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SHORT COMMUNICATION

Propagators in quantum mechanics

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ABSTRACT

We consider one-dimensional non-relativistic quantum mechanics to exhibit that the propagators (Green's functions) for free particle, linear potential and harmonic oscillator, are obtainable from purely classical means.

Keywords: Propagators in quantum mechanics, Green's functions

1. INTRODUCTION

The wave function $\psi(x, t)$ satisfies the Schrödinger equation [1]:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi, \quad (1)$$

which accepts solution via Green's technique [2]:

$$\psi(x, t) = \int_{-\infty}^{\infty} K(x, x', t) \psi(x', 0) dx', \quad (2)$$

where: $K(x, x', t)$ is the corresponding propagator for the potential $V(x)$, with the properties:

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) - i\hbar \frac{\partial}{\partial t}\right) K(x, x', t) = 0, \quad \lim_{t \rightarrow 0} K(x, x', t) = \delta(x - x'). \quad (3)$$

In according with Dirac [3, 4] and Feynman [5-7]:

$$K(x, x', t) \propto \exp\left(\frac{i}{\hbar} \int_0^t L dt\right), \quad (4)$$

being L the Lagrangian of the system under study. In (4) are important all paths with initial and final points $(x', 0)$ and (x, t) , respectively; in this connection we remember the comment from Sommerfeld [8]: 'The causality of the 20th century must not limit itself to the initial state, but must take end-state into consideration as an equally decisive moment'.

Here we determine the classical action integral $\int_0^t L dt$ associated with the path actually traversed between the points $(x', 0)$ and (x, t) , and after we eliminate the constants of integration to establish a posteriori the democracy of all paths between the given events. This approach affords a purely classical means of explicit evaluation of the propagator. In Sec. 2 we exhibit this elementary method to construct the propagators for free particle, harmonic oscillator and constant external field, where $V(x)$ is, at most, a second degree polynomial in x .

2. ELEMENTARY PROCEDURE TO CALCULATE THE PROPAGATOR

Here we find the propagator for some simple systems:

a). $V(x) = 0$.

For free particle we have that $\exp\left(\frac{i}{\hbar} \int_0^t \frac{p^2}{2m} dt\right) = \exp\left(\frac{i}{\hbar} \frac{p^2}{2m} t\right)$ because the linear momentum $p = m \frac{x-x'}{t}$ is a constant, hence from (4):

$$K(x, x', t) = N \exp\left[\frac{im}{2\hbar t} (x - x')^2\right], \quad (5)$$

which satisfies the Schrödinger equation. The relation:

$$\delta(x - a) = \lim_{\sigma \rightarrow 0} \frac{1}{\sigma\sqrt{\pi}} \exp\left[-\frac{(x-a)^2}{\sigma^2}\right], \quad (6)$$

permits to obtain N in (5) to verify (3), therefore the propagator for free particle is given by [1, 9-16]:

$$K(x, x', t) = \sqrt{\frac{m}{2\pi i \hbar t}} \exp \left[-\frac{m}{2i \hbar t} (x - x')^2 \right]. \quad (7)$$

b). $V(x) = kx$.

For this linear potential the classical equations of motion give $\dot{x} = c - \frac{k}{m}t$, $x = x' - \frac{k}{2m}t^2 + ct$, $c = \text{constant}$, $L = \frac{m}{2}\dot{x}^2 - kx$, then from (4):

$$K(x, x', t) = N \exp \left\{ \frac{i}{\hbar} \left[\frac{m}{2t} (x - x')^2 - \frac{k}{2} (x + x') t - \frac{k^2}{24m} t^3 \right] \right\}, \quad (8)$$

which verifies the Schrödinger equation. From (6) and (8) we determine the value $N = \sqrt{\frac{m}{2\pi i \hbar t}}$ to satisfy (3), thus we reproduce the expression reported in the literature [9, 10, 15, 17] for the propagator under a constant external field; the relation (8) with $k = 0$ gives (7) for free particle.

c). $V(x) = \frac{1}{2}m\omega^2x^2$.

For the harmonic oscillator the classical solution is given by:

$$x(t) = A \cos(\omega t + \varphi) = x' \cos(\omega t) - A \sin \varphi \cdot \sin(\omega t), \quad x' = A \cos \varphi, \quad (9)$$

then

$$\int_0^t L dt = \int_0^t \left(\frac{m}{2} \dot{x}^2 - \frac{m}{2} \omega^2 x^2 \right) dt = -\frac{m\omega}{2} [xx' \sin(\omega t) + A \sin \varphi \cdot (x \cos(\omega t) - x')],$$

hence (4) implies:

$$K(x, x', t) = N \exp \left\{ \frac{im\omega}{2\hbar \sin(\omega t)} [(x^2 + x'^2) \cos(\omega t) - 2xx'] \right\}, \quad (10)$$

because from (9) we have that $A \sin \varphi = \frac{[x' \cos(\omega t) - x]}{\sin(\omega t)}$. This expression (10) satisfies the Schrödinger equation and it is easy to see that $N = \sqrt{\frac{m\omega}{2\pi i \hbar \sin(\omega t)}}$ to verify (3) in according with (6), thus we have obtained the formula for the harmonic oscillator propagator [1, 9-12, 14-16, 18-23].

3. CONCLUSIONS

The Lagrangians here considered are quadratic in the velocities where $V(x)$ is, at most, a second degree polynomial [10, 12, 24, 25]. It is simple to check that the propagators (7), (8) and (10) satisfy the Trotter formula [12, 26, 27]:

$$K(x, x', t) = \left(\frac{m}{2\pi i \hbar t}\right)^{r/2} \exp\left\{\frac{i}{2\hbar}\left[\frac{m}{t}(x - x')^2 - (V(x) + V(x'))t\right]\right\}, \quad (11)$$

for $t \ll 1$ with $r = 1$. We find that in the three cases here studied the Fujiwara's result [9] is verified:

$$N = \sqrt{\frac{i}{2\pi\hbar} \frac{\partial^2}{\partial x \partial x'} \int_0^t L dt}. \quad (12)$$

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