The solution of the Schrödinger equation obtained from the solution of the Heisenberg equations

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It is shown that the knowledge of the solution of the Heisenberg equations for a given Hamiltonian allows us to find the corresponding propagator up to a time-dependent phase factor, which gives the solution of the Schrödinger equation.

Keywords: Heisenberg's equations; Schrödinger equation; propagator.

Se muestra que el conocimiento de la solución de las ecuaciones de Heisenberg para un hamiltoniano dado nos permite hallar el propagador correspondiente hasta un factor de fase dependiente del tiempo, el cual da la solución de la ecuación de Schrödinger.

Descriptores: Ecuaciones de Heisenberg; ecuación de Schrödinger; propagador.

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1. Introduction

In the standard formulation of the non-relativistic quantum mechanics, the time evolution of a quantum system can be studied assuming that the state vector (or, equivalently, the wavefunction) changes with the time, with the position and momentum operators being time-independent, or that the state vector is fixed, with the observables changing with the time according to the Heisenberg equations.

In view of the equivalence between these two approaches, one natural question is: Given the solution of the Heisenberg equations for the position and momentum operators, is it possible to use it to find the solution of the Schrödinger equation?

The aim of this paper is to show that the answer is, essentially, yes: If one has the solution of the Heisenberg equations for the position and momentum operators (in the case of spin-0 particles), then one can find the propagator or, equivalently, the time evolution operator, up to a phase factor that only depends on the time. The propagator determines the solution of the Schrödinger equation if the wavefunction at some initial time is given.

A closely related result was obtained in Ref. 1, where the propagator for one-dimensional systems with time-independent forces linear in q and p was calculated making use of the Heisenberg equations, without noticing that a similar procedure is applicable to any Hamiltonian (not necessarily time-independent or quadratic in the coordinates and momenta) if one assumes that the solution of the Heisenberg equations is known, regardless of whether it has the same form of the classical equations of motion or not. Another point missing in Ref. 1 is the fact that actually the Heisenberg equations do not determine the propagator in a unique way.

In Sec. 2 we present the basic equations, which are applied in Sec. 3 to find the propagator in the standard examples considered in the textbooks, starting from the solution of the Heisenberg equations.

2. From the solution of the Heisenberg equations to the propagator

The solution of the Schrödinger equation

$$\mathrm{i}\hbar\frac{\mathrm{d}\,|\psi(t)\rangle}{\mathrm{d}t} = H\,|\psi(t)\rangle \tag{1}$$

can be expressed as

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle, \tag{2}$$

where $U(t,t_0)$ is a unitary operator, called the time development operator, or time evolution operator, and $|\psi(t_0)\rangle$ represents the state of the quantum system at some initial time t_0. Then, Eq. (1) is equivalent to

$$\mathrm{i}\hbar\frac{\partial U(t,t_0)}{\partial t} = HU(t,t_0), \tag{3}$$

with the initial condition

$$U(t_0,t_0) = I, \tag{4}$$

where I is the identity operator. According to Eq. (2), the knowledge of the evolution operator amounts to having the solution of the Schrödinger equation for any initial state.

The evolution operator is usually given in an explicit manner through its matrix elements with respect to the basis formed by the eigenstates of the position operator. For instance, in the case of a particle in one dimension, these matrix elements are

$$K(x',t;x,t_0) \equiv \langle x'|U(t,t_0)|x\rangle. \tag{5}$$

The complex-valued function $K(x',t;x,t_0)$ is known as the propagator and, among other procedures, the path integral can be employed to calculate it (see, *e.g.*, Refs. 2 and 3, see also Ref. 4 and the references cited therein). (Usually a step function $\theta(t-t_0)$ is included on the right-hand side of Eq. (5), see, *e.g.*, Ref. 2, Sec. 2.6.)

If A is an operator representing some observable, the corresponding operator, A_H, in the Heisenberg picture is defined by

$$A_H(t) \equiv U(t,t_0)^{-1} A U(t,t_0). \tag{6}$$

Then, as a consequence of Eq. (3), the operator A_H obeys the Heisenberg equation

$$\mathrm{i}\hbar \frac{\mathrm{d}A_H}{\mathrm{d}t} = \mathrm{i}\hbar \left(\frac{\partial A}{\partial t}\right)_H + [A_H, H_H], \tag{7}$$

which is analogous to the equation appearing in Hamiltonian mechanics for the time derivative of a function defined on the extended phase space, with the commutator replaced by the Poisson bracket.

By contrast with the Schrödinger equation, which is commonly expressed as a partial differential equation, the Heisenberg equations are ordinary differential equations, which, in some cases, can be readily solved (frequently taking advantage of their similarity with classical equations of motion). According to Eq. (6), the solution of the Heisenberg equations involves the evolution operator. Hence, we can expect that the solution of the Heisenberg equations for the coordinates and momentum operators would determine the evolution operator and, hence, the solution of the corresponding Schrödinger equation.

In order to simplify the expressions below, we shall assume that there is one position operator and one momentum operator only. The equations corresponding to more general cases can be readily obtained. The solution of the Heisenberg equations

$$\frac{\mathrm{d}q_H}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}[q_H, H_H], \qquad \frac{\mathrm{d}p_H}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}[p_H, H_H], \tag{8}$$

must be of the form [see Eq. (6)]

$$\begin{aligned} U(t,t_0)^{-1} q U(t,t_0) &= F(q,p,t), \\ U(t,t_0)^{-1} p U(t,t_0) &= G(q,p,t), \end{aligned} \tag{9}$$

where $F(q,p,t)$ and $G(q,p,t)$ are operators made out of q, p, and t (see the examples below). Equations (9) are equivalent to

$$\begin{aligned} \langle x'|qU(t,t_0)|x\rangle &= \langle x'|U(t,t_0)F|x\rangle, \\ \langle x'|pU(t,t_0)|x\rangle &= \langle x'|U(t,t_0)G|x\rangle, \end{aligned}$$

that is,

$$\begin{aligned} x'\langle x'|U(t,t_0)|x\rangle &= \langle x'|U(t,t_0)F|x\rangle, \\ \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x'}\langle x'|U(t,t_0)|x\rangle &= \langle x'|U(t,t_0)G|x\rangle \end{aligned} \tag{10}$$

[see, *e.g.*, Ref. 2, Chap. 2, Eq. (188)]. These last equations constitute a system of differential equations for the propagator $\langle x'|U(t,t_0)|x\rangle$ containing partial derivatives of the propagator with respect to x and x' only. The order of these equations depends on the specific form of the operators F and G. In the examples considered below, Eqs. (10) turn out to be of first order. (By contrast, in all these examples, the Schrödinger equation for the wavefunction is a second-order partial differential equation.)

The system of Eqs. (10) *cannot* determine completely the propagator since if $U(t,t_0)^{-1}qU(t,t_0)$ and $U(t,t_0)^{-1}pU(t,t_0)$ satisfy the Heisenberg equations, then so do $\tilde{U}(t,t_0)^{-1}q\tilde{U}(t,t_0)$ and $\tilde{U}(t,t_0)^{-1}p\tilde{U}(t,t_0)$ if $\tilde{U}(t,t_0) \equiv f(t)U(t,t_0)$, for any non-vanishing complex-valued function $f(t)$. (In other words, if we multiply the operator $U(t,t_0)$ appearing in Eqs. (10) by an arbitrary function of t only, this function can then be eliminated from the equations, leaving them unaltered.) In order for $U(t,t_0)$ and $\tilde{U}(t,t_0)$ to be unitary, the modulus of $f(t)$ must be equal to 1, that is, $f(t)$ is a phase factor. (See the examples below and the discussion given in Sec. 4.)

3. Examples

We now present some standard one-dimensional examples, usually considered in the literature.

3.1. Propagator of a free particle

Even though the propagator of a free particle can be obtained as a particular case of the propagators calculated below, it will be instructive to start with this simple example.

If $H = p^2/2m$, then $H_H = {p_H}^2/2m$ and the Heisenberg equations (8) give

$$\frac{\mathrm{d}q_H}{\mathrm{d}t} = \frac{p_H}{m}, \qquad \frac{\mathrm{d}p_H}{\mathrm{d}t} = 0. \tag{11}$$

The solution of the second equation (11) is $p_H(t) = \text{const.}$, *i.e.*, $U(t,t_0)^{-1}pU(t,t_0) = \text{const.}$ and, by evaluating both sides of this equation at $t = t_0$, we find that

$$U(t,t_0)^{-1}pU(t,t_0) = p$$

[see Eq. (4)].

In a similar manner, from the first equation in (11) we obtain

$$U(t,t_0)^{-1}qU(t,t_0) = \frac{(t-t_0)p}{m} + q$$

[*cf.* Eq. (9)]. Hence,

$$\begin{aligned} pU(t,t_0) &= U(t,t_0)p, \\ qU(t,t_0) &= \frac{t-t_0}{m}U(t,t_0)p + U(t,t_0)q. \end{aligned} \tag{12}$$

The first equation in (12) amounts to

$$\langle x'|pU(t,t_0)|x\rangle = \langle x'|U(t,t_0)p|x\rangle,$$

i.e.,

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x'}K(x',t;x,t_0) = -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}K(x',t;x,t_0)$$

(which means that $K(x',t;x,t_0)$ depends on x and x' only through their difference). Similarly, the second equation in (12) is equivalent to

$$x'K(x',t;x,t_0) = \frac{t-t_0}{m}\left(-\frac{\hbar}{\mathrm{i}}\right)\frac{\partial}{\partial x}K(x',t;x,t_0) + xK(x',t;x,t_0).$$

Thus, we readily obtain

$$K(x',t;x,t_0) = F\exp\left[\frac{\mathrm{i}m(x'-x)^2}{2\hbar(t-t_0)}\right], \tag{13}$$

where the factor F may be a function of $t-t_0$ only. In order to find F we make use of Eq. (4) in the form

$$\lim_{t\to t_0}\int_{-\infty}^{\infty} K(x',t;x,t_0)\,\mathrm{d}x = 1, \tag{14}$$

which gives

$$\lim_{t\to t_0} F\sqrt{\frac{2\pi\mathrm{i}\hbar(t-t_0)}{m}} = 1.$$

This condition determines the function F up to a time-dependent factor whose limit as t goes to t_0 is equal to 1. The simplest choice is

$$F = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar(t-t_0)}} \tag{15}$$

and it can be verified that with this F, the expression given by (13) satisfies Eq. (3) with $H = p^2/2m$.

3.2. One-dimensional harmonic oscillator

Taking H as the standard Hamiltonian for a one-dimensional harmonic oscillator, we obtain the equations

$$\frac{\mathrm{d}q_H}{\mathrm{d}t} = \frac{p_H}{m}, \qquad \frac{\mathrm{d}p_H}{\mathrm{d}t} = -m\omega^2 q_H,$$

which have the form of the classical equations of motion for a one-dimensional harmonic oscillator. Hence,

$$q_H = \cos\omega(t-t_0)\,q + \frac{\sin\omega(t-t_0)}{m\omega}p,$$
$$p_H = -m\omega\sin\omega(t-t_0)\,q + \cos\omega(t-t_0)\,p,$$

which is equivalent to the equations

$$\langle x'|qU(t,t_0)|x\rangle = \cos\omega(t-t_0)\langle x'|U(t,t_0)q|x\rangle + \frac{\sin\omega(t-t_0)}{m\omega}\langle x'|U(t,t_0)p|x\rangle,$$
$$\langle x'|pU(t,t_0)|x\rangle = -m\omega\sin\omega(t-t_0)\langle x'|U(t,t_0)q|x\rangle + \cos\omega(t-t_0)\langle x'|U(t,t_0)p|x\rangle,$$

that is,

$$x'K(x',t;x,t_0) = x\cos\omega(t-t_0)K(x',t;x,t_0) - \frac{\sin\omega(t-t_0)}{m\omega}\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}K(x',t;x,t_0),$$
$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x'}K(x',t;x,t_0) = -m\omega x\sin\omega(t-t_0)K(x',t;x,t_0) - \cos\omega(t-t_0)\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}K(x',t;x,t_0).$$

The solution of these equations is

$$K(x',t;x,t_0) = F\exp\left\{\frac{\mathrm{i}m\omega[(x^2+x'^2)\cos\omega(t-t_0)-2xx']}{2\hbar\sin\omega(t-t_0)}\right\},$$

where F is a function of $t-t_0$ only. In this case, Eq. (14) yields

$$\lim_{t\to t_0} F\sqrt{\frac{2\pi\mathrm{i}\hbar\sin\omega(t-t_0)}{m\omega}} = 1,$$

which is satisfied with F given, *e.g.*, by Eq. (15) or by

$$F = \sqrt{\frac{m\omega}{2\pi\mathrm{i}\hbar\sin\omega(t-t_0)}}.$$

A straightforward computation shows that with this last expression, Eq. (3) is satisfied with the standard Hamiltonian $H = p^2/2m + \frac{1}{2}m\omega^2q^2$.

3.3. Particle in a uniform field

Letting

$$H = \frac{p^2}{2m} - eEq,$$

where e and E are constants, we have

$$\frac{\mathrm{d}q_H}{\mathrm{d}t} = \frac{p_H}{m}, \qquad \frac{\mathrm{d}p_H}{\mathrm{d}t} = eE,$$

with the solution

$$p_H = eE(t-t_0) + p,$$
$$q_H = \frac{eE}{2m}(t-t_0)^2 + \frac{t-t_0}{m}p + q.$$

Proceeding as in the foregoing examples we obtain the equations

$$\langle x'|pU(t,t_0)|x\rangle = eE(t-t_0)\langle x'|U(t,t_0)|x\rangle + \langle x'|U(t,t_0)p|x\rangle,$$
$$\langle x'|qU(t,t_0)|x\rangle = \frac{eE}{2m}(t-t_0)^2\langle x'|U(t,t_0)|x\rangle + \frac{t-t_0}{m}\langle x'|U(t,t_0)p|x\rangle + \langle x'|U(t,t_0)q|x\rangle,$$

which are equivalent to

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x'}K(x',t;x,t_0) = eE(t-t_0)K(x',t;x,t_0) - \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}K(x',t;x,t_0),$$

$$x'K(x',t;x,t_0) = \frac{eE}{2m}(t-t_0)^2K(x',t;x,t_0) - \frac{\hbar}{\mathrm{i}}\frac{(t-t_0)}{m}\frac{\partial}{\partial x}K(x',t;x,t_0) + xK(x',t;x,t_0).$$

One can readily find that the solution of this system of equations is given by

$$K(x',t;x,t_0) = F\exp\left\{\frac{\mathrm{i}m}{2\hbar T}\left[(x'-x)^2 + \frac{eET^2(x'+x)}{m}\right]\right\},$$

where $T \equiv t - t_0$, and F is a function of $t - t_0$ only. In order to satisfy Eqs. (3) and (4) with the Hamiltonian specified above, the function F has to be taken as

$$F = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar T}}\exp\left[-\frac{\mathrm{i}(eE)^2T^3}{24\hbar m}\right].$$

Alternatively, Eqs. (3) and (4) are satisfied with

$$F = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar T}}$$

if we take $H = p^2/2m - eEq - (eE)^2T^2/8m$.

4. Concluding remarks

As we have shown, the solution of the Heisenberg equations for the position and momentum operators allows us to find the propagator up to a time-dependent phase factor. This indeterminacy is a consequence of the fact that if we replace the Hamiltonian, H, by $H + h(t)$, where $h(t)$ is a multiple of the identity operator that depends on the time only, then this additional term commutes with all operators, and the Heisenberg equations (8) are left unchanged. On the other hand, the term $h(t)$ does not disappear from the Schrödinger equations (1) and (3), and even the addition of a constant to the Hamiltonian modifies the time evolution operator.

Whereas the Schrödinger equation is closely related to the Hamilton–Jacobi equation, the Heisenberg equations are similar to the Hamilton equations expressed in terms of the Poisson bracket; a term $h(t)$ added to the Hamiltonian has no effect in the Hamilton or the Heisenberg equations, but such a term has consequences on the Schrödinger and the Hamilton–Jacobi equation. (In the case of the Schrödinger equation, the addition of a term $h(t)$ to the Hamiltonian produces an additional time-dependent phase factor on the state vector, the wavefunction, or the time evolution operator.)

The result presented in this paper is analogous to the fact that, in classical mechanics, one can use the solution of the Hamilton equations to find a complete solution of the Hamilton–Jacobi equation. The solution of the system of equations (10) constitute a relatively easy way of finding the propagator, in comparison with other standard procedures, *provided that we already have the solution of the Heisenberg equations* (which, in general, may be a difficult task). An even simpler procedure consists in making use of the conserved operators that represent the initial position of the particle [5, 6], since one has to solve fewer equations. However, the relevant point here is that the solution of the Heisenberg equations can be used to obtain the evolution operator.

1. P. Nardone, *Am. J. Phys.* **61** (1993) 232.
2. K. Gottfried and T.-M. Yan, *Quantum Mechanics: Fundamentals*, 2nd ed. (Springer-Verlag, New York, 2003).
3. H.J.W. Müller-Kirsten, *Introduction to Quantum Mechanics* (World Scientific, Singapore, 2006).
4. F.A. Barone, H. Boschi-Filho and C. Farina, *Am. J. Phys.* **71** (2003) 483.
5. V.V. Dodonov, I.A. Malkin and V.I. Man'ko, *Int. J. Theor. Phys.* **14** (1975) 37.
6. G.F. Torres del Castillo, *Rev. Mex. Fís.* **61** (2015) 376.