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The Free-Particle Green's Function in One Spatial and One Time Dimension

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Abstract

This paper will solve the one-dimensional free particle case of the Schrödinger equation, with an added Dirac delta. The purpose of the Dirac delta, which in this case is in terms of position and time, is to represent an impulse at a certain position and time; the solution represents the wave function response to this impulse. While the homogeneous case of the Schrödinger equation represents a particle peacefully existing, this particle responds to an instantaneous disturbance to a system at some point.

The solution will use a Green's function. This is different from other solutions because it pieces together two approaches that both make an educated guess as to the form of a function or a component of the solution. This guess step is different in both approaches, and by including two, we create a more comprehensive solution. Most other papers and lecture notes only verify a solution, not solve it through deduction as this paper demonstrates.

Keywords: Schrödinger equation, Green's functions, quantum mechanics, Dirac delta, partial differential equations (PDEs)

1. Introduction

The Schrödinger equation is a fundamental equation in quantum mechanics that governs the time evolution of quantum states.

In this paper, we solve the one-dimensional time-dependent Schrödinger equation for a free particle subject to a Dirac delta impulse at a specific position and time, using a Green's function. This is analogous to a particle having an instantaneous disturbance at a particular point and time (similar to dipping your finger into a still pond), but otherwise being in free space at all other moments. The primary motivation is to develop an airtight solution to the differential equation using two parallel derivations. The Green's function propagator we derive is a standard textbook result, and the contribution of our paper is expository and pedagogical.

There is existing literature on Green's functions for the Schrödinger equation. However, most papers verifying the form of Green's function for free particles often lack detailed deductions from basic principles. Some assume the form, often treating it as a classical result. While these approaches might be valid, there is still a need for a full derivation. It is difficult to find accessible full derivations that are not done from a perspective of verification. For example, although Fourier transform solutions are common, the phase shift $x - x'$ in is usually assumed and then verified afterwards to be true. In order to create an airtight solution, we combine two distinct methods: one based on Fourier transforms and another using the time-evolution operator and deducing the components of the Green's function.

In the Fourier transform approach, we assume the phase to be $x - x'$. In the time-evolution approach, we make an educated speculation that the Green's function kernel K is proportional to the time-evolution operator. By demonstrating that both methods converge to the same result, we have a more convincing bottom-up derivation that should enhance understanding of this classic result.

This paper thus contributes a thorough, accessible derivation suitable for advanced students and researchers, filling a niche in the pedagogical literature.

2. Methods

The Hamiltonian is quantized to form the free-particle Schrödinger equation $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$.

For the homogeneous case, separation of variables yields plane-wave solutions $\psi(x,t) = A\exp(ikx - i\omega t) + B\exp(-ikx - i\omega t)$, with $\omega = \frac{\hbar k^2}{2m}$.

The inhomogeneous case, incorporating a Dirac delta source $\delta(x - x')\delta(t - t')$, is solved using Green's functions via two complementary approaches. The first employs a Fourier transform in space, assuming a form $G(x,t;x',t') = \Theta(t - t')\int\frac{dk}{2\pi}\exp(ik(x - x'))g_k(t - t')$, leading to $g_k(\tau) = \exp\left(-i\frac{\hbar k^2}{2m}\tau\right)$, an evaluation via Gaussian integration. The second approach deduces the inclusion of the time-evolution operator $U = \exp(-iH(t - t')/\hbar)$, thereby expressing G in position representation by inserting momentum eigenstates and similarly evaluating the integral.

To address non-normalizability of the free-particle wave function, an infinite square well potential $V(x) = 0$ for $0 < x < a$ and infinite elsewhere is introduced. The time-independent Schrödinger equation is solved with boundary conditions $\Psi(0) = \Psi(a) = 0$, yielding $\Psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$ and discrete energies $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$.

3. The Schrödinger Equation

The Schrödinger equation is an equation in quantum mechanics. It is defined as follows:

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle\,. \tag{1}$$

$|\psi\rangle$ is a state ket, representing a particle's state and storing information about it such as its position, velocity, and sometimes instant in time (Sakurai, 1967).

According to classical mechanics, the Hamiltonian of a free particle is $H = \frac{p^2}{2m}$. In quantum mechanics, the momentum operator is

$$p = -\, i\hbar \frac{\partial}{\partial x} \,. \tag{2}$$

To obtain the quantum free particle Hamiltonian, we can apply the momentum operator twice:

$$p^2 = \left(-\, i\hbar \frac{\partial}{\partial x}\right)\left(-\, i\hbar \frac{\partial}{\partial x}\right) = -\, \hbar^2 \frac{\partial^2}{\partial x^2} \,. \tag{3}$$

Therefore, the Hamiltonian is

$$H = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \,. \tag{4}$$

Substituting into the Schrödinger equation, we get:

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} |\psi\rangle \tag{5}$$

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}\right) |\psi\rangle = 0 \,. \tag{6}$$

We have a second-degree linear operator applied to a wave function that yields zero. First, we are interested in solving for the wave function $|\psi\rangle$ in this homogeneous case. Second, we are also interested in seeing the properties of this linear operator applied to the Green's function, constituting the inhomogeneous case.

4. Homogeneous Case

We take ψ to be a function of position and time, $\psi(x, t)$. We first assume that ψ is separable into independent functions of position and time, so $\psi(x, t) = \phi(x)\tau(t)$. Then, we get

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}\right) \phi(x)\tau(t) = 0 \tag{7}$$

$$\phi(x) i\hbar \frac{\partial}{\partial t} \tau(t) + \tau(t) \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \phi(x) = 0 \tag{8}$$

$$i\hbar \frac{1}{\tau(t)} \frac{\partial}{\partial t} \tau(t) = -\, \frac{\hbar^2}{2m} \frac{1}{\phi(x)} \frac{\partial^2}{\partial x^2} \phi(x) \,. \tag{9}$$

Since the left side depends only on t and the right side depends only on x, both sides must equal some constant E. We can then solve this as two ordinary differential equations:

$$\frac{\partial}{\partial t} \tau(t) = \frac{-i}{\hbar} E \tau(t) \,. \tag{10}$$

We then find its solution:

$$\tau(t) = A\exp\left(\frac{-i}{\hbar}Et\right). \tag{11}$$

Next, we find the ODE in terms of x:

$$-\frac{\hbar^2}{2m}\frac{1}{\phi(x)}\frac{\partial^2}{\partial x^2}\phi(x) = E \tag{12}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) = E\phi(x). \tag{13}$$

Notice that this is the same as an eigenvalue equation with the Hamiltonian operator, $H\phi = E\phi$, so it can be said that the constant E is an eigenvalue of energy. First, note that $A^n|a'\rangle = a'|a'\rangle$ implies $f(A)|a'\rangle = f(a')|a'\rangle$ for analytic f:

$$f(A)|a'\rangle = \sum_{n=0}^{\infty}\frac{f^{(n)}(A)}{n!}A^n|a'\rangle, \tag{14}$$

and applying A to $|a'\rangle$ times yields

$$f(A)|a'\rangle = \sum_{n=0}^{\infty}\frac{f^{(n)}(A)}{n!}(a')^n|a'\rangle = f(a')|a'\rangle. \tag{15}$$

Therefore, as the Hamiltonian is an analytic function of momentum:

$$H|\phi\rangle = E|\phi\rangle = \frac{p^2}{2m}|\phi\rangle, \tag{16}$$

further separated into

$$\frac{\partial^2}{\partial x^2}\phi(x) = \frac{-2mE}{\hbar^2}\phi(x). \tag{17}$$

Since this is a second-order linear ODE, there are potentially two solutions, each having the negative exponential argument of the other. The argument is

$$\pm\sqrt{\frac{-2mE}{\hbar^2}}, \tag{18}$$

and we set $k = \sqrt{\frac{2mE}{\hbar^2}}$. Quickly substituting $E = \frac{p^2}{2m}$ shows that $k = \frac{p}{\hbar}$ and $p = \hbar k$, so k is the wave vector. The solutions are therefore

$$\phi(x) = M\exp(ikx) + N\exp(-ikx). \tag{19}$$

We can finally combine our two functions:

$$\psi(x,t) = \phi(x)\tau(t) = A\exp\left(ikx - \frac{i}{\hbar}Et\right) \tag{20}$$

or

$$\psi(x,t) = B\exp\left(-\ ikx - \frac{i}{\hbar}Et\right). \tag{21}$$

Using our definition for k, we can rearrange to state that

$$\frac{E}{\hbar} = \frac{\hbar k^2}{2m} = \omega\,. \tag{22}$$

As $E = \hbar\omega$, ω is the particle's angular frequency. so

$$\psi_1(x,t) = \phi(x)\tau(t) = A\exp(ikx - i\omega t) \tag{23}$$

or

$$\psi_2(x,t) = B\exp(-\ ikx - i\omega t)\,. \tag{24}$$

5. Inhomogeneous case and Green's function

The Green's function, in one spatial (x) and one temporal (t) dimension, for fixed x' and t' is

$$LG\left(x,t;x'\ ,t'\right) = \delta\left(x - x'\ \right)\delta(t - t')\,, \tag{25}$$

where the Dirac delta is the distribution defined as

$$\delta(\chi) = 0\ \ for\ \ \chi \neq 0\ \ and\ \ singular\ \ at\ \ \chi = 0 \tag{26}$$

such that

$$\int_{-\infty}^{+\infty} \delta(\chi)d\chi = 1\,. \tag{27}$$

L is a second-degree linear differential operator in terms of x and t with no cross-terms, p, q, u, v, w analytic, in the form

$$L = p(x,t)\frac{\partial}{\partial t} + q(x,t)\frac{\partial^2}{\partial t^2} + u(x,t)\frac{\partial}{\partial x} + v(x,t)\frac{\partial^2}{\partial x^2} + w(x,t)\,. \tag{28}$$

Notice that our previous linear operator can easily be cast into this form:

$$L = \left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right). \tag{29}$$

Applying it to our above case yields

$$\left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)G = \delta(x - x')\delta(t - t')\,. \tag{30}$$

This is the inhomogeneous case, which is significant as (x', t') is the "source". It is the exact position and time at which the system is disturbed. Imagine, for example, a lake that is peaceful until you suddenly poke your finger in it, exciting the system. The Green's function represents how the lake evolves in response to that instantaneous point source. Considering our situation, it is fitting to use an outgoing Green's function, meaning that $G(x, t; x', t') = 0$ when $t < t'$. There is no activity before our instantaneous source impulse "excites" the system, so there is no energy prior to t'. Therefore, the Green's function propagator is 0 prior to t'.

In terms of space, we will assume an infinite domain from $x \in R$, and that

$$\lim_{|x| \to \infty} G(x, t; x', t') = 0 \, , \tag{31}$$

as this inhomogeneous wave function should stay bounded at ∞.

5.1. First Solution

This solution makes an educated guess about the Fourier series' small variable $R = x - x'$. The second solution does not make this assumption; it instead makes a cautious deduction that the time-evolution operator is included in the Green's function, which this first solution rigorously derives. So, both solutions are missing something and fill each other's gaps.

First, we observe that the Green's function must include a step function as a factor, because we are working with the outgoing Green's function. The step function would ensure that, firstly, the Green's function is 0 prior to t', and that there is a discontinuous "jump" at t'. Thus, we define the step function as

$$\Theta(t) = I_{\{t \geq 0\}} \, , \tag{32}$$

where I_A is the indicator function for the set A, such that

$$\frac{d\Theta(t-t')}{dt} = \delta(t - t') \, . \tag{33}$$

Therefore, we write:

$$G(x, t; x', t') = \Theta(t - t') K(x, t; x', t') \tag{34}$$

We make an educated guess that K is the Fourier transform of a function f. The Fourier transform is

$$F(r) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{irt} f(t) dt \, . \tag{35}$$

We will define our Fourier transform K in terms of the wave vector k, which is proportional to p by $p = \hbar k$. For brevity, we will write $R = x - x'$ and $\tau = t - t'$ from now on.

$$K(x, t; x', t') = \int_{\mathbb{R}} \frac{dk}{2\pi} e^{ikR} g_k(\tau) \, . \tag{36}$$

$g_k(\tau)$ is a function of both k and t. Now, we want to extract this kernel, so we re-substitute this new expression for G back into our differential equation:

$$\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\Theta(t-t')K=\delta(t-t')\delta(x-x') \tag{37}$$

$$i\hbar\delta(\tau)K+i\hbar\Theta(\tau)\frac{\partial K}{\partial t}+\frac{\hbar^2}{2m}\Theta(\tau)\frac{\partial^2 K}{\partial x^2}=\delta(x-x')\delta(\tau)\,. \tag{38}$$

The second derivative of K with respect to position is

$$\frac{\partial^2 K}{\partial x^2}=\frac{\partial^2}{\partial x^2}\int_{\mathbb{R}}\frac{dk}{2\pi}e^{ikR}g_k(\tau)\,, \tag{39}$$

where we can differentiate under the integral sign:

$$\int_{\mathbb{R}}\frac{dk}{2\pi}g_k(\tau)\frac{\partial^2}{\partial x^2}e^{ikR}=\int_{\mathbb{R}}\frac{dk}{2\pi}g_k(\tau)(ik)^2e^{ikR}=-\int_{\mathbb{R}}\frac{dk}{2\pi}k^2g_k(\tau)e^{ikR}\,. \tag{40}$$

Supposing $\tau>0$, we get a homogeneous differential equation in terms of time:

$$i\hbar\frac{\partial}{\partial t}\left(\int_{\mathbb{R}}\frac{dk}{2\pi}e^{ikR}g_k(\tau)\right)+\frac{\hbar^2}{2m}\left(-\int_{\mathbb{R}}\frac{dk}{2\pi}k^2g_k(\tau)e^{ikR}\right)=0 \tag{41}$$

$$i\hbar\int_{\mathbb{R}}\frac{dk}{2\pi}e^{ikR}\frac{\partial g_k(\tau)}{\partial t}=\frac{\hbar^2}{2m}\int_{\mathbb{R}}\frac{dk}{2\pi}k^2g_k(\tau)e^{ikR}\,. \tag{42}$$

Because the Fourier transform is one-to-one, we equate the integrands:

$$i\hbar\frac{1}{2\pi}e^{ikR}\frac{\partial g_k(\tau)}{\partial t}=\frac{\hbar^2}{2m}\frac{1}{2\pi}k^2g_k(\tau)e^{ikR} \tag{43}$$

$$\frac{\partial g_k(\tau)}{\partial t}=\frac{-i\hbar}{2m}k^2g_k(\tau)\,. \tag{44}$$

The solution is

$$g_k(\tau)=\exp\left(\frac{-i\hbar k^2}{2m}\tau\right). \tag{45}$$

Notably, it is the time-evolution operator:

$$\exp\left(\frac{-i\hbar^2k^2}{2m\hbar}\tau\right)=\exp\left(\frac{-ip^2}{2m\hbar}\tau\right)=\exp\left(\frac{-iH}{\hbar}\tau\right). \tag{46}$$

Finally, we would like to solve for K, which now is

$$K(x,t;x',t')=\int_{\mathbb{R}}\frac{dk}{2\pi}\exp(ikR)\,\exp\left(\frac{-i\hbar k^2}{2m}\tau\right) \tag{47}$$

$$= \int_{\mathbb{R}} \frac{dk}{2\pi} \exp\left(i\left(\frac{-\hbar k^2}{2m}\tau + Rk\right)\right) = \int_{\mathbb{R}} \frac{dk}{2\pi} \exp\left(i\frac{-\hbar\tau}{2m}\left(k^2 - \frac{2mR}{\hbar\tau}k\right)\right). \tag{48}$$

We can use the scaled Gaussian for this:

$$\int_{\mathbb{R}} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}} \tag{49}$$

for $\alpha \in C$.

Completing the square in K yields

$$K(x, t; x', t') = \int_{\mathbb{R}} \frac{dk}{2\pi} \exp\left(i\frac{-\hbar\tau}{2m}\left(\left(k - \frac{mR}{\hbar\tau}\right)^2 - \left(\frac{mR}{\hbar\tau}\right)^2\right)\right) \tag{50}$$

$$= \int_{\mathbb{R}} \frac{dk}{2\pi} \exp\left(-\, i\frac{\hbar\tau}{2m}\left(k - \frac{mR}{\hbar\tau}\right)^2 + \frac{i}{2}\left(\frac{mR^2}{\hbar\tau}\right)\right) \tag{51}$$

$$= \exp\left(\frac{i}{2}\frac{mR^2}{\hbar\tau}\right)\frac{1}{2\pi}\int_{\mathbb{R}} \exp\left(-\, i\frac{\hbar\tau}{2m}\left(k - \frac{mR}{\hbar\tau}\right)^2\right) dk\,. \tag{52}$$

For $\tau \neq 0$, we can shift the integral to the right by $\frac{mR}{\hbar\tau}$ so $\alpha = \frac{i\hbar\tau}{2m}$ and the integral is equal to

$$\sqrt{\frac{\pi}{\alpha}} = \sqrt{\frac{\pi}{\frac{i\hbar\tau}{2m}}} = \sqrt{\frac{2\pi m}{i\hbar\tau}}\,. \tag{53}$$

Finally,

$$K(x, t; x', t') = \sqrt{\frac{m}{2\pi i\hbar\tau}} \exp\left(i\frac{mR^2}{2\hbar\tau}\right). \tag{54}$$

Therefore, our principal solution is

$$G_0(x, t; x', t') = \sqrt{\frac{m}{2\pi i\hbar(t-t')}}\Theta(t - t') \exp\left(i\frac{m(x-x')^2}{2\hbar(t-t')}\right), \tag{55}$$

and with homogeneous solutions added,

$$G(x, t; x', t') = A\psi_1(x, t) + B\psi_2(x, t) + G_0(x, t; x', t') \tag{56}$$

$$= A \exp(ikx - i\omega t) + B \exp(-\, ikx - i\omega t) \tag{57}$$

$$+ \sqrt{\frac{m}{2\pi i\hbar(t-t')}}\Theta(t - t') \exp\left(i\frac{m(x-x')^2}{2\hbar(t-t')}\right). \tag{58}$$

K is the path integral kernel. This result can be obtained with Feynman's path integral formulation, according to Sakurai's *Advanced Quantum Mechanics.*

5.2. Second Approach

First, we will rewrite the Hamiltonian as H instead of the differential operator, so that our eventual solution includes the Hamiltonian:

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)G = \delta(x - x')\delta(t - t') \tag{59}$$

Our first observation is that we can construct an outgoing Green's function by having a step function as a factor. So where K is a function of possibly, but not certainly, x and t,

$$G(x,t;x',t') = \Theta(t - t')K(x,t;x',t')\,. \tag{60}$$

Rearranging HG to the right and substituting our new definition of G,

$$i\hbar\frac{\partial}{\partial t}(\Theta(t - t')K(x,t;x',t')) = H(\Theta(t - t')K(x,t;x',t')) + \delta(x - x')\delta(t - t') = i\hbar\left(\delta(t - t')K(x,t;x',t') + \Theta(t - t')\frac{\partial K}{\partial t}\right) \tag{61}$$

$$= H\Theta(t - t')K + \delta(x - x')\delta(t - t')\,. \tag{62}$$

We are inclined to match the terms with Θ and the terms with δ. If they did not correspond, then

$$\delta(t - t')K = H\Theta(t - t')K \tag{63}$$

$$\delta(t - t') = H\Theta(t - t')\,, \tag{64}$$

which is a contradiction. Hence, the following must be true:

$$i\hbar\delta(t - t')K(x,t;x',t') = \delta(x - x')\delta(t - t') \tag{65}$$

$$i\hbar\Theta(t - t')\frac{\partial K}{\partial t} = H\Theta(t - t')K\,. \tag{66}$$

The first is 0 on both sides for $t \neq t'$, but does not imply directly that

$$i\hbar K(x,t;x',t') = \delta(x - x') \tag{67}$$

for $t = t'$. It may just happen that there are time-dependent components of K that are equal to 1 when $t = t'$.

However, even if the entirety of K is not equal to $\delta(x - x')$, we can deduce that specifically the position-dependent component of K is equal to $\delta(x - x') = \langle x|x'\rangle$, so K is proportional to $\langle x|x'\rangle$:

$$K \propto \delta(x - x') = \langle x|x'\rangle\,. \tag{68}$$

Additionally, at least for $t \geq t'$,

$$i\hbar\frac{\partial K}{\partial t} = HK\,, \tag{69}$$

which resembles the time-evolution Schrödinger equation:

$$i\hbar\frac{\partial U}{\partial t} = HU\,. \tag{70}$$

This also allows us to speculate that

$$K \propto U\,, \tag{71}$$

and as our Hamiltonian is time-independent ($t \geq t'$, of course), our time-evolution operator is

$$U(t) = \exp\left(-\frac{i}{\hbar}H(t - t')\right). \tag{72}$$

We have displaced the time origin by t'; this does not change any of our following operations, and we will find that this choice of origin corresponds with our final solution. With these two statements of proportionality, we can set up such that U is applied to $\langle x|x'\rangle$. From this equation from earlier,

$$i\hbar\delta(t - t')K(x,t;x',t') = \delta(x - x')\delta(t - t')\,. \tag{73}$$

It is clear that the constant coefficient of K is $-\,i/\hbar$. So, we have, with an educated deduction, that

$$K = \frac{-i}{\hbar}U\langle x|x'\rangle\,. \tag{74}$$

Now, we know that for p,

$$i\hbar\frac{\partial}{\partial x}\langle x|\alpha\rangle = \langle x|p|\alpha\rangle\,, \tag{75}$$

so there are two forms of the momentum operator: one applied to the entire position wave, which is a differential operator, and the other applied to the ket, which is a matrix operator. Right now, our time-evolution operator U is an analytic function of H, which is an analytic function of p. This means that U is an analytic function of p. Next, and to further determine properties of U, we can substitute K back into the differential equation:

$$= i\hbar\left(\delta(t - t')K(x,t;x',t') + \Theta(t - t')\frac{\partial K}{\partial t}\right) = H\Theta(t - t')K + \delta(x - x')\delta(t - t') \tag{76}$$

$$= \delta(t - t')\langle x|U|x'\rangle + \Theta(t - t')\frac{\partial}{\partial t}\langle x|U|x'\rangle = H\Theta(t - t')\langle x|U|x'\rangle + \delta(x - x')\delta(t - t')\,. \tag{77}$$

Given that the $\delta\left(t - t'\right)$ terms are equal to each other, we can integrate them both over all time:

$$\delta(t - t')\langle x|U|x'\rangle = \delta(x - x')\delta(t - t') \tag{78}$$

$$\int_{-\infty}^{\infty} dt\,\delta(t - t')\langle x|U(t)|x'\rangle = \int_{-\infty}^{\infty} dt\,\delta(x - x')\delta(t - t') = \delta(x - x')\,. \tag{79}$$

$\langle x|$ and $|x'\rangle$ are independent of time, so

$$\langle x|\left(\int_{-\infty}^{\infty} dt\,\delta(t - t')U(t)\right)|x'\rangle = \delta(x - x') \tag{80}$$

$$\langle x|U(t')|x'\rangle = \langle x|x'\rangle \,. \tag{81}$$

Therefore, $U(t')$ must equal 1, so

$$U(t) = \exp\left(-\frac{i}{\hbar}H(t - t')\right) . \tag{82}$$

Finally, to obtain actual values and not mere operators, we sandwich a complete set of momentum eigenkets to the right of U. This is because the momentum and time-evolution operator commute, as time evolution is an analytic function of momentum, so momentum eigenkets are simultaneous eigenkets of both momentum and time evolution (for a free particle with constant Hamiltonian).

$$K =- \frac{i}{\hbar}\langle x|U\left(\int_{\mathbb{R}} |p'\rangle\langle p'|dp\right)|x'\rangle =- \frac{i}{\hbar}\int_{\mathbb{R}} \langle x|U|p'\rangle\langle p'|x'\rangle\, dp' \tag{83}$$

$$=- \frac{i}{\hbar}\int_{\mathbb{R}} \exp\left(-\frac{i}{\hbar}\frac{(p')^2}{2m}(t - t')\right) \langle p'\rangle\langle p'|x'\rangle\, dp' \,. \tag{84}$$

Finding the form of $\langle x\rangle$,

$$\langle x'|p|\alpha\rangle =- i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle \,. \tag{85}$$

If we set $|p'\rangle = |\alpha\rangle$,

$$\langle x'|p|p'\rangle = p'\langle x'|p'\rangle =- i\hbar\frac{\partial}{\partial x'}\langle x'|p'\rangle \,. \tag{86}$$

We can suppose p' is fixed, and that $V(x') = \langle x'|p'\rangle$. Then, we get an easy ODE:

$$p'V(x') =- i\hbar\frac{\partial}{\partial x'}V(x') \tag{87}$$

$$V(x') = \langle x'|p'\rangle = N\exp\left(\frac{i}{\hbar}p'x'\right) \,. \tag{88}$$

N is

$$\delta(x'' - x') = \frac{1}{2\pi}\int_{\mathbb{R}} \exp\ (i(x'' - x')k)\ dk = \langle x''|x'\rangle = \int_{\mathbb{R}} dp'\langle x''|p'\rangle\langle p'|x'\rangle \,, \tag{89}$$

and setting

$$k = p/\hbar \,, \tag{90}$$

we find that $N^2 = \frac{1}{2\pi\hbar}$. Back to K:

$$K =- \frac{i}{\hbar}\int_{\mathbb{R}}\left(\frac{1}{2\pi\hbar}\right) \exp\left(-\frac{i}{\hbar}\frac{(p')^2}{2m}(t - t')\right) \exp\left(\frac{i}{\hbar}p'(x - x')\right) dp' \,, \tag{91}$$

which simplifies to, where $\tau = t - t'$ and $R = x - x'$,

$$K = -\frac{i}{\hbar}\int_{\mathbb{R}}\left(\frac{1}{2\pi\hbar}\right)\exp\left(-\frac{i\tau}{2m\hbar}\left(p' - \frac{mR}{\tau}\right)^2 + \frac{imR^2}{2\hbar\tau}\right)dp' \tag{92}$$

$$= -\frac{i}{\hbar}\frac{1}{2\pi\hbar}\exp\left(\frac{imR^2}{2\hbar\tau}\right)\int_{\mathbb{R}}\exp\left(-\frac{i\tau}{2m\hbar}\left(p' - \frac{mR}{\tau}\right)^2\right)dp' \,. \tag{93}$$

By the same Gaussian integral formula, we get

$$K = -\frac{i}{\hbar}\frac{1}{2\pi\hbar}\exp\left(\frac{imR^2}{2\hbar\tau}\right)\sqrt{\frac{2\pi m\hbar}{i\tau}} \tag{94}$$

$$= \sqrt{\frac{m}{2\pi i\hbar\tau}}\exp\left(\frac{imR^2}{2\hbar\tau}\right) = \sqrt{\frac{m}{2\pi i\hbar(t-t')}}\exp\left(\frac{im(x-x')^2}{2\hbar(t-t')}\right), \tag{95}$$

which confirms our original solution.

6. Discussion

Previous derivations and verifications of this Green's function solution often feel incomplete, as if one has to know the result beforehand to make these derivations. For example, the lecture notes for Physics 221B at UC Berkeley state a solution $\langle x|U|x'\rangle$, then verify the solution works afterwards (Littlejohn, 2020). Our derivation is more robust. Even though the individual solutions involve guesses—the Fourier transform approach guesses $R = x - x'$ and the time-evolution approach guesses that the time-evolution operator is included based on some proportionality conditions—the combination of both fills in each other's gaps. Additionally, the Fourier transform solution always assumes that the solution is continuous, so having the alternative solution further makes the derivation airtight.

This result is a foundational part of quantum mechanics and is mostly used as a concept in teaching. Therefore, it's often accepted to take this solution as a known result. However, it's also important to have a complete derivation to ensure people's foundational quantum mechanics knowledge is robust.

Beyond this, it is possible to investigate the free particle in higher spatial dimensions (which is mostly similar to this), and even potential systems, where we add a potential term $V(x)$ to the Hamiltonian. For example, we could investigate the infinite square well with a Green's function, by including the Dirac delta impulse, and other things like quantum tunnelling, by defining a potential region with $V(x) = 0$, and another with $V(x) = 1$.

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No generative AI was used in the creation of this paper.

Author Biography

Ryan Ng is a senior high school student at Renaissance College with a strong interest in many diverse fields, such as mechanics, general relativity, complex analysis, abstract algebra, critical theory, intersectionality, feminist peace theory, and evolutionary economics.

His work in "The free-particle Green’s function in one spatial and one time dimension" constructs an alternative pedagogical approach to the Green's function impulse case of the Schrödinger equation, using two parallel derivations. He has also done work constructing a completely contained derivation of Ehrenfest's theorem that includes alternative derivation methods for certain operator relations, and an analysis of radially symmetric potential wells, in particular, an infinitesimally thin ring.

In high school, Ryan has written reports on theoretical fluid dynamics, experimentally investigating the relationship between a rigid body's pivot point and its rotational properties. He has also conducted a study on intersectional feminism in Hong Kong.

Ryan hopes to continue pursuing physics research at university while exploring the many fields in academia.

Mentor Contribution Statement

As Ryan's mentor, I provided conceptual guidance and methodological feedback throughout the development of his paper on the Green's function. My role was pedagogical in nature: I helped Ryan identify the research problem and suggested structuring the problem. I also offered explanations of the mathematical foundations underlying each method.

All analytical work, derivations, and manuscript writing were carried out by Ryan independently.