GREEN FUNCTIONS AND THE SCHRÖDINGER EQUATION

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Reference: Tom Lancaster and Stephen J. Blundell, *Quantum Field Theory for the Gifted Amateur*, (Oxford University Press, 2014), Section 16.2.

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We've seen how a Green (or Green's) function can be used to solve a differential equation with a forcing term of the form

$$Lx(t) = f(t) \tag{1}$$

where L is a differential operator (such as $L = \frac{d^2}{dt^2} + k$ for the harmonic oscillator), x is the function to be found and f is a specified forcing function. The solution requires finding a Green function that satisfies

$$LG\left(t,t'\right) = \delta\left(t-t'\right) \tag{2}$$

From here, the solution is given by

$$x(t) = \int_{-\infty}^{\infty} G\left(t,t'\right) f\left(t'\right) dt' \tag{3}$$

In section 16.2, L&B describe what they claim is a Green function for the Schrödinger equation. The problem with defining a Green function for the Schrödinger equation is that there is no forcing term. The Schrödinger equation can be written as

$$\left(H - i\frac{\partial}{\partial t}\right)\phi(x,t) = 0 \tag{4}$$

where H is the hamiltonian and $\phi(x,t)$ is the (one-dimensional) wave function to be found. L&B introduce what they call the Green function $G^{+}(x,t_x,y,t_y)$ by their equation 16.13:

$$\phi(x,t_x) = \int dy G^{+}(x,t_x,y,t_y)\,\phi(y,t_y) \tag{5}$$

This isn't of the form 3 in which the Green function is integrated over the forcing term to generate the solution $x(t)$. Rather, the Green function is integrated over the wave function ϕ at earlier times ($t_y < t_x$) to get the wave function at time t_x. This leads to a problem as we now see.

If we define the Green function as in their equation 16.22, so that

$$\left(H - i\frac{\partial}{\partial t_x}\right) G^+(x, t_x, y, t_y) = -i\delta(x - y)\,\delta(t_x - t_y) \tag{6}$$

then applying this to 5 leads to

$$\left(H - i\frac{\partial}{\partial t_x}\right)\phi(x, t_x) = \int dy \left(H - i\frac{\partial}{\partial t_x}\right) G^+(x, t_x, y, t_y)\,\phi(y, t_y) \tag{7}$$

$$= -i\int \delta(x - y)\,\delta(t_x - t_y)\,\phi(y, t_y) \tag{8}$$

$$= -i\phi(x, t_x)\,\delta(0) \tag{9}$$

where setting $x = y$ due to the delta function also sets $t_x = t_y$. This doesn't agree with 4, and in fact appears to be infinite due to the $\delta(0)$.

This problem appears to cause quite a bit of confusion in physics blogs. The clearest explanation of how a Green function works with the Schrödinger equation that I've found is on Physics Stack Exchange (link here, valid at the time of writing). The situation appears to be as follows. We can define a Green function in the usual way so that it satisfies

$$\left(H - i\frac{\partial}{\partial t_x}\right) G(x, t_x, y, t_y) = -i\delta(x - y)\,\delta(t_x - t_y) \tag{10}$$

(The $-i$ on the RHS is just for convenience; we could equally well divide it out and incorporate it into the definition of G as is done in the Stack Exchange post.) We now propose that G has the form

$$G^+(x, t_x, y, t_y) = \theta(t_x - t_y)\,K(x, t_x, y, t_y) \tag{11}$$

where $\theta(t_x - t_y)$ is the usual Heaviside step function (zero for $t_x < t_y$ and 1 for $t_x > t_y$). K is some function yet to be determined. The + superscript on G^+ indicates that it is non-zero only if $t_x > t_y$.

We now suppose that for $t_x = t_y = t$, K satisfies

$$K(x, t, y, t) = \delta(x - y) \tag{12}$$

In other words, at a single time, K is non-zero only at a single point. Since our ultimate goal is to define a propagator for the wave function, this is equivalent to saying that a particle can't move anywhere in zero time.

Now we apply the Schrödinger operator to G, and use the fact that

$$\frac{d\theta(t_x - t_y)}{dt_x} = \delta(t_x - t_y) \tag{13}$$

We get

$$\frac{\partial}{\partial t_x}G(x,t_x,y,t_y)=\delta(t_x-t_y)K(x,t_x,y,t_y)+\theta(t_x-t_y)\frac{\partial}{\partial t_x}K(x,t_x,y,t_y) \tag{14}$$

The delta function in the first term on the RHS restricts t_x to $t_x = t_y$ so using 12 we have

$$\frac{\partial}{\partial t_x}G(x,t_x,y,t_y)=\delta(t_x-t_y)\delta(x-y)+\theta(t_x-t_y)\frac{\partial}{\partial t_x}K(x,t_x,y,t_y) \tag{15}$$

We therefore have

$$\left(H-i\frac{\partial}{\partial t_x}\right)G(x,t_x,y,t_y)=-i\delta(t_x-t_y)\delta(x-y)+\theta(t_x-t_y)\left(H-i\frac{\partial}{\partial t_x}\right)K(x,t_x,y,t_y) \tag{16}$$

Comparing this with the original definition 10 we see that we can cancel the terms involving the delta functions and we are left with

$$\theta(t_x-t_y)\left(H-i\frac{\partial}{\partial t_x}\right)K(x,t_x,y,t_y)=0 \tag{17}$$

Therefore, the actual evolution equation should be

$$\phi(x,t_x)=\int dy\; K(x,t_x,y,t_y)\phi(y,t_y) \tag{18}$$

If we now apply the Schrödinger operator $\left(H-i\frac{\partial}{\partial t_x}\right)$ to both sides of this equation, we get zero on both sides, as required.

This derivation relies on K satisfying 12 which, as we've said above, makes sense since, if $t_x = t_y$ in 18, the particle can't go anywhere and we'd expect that $\phi(x,t_x)=\phi(y,t_y)$. The actual form of K depends on the particular problem.

In their example 16.3, L&B show that G^+ has the form

$$G^+(x,t_x,y,t_y)=\theta(t_x-t_y)\sum_n\phi_n(x)\phi_n^*(y)e^{-iE_n(t_x-t_y)} \tag{19}$$

where ϕ_n is an eigenfunction of H with energy E_n.

In their example 16.4, they demonstrate that this G^+ satisfies 10 by a method similar to our derivation above. The final step (getting equation 16.27) might require a bit of clarification. They arrive at the result

$$\left(H-i\frac{\partial}{\partial t_x}\right)G^+(x,t_x,y,t_y)=-i\delta(t_x-t_y)\sum_n\phi_n(x)\phi_n^*(y)e^{-iE_n(t_x-t_y)} \tag{20}$$

To get the next step, note that the delta function sets $t_x=t_y$ so the exponential terms are all 1 and we end up with

$$\left(H-i\frac{\partial}{\partial t_x}\right)G^+(x,t_x,y,t_y)=-i\delta(t_x-t_y)\sum_n\phi_n(x)\phi_n^*(y) \tag{21}$$

$$=-i\delta(t_x-t_y)\sum_n\langle x|n\rangle\langle n|y\rangle \tag{22}$$

$$=-i\delta(t_x-t_y)\langle x|\left(\sum_n|n\rangle\langle n|\right)|y\rangle \tag{23}$$

$$=-i\delta(t_x-t_y)\langle x|y\rangle \tag{24}$$

$$=-i\delta(t_x-t_y)\delta(x-y) \tag{25}$$

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