!

[1] $\hbar = 1$, energy is frequency, and momentum is wavenumber.

[2] 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.

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.

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.

2.1 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.

3 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. [3]

4 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?

[3] 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.

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?

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.

5 Equivalence to the Lippmann Schwinger equation and Born series

The usual scattering equations are the Lippmann-Schwinger equation and the Born series. They are difficult to understand, and the unnormalised solutions can't be interpreted the same way normalised quantum states can. But they are used in real life to make accurate predictions of the results of real life experiments, so they must be correct in some sense. Indeed, there is a very easy way to recover these equations from the inhomogeneous method.

Here is the Lippmann-Schwinger equation:

$$\alpha = \beta + (\omega - T + i\varepsilon)^{-1} V \alpha \tag{28}$$

α and β are unnormalised quantum states whose interpretation is problematic. Rearranging,

$$(1 + i(\varepsilon - i\omega + iT)^{-1} V)\alpha = \beta \tag{29}$$

Compare this to equation 21:

$$(1 + i(\varepsilon + \partial + iT)^{-1} V)\psi = Gf \tag{30}$$

They're almost the same, only instead of ∂, the Lippmann-Schwinger equation has a $-i\omega$.

How could we possibly convert ∂ to $-i\omega$?

Well, through a time Fourier transform, of course.

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.

Define the time Fourier transform:

$$\psi_\omega(\omega) = \int_t e^{i\omega t}\psi(t) \tag{31}$$

Applying this to both sides of equation 21, one gets

$$(1 + iG_\omega V)\psi_\omega = G_\omega f_\omega, \text{ where} \tag{32}$$

$$G_\omega = (\varepsilon - i\omega + iT)^{-1} \tag{33}$$

This is the Lippmann-Schwinger equation! Thus the exact meanings of the mystery states α and β are now clear.

$$\alpha = \psi_\omega \tag{34}$$

$$\beta = G_\omega f_\omega \tag{35}$$

α is just the Fourier transform of the time evolution with V, and β is just the Fourier transform of the time evolution without V. Interestingly, both need the Heaviside in order for the equation to hold. Doing the inverse Fourier transform of the Lippmann-Schwinger equation, one would get those same Heavisides. One could say they were there all along.

6 Further directions

There is a lot more to say about this inhomogeneous method. I haven't even gotten to cross sections. I'm writing a follow-up post right now. Stay tuned.