Alternative method for determining the Feynman propagator of a non-relativistic quantum mechanical problem

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Abstract:

A direct procedure for determining the propagator associated with a quantum mechanical problem was given by the Path Integration Procedure of Feynman. The Green function, which is the Fourier Transform with respect to the time variable of the propagator, can be derived later. In our approach, with the help of a Laplace transform, a direct way to get the energy dependent Green function is presented, and the propagator can be obtained later with an inverse Laplace transform. The method is illustrated through simple one dimensional examples and for time independent potentials, though it can be generalized to the derivation of more complicated propagators.

Introduction

In contrast of the Hamiltonian emphasis in the original formulation of quantum mechanics, Feynmans approach could be referred to as Lagrangian and it emphasized the propagator $K(x,t,x',t')$ which takes the wave function $\psi(x',t')$ at the point x' and time t' to the point x, at time t i.e.

$$\psi(x,t) = \int K(x,t,x',t')\psi(x',t')dx' \tag{1}$$

While this propagator could be derived by the standard methods of quantum mechanics, Feynman invented a procedure by summing all time dependent paths connecting points x, x' and this became an alternative formulation of quantum mechanics whose results coincided with the older version when all of them where applicable, but also became relevant for problems that the original methods could not solve.

Introduction

In Feynmans approach the first step is deriving the propagator $K(x,t,x',t')$ and later the energy dependent Green functions $G(x,x',E)$. In this paper we invert the procedure, we start by deriving the $G(x,x',E)$ which is a simpler problem, at least in the one dimensional single particle case we will be discussing here. Once we have $G(x,x',E)$ the $K(x,t,x',t')$ is given by the inverse Laplace transform and can be written as

$$K(x,x',t) = \frac{1}{2\pi\hbar i}\int_{i\hbar c-\infty}^{i\hbar c+\infty} \exp(-iEt/\hbar)G(x,x',E)dE \tag{2}$$

where c is a constant that allows the upper line $i\hbar c + E$ in the complex plane of E to be above all the poles of $G(x,x',E)$. For compactness in the notation from now on we will take $t' = 0$ so we write $K(x,t,x',t')$ as $K(x,x',t)$. The real hard part in our approach will be the determination by (2) of $K(x,x',t)$ but this is a well defined problem in mathematics and procedures have been developed to solve it.

Introduction

This is then the program we plan to follow. In section 2 we show that for a single particle in one dimension (the initial case of our analysis) all we need to know are two independent solutions $u_E^{\pm}$ of the equation.

$$[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E]u_E^{\pm}(x,E) = 0 \tag{3}$$

to be able to derive $G(x, x', E)$ in section 3. We then consider in section 4, two elementary cases, the free one dimensional particle and the harmonic oscillator. In the first case the integral (2) is trivial to evaluate. In the case of the harmonic oscillator the evaluation of (2) requires a more careful analysis but it can be carried out. In all cases our final result is identical to the one in the book of Grosche and Steiner[1] that use Feynmans method to derive the results. Thus we have an alternative method for deriving $K(x, x', t)$.

The Hamiltonian and the propagator equation

We start with the simplest Hamiltonian of one particle in one dimension *i.e.*

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \tag{4}$$

with thus far an arbitrary potential $V(x)$.

>From the equation (1) that defines the properties of the propagator it must satisfy the equation

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) - i\hbar\frac{\partial}{\partial t}\right]K(x, x', t) = 0 \tag{5}$$

and besides if $t = 0$ it becomes

$$K(x, x', 0) = \delta(x - x') \tag{6}$$

We proceed now to take the Laplace transform of (5)

The Hamiltonian and the propagator equation

$$\int_0^\infty \exp(-st)\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)-i\hbar\frac{\partial}{\partial t}\right]K(x,x',t)ds=0$$

$$= \quad -\frac{\hbar^2}{2m}\frac{\partial^2\bar{G}(x,x',s)}{\partial x^2}+V(x)\bar{G}(x,x's)-i\hbar\int_0^\infty e^{-st}\frac{\partial K(x,x',t')}{\partial t}dt \tag{7}$$

where

$$\bar{G}(x,x',s)\equiv\int_0^\infty e^{-st}K(x,x',t)dt \tag{8}$$

We note though that

$$\int_0^\infty e^{-st}\frac{\partial K(x,x',t)}{\partial t}dt=\int_0^\infty\frac{\partial}{\partial t}\left[e^{-st}K(x,x',t)\right]dt$$
$$+s\int_0^\infty e^{-st}K(x,x',t)dt=\delta(x-x')+s\bar{G}(x,x',s) \tag{9}$$

where we made use of (6) and (8).

The Hamiltonian and the propagator equation

With the help of (9) we see that $\bar{G}(x, x', s)$ satisfies

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - i\hbar s \right] \bar{G}(x, x's) = i\hbar\delta(x - x') \tag{10}$$

where we now have that the partial derivative with respect to x becomes the ordinary one as there is no longer a time variable.

We integrate with respect to the variable x in the interval $x' - \epsilon \leq x \leq x' + \epsilon$ and in the limit $\epsilon \to 0$. Eq.(10) leads to the equations

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d\bar{G}}{dx}\right)_{x=x'+0} + \frac{\hbar^2}{2m}\left(\frac{d\bar{G}}{dx}\right)_{x=x'-0} \right] = i\hbar \tag{11}$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - i\hbar s \right] \bar{G}(x, x', s) = 0 \qquad x \neq x' \tag{12}$$

We proceed now to indicate how we can derive $K(x, x', t)$ with the help of $\bar{G}(x, x', s)$ of the corresponding problem satisfying (11) and (12).

Green function and its inverse Laplace Transform

Our interest is not to stop at Eq. (11), (12) for $\bar{G}(x, x', s)$ but actually to get $K(x, x', t)$ for which we can use the inverse Laplace transform $[2]$ to get

$$K(x, x', t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \bar{G}(x, x', s) e^{st} ds \tag{13}$$

where the integration takes place along a line in the complex plane s parallel to the imaginary axis and at a distance c to it so that all singularities of $\bar{G}(x, x', s)$ in the s plane are on the left of it.
To have a more transparent notation rather than the s plane we shall consider an energy variable E proportional to it through the relation

$$E = i\hbar s \quad \text{or} \quad s = -i(E/\hbar) \tag{14}$$

Green function and its inverse Laplace Transform

and define $G(x,x',E)$ by

$$G(x,x',E) \equiv \bar{G}(x,x',-iE/\hbar) \tag{15}$$

The energy Green Function, which must be symmetric under interchange of x and x', has then the property

$$G(x,x',E) = G(x',x,E) \tag{16}$$

which combines with the two equations (11), (12) to give in this notation

$$\left[\frac{dG}{dx}\right]_{x=x'+0} - \left[\frac{dG}{dx}\right]_{x=x'-0} = -\frac{2m}{\hbar^2} \tag{17}$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E\right]G(x,x',E) = 0 \qquad \text{for} \quad \mathrm{x} \neq \mathrm{x}' \tag{18}$$

Green function and its inverse Laplace Transform

Let us first consider the case when $x < x'$ and proceed to show that the equations (16), (17), (18) determine in a unique way the Green function of the problem. For this purpose we introduce with the notation $u_E^{\pm}(x)$ two linearly independent solutions of the equation (18)

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E \right] u_E^{\pm}(x) = 0 \tag{19}$$

>From this equation we see that

$$u_E^{-}(x)\frac{d^2 u_E^{+}(x)}{dx} - u_E^{+}\frac{d^2 u_E^{-}(x)}{dx} = \frac{d}{dx}\left(u_E^{-}\frac{du_E^{+}}{dx} - u_E^{+}\frac{du_E^{-}}{dx} \right) = 0 \tag{20}$$

Thus the Wronskian of the problem is independent of x, *i.e.*

$$W(E) = u_E^{-}(x)\frac{du_E^{+}}{dx} - u_E^{+}(x)\frac{du_E^{-}}{dx} \tag{21}$$

Green function and its inverse Laplace Transform

As $G(x, x', E)$ satisfies (18) we can write it for $x < x'$ as

$$G(x, x', E) = F(x', E) u_E^+(x), \tag{22}$$

choosing one of the two solutions of equation (18) and $F(x', E)$ is as yet an undetermined function of x', E.

We see from the symmetry of $G(x, x', E)$ that it must satisfy the same equation (18) in x' so that from (22) we get

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx'^2} + V(x') - E \right] F(x', E) = 0 \tag{23}$$

and thus $F(x', E)$ must be a linear combination of the two independent solutions $u_E^{\pm}(x)$ *i.e.*

$$F(x', E) = a_+(E) u_E^+(x') + a_-(E) u_E^-(x') \tag{24}$$

and our Green function becomes

$$G(x, x', E) = \Big[a_+(E) u_E^+(x') + a_-(E) u_E^-(x') \Big] u_E^+(x), \tag{25}$$

while for the other case, *i.e.* $x > x'$, the symmetry of the Green function demands

$$G(x, x', E) = \Big[a_+(E) u_E^+(x) + a_-(E) u_E^-(x) \Big] u_E^+(x'), \tag{26}$$

Replacing (25) and (26) in (17) we find that the coefficient $a_+(E)$ vanishes and $a_-(E)$ satisfies

$$a_-(E) W(E) = -\frac{2m}{\hbar^2}. \tag{27}$$

Thus from (25), (26) and (27) we get that

Green function and its inverse Laplace Transform

$$G(x,x',E) = -\frac{2m}{\hbar^2} W^{-1}(E) \begin{cases} u_E^-(x')u_E^+(x) & \text{if } x < x' \\ u_E^-(x)u_E^+(x') & \text{if } x > x' \end{cases} \tag{28}$$

We now have the explicit Green function of our problem once we can obtain two independent solutions of the equations (18).

Conclusion

Once $G(x, x', E)$ has been determined, the propagator $K(x, x', t)$ is given by the inverse Laplace transform (13) which in terms of the E variable becomes

$$K(x, x', t) = \frac{1}{2\pi\hbar i}\int_{i\hbar c-\infty}^{i\hbar c+\infty} \exp(-iEt/\hbar) G(x, x', E) dE \qquad (29)$$

where now the integral takes place in the E plane over a line parallel to the real axis with all the poles of $G(x, x', E)$ below it.
We proceed to give the results of some specific examples of our method.

Specific examples: The free particle

The potential $V(x)$ is taken as zero and so the equation (18)becomes

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-E\right]G(x,x',E)=0 \tag{30}$$

We introduce the variable k through the definition

$$E=\frac{\hbar^2k^2}{2m} \quad , \quad dE=\frac{\hbar^2k}{m}dk \tag{31}$$

and thus the $u_E^{\pm}(x)$ for this problem satisfy the equation

$$\left[\frac{d^2}{dx}+k^2\right]u_E^{\pm}(x)=0, \quad u_E^{\pm}(x)=\exp(\pm ikx) \tag{32}$$

with the Wronskian (21) given by

$$W(E)=2ik \tag{33}$$

Specific examples: The free particle

Thus from the two cases of (28) our function $G(x, x', E)$ is written compactly as

$$G(x, x'E) = \frac{im}{\hbar k} \exp[ik|x - x'|] \tag{34}$$

The propagator $K(x, x', t)$ is given by (29) in terms of $G(x, x', E)$ and substituting (34) in it we get

$$\begin{aligned} K(x, x', t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp[ik|x - x'| - i(\hbar k^2/2m)t]dk \\ &= \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left[\frac{im(x - x')^2}{2\hbar t}\right] \end{aligned} \tag{35}$$

which is also the result obtained by Feynmans method.

Specific examples: The harmonic oscillator

The potential $V(x)$ is proportional to x^2 and thus $u_E^{\pm}(x)$ satisfies the equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2-E\right]u_E^{\pm}(x)=0 \tag{36}$$

where ω is the frequency of the oscillator

We introduce the variables

$$z=\sqrt{\frac{2m\omega}{\hbar}}x \quad , \quad p=\frac{E}{\hbar\omega}-\frac{1}{2} \tag{37}$$

in terms of which the equation (36) takes the form

$$\left[\frac{d^2}{dz^2}-\frac{z^2}{4}+p+\frac{1}{2}\right]u_E^{\pm}(x)=0 \tag{38}$$

Specific examples: The harmonic oscillator

Two independent solutions of (38) are given by parabolic cylinder functions$[3]$*i.e.*

$$u_E^{\pm}(x) = D_p(\pm z) \qquad (39)$$

Following an analysis similar to that of the free particle we get

$$G(x, x', E) = \sqrt{\frac{2m}{\pi\hbar^3\omega}}\Gamma\left(\frac{1}{2} - \frac{E}{\hbar\omega}\right)D_{\frac{E}{\hbar\omega}-\frac{1}{2}}\left(\sqrt{\frac{2m\omega}{\hbar}}x_>\right)D_{\frac{E}{\hbar\omega}-\frac{1}{2}}\left(-\sqrt{\frac{2m\omega}{\hbar}}x_<\right). \qquad (40)$$

where

$$x_> = \max\{x, x'\}, \quad x_< = \min\{x, x'\} \qquad (41)$$

We want though to obtain $K(x, x', t)$ of (29) from (40) and we find out

$$K(x, x', t) = \left(\frac{m\omega}{2\pi i\hbar \sin \omega t}\right)^{1/2} \exp\left\{\frac{im\omega}{2\hbar \sin \omega t}\left[(x'^2 + x^2)\cos \omega t - 2xx'\right]\right\} \tag{42}$$

Again the result coincides with the one obtained from Feynman's method. We have treated the simplest Hamiltonians but the method can be generalized to many particles with angular momentum as well as to relativistic and time dependent problems.

References

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