A QUANTUM-MECHANICAL PARTICLE IN A TIME-DEPENDENT POTENTIAL FIELD

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The behavior of a particle moving according to the laws of quantum mechanics in a field, which potential changes over time, is studied. The method of unitary transformations for solving the temporal Schrödinger equation is considered. The reduced Hamiltonian of the system of a quantum-mechanical particle in time-dependent potential is obtained, as well as the total operator of the evolution of such a system. We find a new version of the unitary transformation, which, compared to the known ones, simplifies solving the problem in analytical form. This transformation associates the linear potential quantum model with time-dependent parameters and free-particle system. Based on the constructed evolution operator, we consider the wave packet dispersion. It is shown that the wave packet dispersion for this model is the same as that for a free particle. This conclusion is the general result of the behavior of a quantum-mechanical particle moving in the field of a time-dependent linear potential.

Keywords: quantum-mechanical particle, temporal Schrödinger equation, evolution operator, linear potential, unitary transformation, dispersion of wavepackage.

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1. Introduction

Study of time-dependent quantum systems is not only of academic interest, but is currently finding ever-widening applications in such fields of physics as quantum optics [1–3], quantum informatics [4, 5], physics of semiconductors [6, 7], etc. Schrödinger equations with a potential depending on time, which have analytical solutions, are of special interest. The best known exactly solved cases are time-dependent quantum harmonic oscillator [8–10] and time-linear potential [11–13].

Most of the works utilized the Lewis – Riesenfeld invariants technique [14] or the group-theory approach [15], which lead to exact wave functions of the irregular shape. But to solve these problems, it would be more rational to use the method of unitary transformations with further construction of the system evolution operator. The known research in this field [12] used the reduction of the Schrödinger equation with linear potential to the generalized oscillator equation. In addition, the Airy function was used to find wave packets. It should be emphasized that for such simple examples as time-dependent oscillator and linear potential, the problem of solving the Schrödinger equation is not easy, as the discussion in the literature suggests.

The objective of this work is to develop a simpler algorithm for finding the exact Schrödinger equation with time-dependent linear potential using a unitary transformation with direct conversion of this model to the case of a free particle, finding an exact solution and studying its capabilities and properties. The obtained results can be applied in scientific research on quantum physics. Moreover, despite the fact that in quantum mechanics courses the matter of time-dependent system description is rather neglected, a teacher can face with the problem of finding a fairly simple exactly solved example, which is fit for students. Therefore, this approach can be used in quantum mechanics teaching.

2. Lewis – Riesenfeld invariant method

The Schrödinger equation describing the motion of a particle in a potential field, which clearly depends on time, has the form

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \left(\frac{\widehat{\mathbf{p}}^2}{2m} + V(x,t)\right)\Psi(x,t). \tag{1}$$

Suppose that for a given system, in addition to the Hamiltonian operator $\widehat{H}(t)$, there is also a Hermitian operator $\widehat{I}(t)$ such that it is invariant, i.e. obeys the relation

$$\frac{d\widehat{I}}{dt} \equiv \frac{\partial \widehat{I}}{\partial t} - \frac{i}{\hbar}\left[\widehat{I}, \widehat{H}\right] = 0. \tag{2}$$

Substituting this operator into the left side of the equation (1), we find:

$$i\hbar\frac{\partial}{\partial t}\left(\widehat{I}\Psi(x,t)\right) = \widehat{H}\left(\widehat{I}\Psi(x,t)\right), \tag{3}$$

therefore, the action of this operator on the state vector will also be a solution of the equation (1). If we assume that the operator $\widehat{I}(t)$ is clearly independent of time, then it will be included in the complete set of operators. This means that its eigenfunctions

$$\widehat{I}(t)\varphi_\lambda(x,t) = \lambda\varphi_\lambda(x,t) \tag{4}$$

can differ from the eigenfunctions of the operator $\widehat{H}$ only by the phase factor

$$\Psi_\lambda(x,t) = e^{i\alpha_\lambda}\varphi_\lambda(x,t). \tag{5}$$

It follows from the equations (2)–(5) that the function α_λ must be a function of time only and satisfy the equation:

$$\frac{d\alpha_\lambda(t)}{dt} = \varphi_\lambda^{-1}\left(i\frac{\partial}{\partial t} - \frac{\widehat{H}}{\hbar}\right)\varphi_\lambda. \tag{6}$$

Thus, to solve the problem, it is necessary to find a suitable invariant or invariants, solve the problem of eigenfunctions, and construct a wave function that is a solution to the equation (1). For such simple examples as time-dependent oscillators and linear potentials, the problem is mathematically too complicated.

3. Unitary transformation method

One of widely accepted techniques for the exact solution of the Schrödinger equation is the method of unitary transformations [12], which is reduced to simple algebraic operations. Using this method, the Schrödinger equation with time-dependent potential is transformed into the equation for a free particle. The method of unitary transformations can be considered as the further development of the evolution operator method.

As far as is known, the system evolution operator is such an operator $\widehat{U}(t)$ that separates the time dependence from the wave function, leaving it dependent only on the spatial coordinates, i.e. the system evolution operator transforms the Schrödinger temporal equation into a stationary one. It is introduced using the relationship

$$\Psi(x,t) = \widehat{U}(t)\Psi(x), \tag{7}$$

where $\Psi(x)$ is the value of the wave function at the moment $t = 0$. At the same time, the operator $\widehat{U}(t)$ changes continuously with time and is unitary: $\widehat{U}^{+}(t)\widehat{U}(t) = 1$. At the initial moment, it coincides with the unity operator: $\widehat{U}(0) = 1$. The unitarity of this operator is necessary for preserving the normalization condition of the wave function, based on the properties of the Dirac representation, when the effect of the operator is transferred from the space vector to the state vector, it becomes the Hermite-conjugate one:

$$\left\langle \widehat{U}(t)\Psi|\widehat{U}(t)\Psi \right\rangle = \left\langle \Psi|\widehat{U}^{+}(t)\widehat{U}(t)\Psi \right\rangle = \langle \Psi|\Psi \rangle .$$

To determine the form of the operator $\widehat{U}(t)$, let's substitute the equation (7) into the unsteady-state Schrödinger equation (1) and obtain:

$$i\hbar \frac{\partial \widehat{U}(t)}{\partial t}\Psi(x) = \widehat{H}\widehat{U}(t)\Psi(x). \tag{8}$$

Since this equation is valid for an arbitrary function $\Psi(x,t)$, for the evolution operator we get the equation

$$i\hbar \frac{\partial \widehat{U}(t)}{\partial t} = \widehat{H}\widehat{U}(t). \tag{9}$$

In the case of a free particle, when the Hamiltonian $\widehat{H}_0 = -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}$ does not depend on time, the equation (9) can be integrated and the evolution operator can be represented in exponential form

$$\widehat{U}(t) = \exp\left(-\frac{i}{\hbar}\widehat{H}_0 t\right). \tag{10}$$

The obtained relation (10) enables to simplify finding the evolution operator for a particle in a time-dependent potential field by means of the unitary transformation, which converts the Hamiltonian of the interacting particle into the Hamiltonian for the free one.

In general terms, such transformation can be written as a set of equations:

$$\Psi(x,t) = A(t)e^{i\Phi(x,t)}\Psi_1(x,t), \quad x' = \frac{x}{C(t)} + B(t), \quad t' = D(t). \tag{11}$$

It takes into account the scaling and phase transformation of the wave function, as well as the scaling transformations of the coordinates and time along with the coordinate shift. Unfortunately, there is no general selection method for such a transformation. Besides, the successful selection of the corresponding functions could significantly simplify the solution of the problem.

4. Evolution operator for a particle in the time-dependent potential field

Let's consider a quantum-mechanical particle moving in the field of uniform force $F(t)$, which is determined by the potential energy of the form

$$V(x,t) = -F(t)x.$$

An instance of the practical application of such a problem is the case of the motion of a particle in the time-dependent electric field of a parallel-plate capacitor, as well as various physical processes modeling [16].

The Schrödinger temporal equation for our system (1) can be written as

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left(\frac{\widehat{\mathbf{p}}^2}{2m} - F(t)x\right)\Psi(x,t).$$

The equation (9) for the evolution operator in this case could not be solved by a simple substitution of the Hamiltonian, since it would not be commutative:

$$\left[\widehat{H}(t), \widehat{H}(\tau)\right] = i\hbar\frac{\widehat{\mathbf{p}}}{m}\left[F(\tau) - F(t)\right] \neq 0. \tag{12}$$

Then, for the evolution operator, we choose a special case of the unitary transformation (11) in the form

$$\widehat{U}(t) = e^{i\alpha(t)\,x}\widehat{\widehat{U}}(t), \tag{13}$$

where $\alpha(t)$ is some real-valued function, and $\widehat{\widehat{U}}(t)$ is the reduced unitary operator. In this case, the initial data are supplemented by another equation and represent the system:

$$\alpha(0) = 0, \quad \widehat{U}(0) = 1.$$

Substituting (13) into (9), we get the following expression:

$$i\hbar\left(\frac{\partial\widehat{\widehat{U}}(t)}{\partial t} + ix\frac{\partial\alpha(t)}{\partial t}\widehat{\widehat{U}}(t)\right) = e^{-i\alpha(t)x}\frac{\widehat{\mathbf{p}}^2}{2m}\left(e^{i\alpha(t)x}\widehat{\widehat{U}}(t)\right) - F(t)x\widehat{\widehat{U}}(t) \tag{14}$$

where $e^{-i\alpha(t)x}\dfrac{\widehat{\mathbf{p}}^2}{2m}e^{i\alpha(t)x}$ can be replaced by $\widehat{\mathcal{H}}(\widehat{\mathbf{p}}, t)$ – the reduced Hamiltonian, for which we have

$$\widehat{\mathcal{H}}(\widehat{\mathbf{p}}, t) = e^{-i\alpha(t)x}\frac{\widehat{\mathbf{p}}^2}{2m}e^{i\alpha(t)x} = \frac{\widehat{\mathbf{p}}^2}{2m} + \frac{\hbar\alpha(t)}{m}\widehat{\mathbf{p}} + \frac{\hbar^2\alpha^2(t)}{2m} = \frac{(\widehat{\mathbf{p}} + \hbar\alpha)^2}{2m}. \tag{15}$$

Due to the fact that $\widehat{\mathcal{H}}(\widehat{\mathbf{p}}, t)$ depends only on momentum and time and does not depend on the coordinate, we come to the equality

$$\left[\widehat{H}(t), \widehat{H}(\tau)\right] = 0,$$

which permits writing the reduced evolution operator $\widehat{\widehat{U}}(t)$ in the exponential form (10).

The solution of the equation (14) will be the set:

$$\begin{aligned} &\alpha(t) = \frac{1}{\hbar}\int\limits_0^t F(\tau)d\tau, \\ &\widehat{\widehat{U}}(t) = \exp\left\{-\frac{i}{\hbar}\int\limits_0^t \widehat{\mathcal{H}}(\widehat{\mathbf{p}}, \tau)d\tau\right\} = \exp\left\{-\frac{i}{\hbar}\left(\widehat{H}_0 t + \frac{\hbar\beta(t)}{m}\widehat{\mathbf{p}} + \frac{\hbar^2\gamma(t)}{2m}\right)\right\} \end{aligned} \tag{16}$$

where the notations are introduced to make the formulation more succinct:

$$\beta(t) = \int\limits_0^t \alpha(\tau)d\tau, \quad \gamma(t) = \int\limits_0^t \alpha^2(\tau)d\tau, \quad \widehat{H}_0 = \frac{\widehat{\mathbf{p}}^2}{2m}.$$

So, the total evolution operator of the system (13) is given by

$$\widehat{U}(x,\widehat{\mathbf{p}},t)=e^{i\alpha(t)x}\exp\left\{-\frac{i}{\hbar}\left(\widehat{H}_0t+\frac{\hbar\beta(t)}{m}\widehat{\mathbf{p}}+\frac{\hbar^2\gamma(t)}{2m}\right)\right\}, \tag{17}$$

which is the general form of the evolution operator for a particle placed in the linear potential field with any time-dependent force $F(t)$.

5. Wave packet dispersion

The evolution operator enables to describe the dynamics of the system under consideration completely. One of the most important questions is studying the influence of the force acting on the particle on the wave packet dispersion.

Let's consider the classical trajectory of a particle, which is given by the expression

$$\langle x\rangle(t)=\langle\Psi(t)|x|\Psi(t)\rangle$$

where $|\Psi(t)\rangle=\widehat{U}^{+}(t)|\Psi_0\rangle$, and $|\Psi_0\rangle$ is the initial state vector. This means, that it is necessary to find a matrix element

$$\overline{x}(t)\equiv\langle x\rangle(t)=\left\langle\Psi_0\left|\widehat{U}^{+}(t)x\widehat{U}(t)\right|\Psi_0\right\rangle.$$

From the explicit form of the evolution operator (17), it is clear that the phase function and term including $\gamma(t)$ will commute with x. In this case, it is necessary to calculate only the

$$\overline{x}(t)=\left\langle\Psi_0\left|\exp\left(i\frac{\beta(t)}{m}\widehat{\mathbf{p}}\right)\exp\left(\frac{i}{\hbar}\widehat{H}_0t\right)x\,\exp\left(-\frac{i}{\hbar}\widehat{H}_0t\right)\exp\left(-i\frac{\beta(t)}{m}\widehat{\mathbf{p}}\right)\right|\Psi_0\right\rangle \tag{18}$$

Applying the evolution operator $\widehat{U}_0$ for a free particle in the form

$$\widehat{U}_0(\widehat{\mathbf{p}},t)=\exp\left(-\frac{i}{\hbar}\widehat{H}_0t\right), \tag{19}$$

we get: $\exp\left(\frac{i}{\hbar}\widehat{H}_0t\right)x\,\exp\left(-\frac{i}{\hbar}\widehat{H}_0t\right)=x+\frac{\widehat{\mathbf{p}}}{m}t$. The remaining part of the operator specifies translations in the x-space

$$\exp\left(i\frac{\beta(t)}{m}\widehat{\mathbf{p}}\right)x\,\exp\left(-i\frac{\beta(t)}{m}\widehat{\mathbf{p}}\right)=x+\frac{\hbar\beta(t)}{m}. \tag{20}$$

Thus, we can write the expression (18) in the form

$$\overline{x}(t)=\langle x\rangle_0+\frac{\langle p\rangle_0}{m}t+\frac{\hbar\beta(t)}{m},$$

which coincides with the solution of the classical problem regarding the trajectory of a particle $x_{\text{class}}(t)$. In addition, $\hbar\alpha(t)$ corresponds to the force $F(t)$ momentum, and $\frac{\hbar\beta(t)}{m}$ describes the nonlinear time dependence of $x_{\text{class}}(t)$ due to inhomogeneous acceleration.

We define the dispersion of the wave packet as

$$[\Delta x(t)]^2 = \left\langle \Psi_0 \left| \widehat{U}^+(t) \, [x - \overline{x}(t)]^2 \, \widehat{U}(t) \right| \Psi_0 \right\rangle . \tag{21}$$

In order to identify the effect of force on dispersion, the expression (21) should be rearranged to an expression including the dispersion of a free particle $[\Delta x_0(t)]^2$. In view of this, we write down the expected value $\bar{x}_0(t)$ of the the free particle coordinate:

$$\overline{x}_0(t) = \left\langle \Psi_0 \left| \widehat{U}_0^+(t) \, x \, \widehat{U}_0(t) \right| \Psi_0 \right\rangle = \langle x \rangle_0 + \frac{\langle p \rangle_0}{m} t.$$

Thereafter,

$$\overline{x}(t) = \overline{x}_0(t) + \frac{\hbar \beta(t)}{m} \tag{22}$$

and the evolution operator (17) could be rewritten as

$$\widehat{U}(x, \widehat{\mathbf{p}}, t) = \exp\left[i \left(\alpha(t) x - \frac{\hbar \gamma(t)}{2m} \right) \right] \widehat{U}_0(\widehat{\mathbf{p}}, t) \exp\left(-i \frac{\beta(t)}{m} \widehat{\mathbf{p}} \right).$$

Therefore, the equation (21) with application of (20) takes the form

$$\begin{aligned} [\Delta x(t)]^2 = \left\langle \Psi_0 \left| \left\{ \widehat{U}^+ \left(x - \overline{x}(t) \right) \widehat{U} \right\}^2 \right| \Psi_0 \right\rangle = \\ = \left\langle \Psi_0 \left| \left[\widehat{U}_0^+ \left(x + \frac{\hbar \beta(t)}{m} - \overline{x}(t) \right) \widehat{U}_0 \right]^2 \right| \Psi_0 \right\rangle . \end{aligned} \tag{23}$$

Substituting (22), we finally find that

$$[\Delta x(t)]^2 = \left\langle \Psi_0 \left| \widehat{U}_0^+ \, [x - \overline{x}(t)]^2 \, \widehat{U}_0 \right| \Psi_0 \right\rangle \equiv [\Delta x_0(t)]^2 .$$

Thus, we come to the conclusion that the dispersion of the wave packet for a particle moving under the action of a spatially uniform but arbitrary time-dependent force will be the same as for a particle moving independently of the applied force.

Direct calculations for the dispersion result in the following:

$$[\Delta x(t)]^2 = (\Delta x_0)^2 + (\Delta p_0)^2 \frac{t^2}{m^2} + \left(\langle xp + px \rangle_0 - 2 \langle x \rangle_0 \langle p \rangle_0 \right) \frac{t}{m}.$$

It should be emphasized that the last term, which is linear in time, can be measured utilizing relevant choice of the initial state vector $|\Psi_0\rangle$.

6. Discussion of the obtained results

To explain the outcome, we recall that the spreading of the wave packet, which describes a quantum-mechanical particle, stems from the fact that frequency ω of each Fourier component of the wave packet is determined by the kinetic energy of the particle and this induces a nonlinear dependence $\omega(k) = \dfrac{\hbar k^2}{2m}$. As a result, the phase velocity of the particle is different for each harmonic component. As a consequence, the shape of the wave packet varies with time, although the group velocity remains constant. That is, even empty space is a dispersive medium for a quantum-mechanical particle. Note that in electrodynamics, an electromagnetic pulse never changes its shape until it enters the dispersive medium.

Let's consider how the dispersion relation arises from the obtained result. For this purpose, we express the wave function of an arbitrary state $\Psi(x,t)$ in terms of the initial state $\Psi_0(x)$

$$\Psi(x,t) = \widehat{U}(t)\Psi_0(x) = \int\limits_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \left\langle x \left| \widehat{U}(t) \right| p \right\rangle \Psi_0(p).$$

For the considered case, the explicit form of this function will be

$$\Psi(x,t) = \exp\left[i\left(\alpha(t) - \frac{\hbar\gamma(t)}{2m}\right)\right] \int\limits_{-\infty}^{\infty} dk\, \Psi_0(k)\, e^{i\Phi(x,k,t)}$$

where we introduce the phase function for each Fourier component

$$\Phi(x,k,t) = kx - \frac{\hbar k^2}{2m}t - \frac{\hbar\beta(t)}{m}k.$$

Due to the fact that the interaction energy is defined by the probability $|\Psi(x,t)|^2$, the factor outside the integral does not give any contribution. The phase rate for each Fourier component is given by the surface $\Phi = \text{const}$ velocity. Hence, we have for a fixed k

$$d\Phi(x,k,t) = \left(\frac{\partial\Phi}{\partial x}\right)_k dx + \left(\frac{\partial\Phi}{\partial t}\right)_k dt.$$

We obtain an expression for the phase velocity

$$V_{\text{ph}} = \frac{dx}{dt} = -\left(\frac{\partial\Phi}{\partial t}\right)_k \Big/ \left(\frac{\partial\Phi}{\partial x}\right)_k = V_{\text{ph}}^{(0)} + \frac{\hbar\alpha(t)}{m}$$

where $\alpha(t) = \beta'(t)$ and $V_{\text{ph}}^{(0)} = \dfrac{\hbar k}{2m}$ is a phase velocity for a free particle.

Therefore, the phase velocity of the wave packet for a particle in the potential field differs from the phase velocity for a free particle only by the second addend. But from the explicit form of this term, it is clear that it does not depend on k and, consequently, does not make changes in the dispersion. Thus, the dispersion calculated for $|\Psi(x,t)|^2$ will be the same as for a free particle $\left|\widehat{U}(t)\Psi_0(x)\right|^2$.

7. Conclusions

In this paper, we suggest a simple version of the unitary transformation, which reduces the quantum problem of motion in a linear potential field with time-dependent parameters to the system of a free particle. This transformation enables one to construct the evolution operator and obtain the solution of Schrödinger temporal equation in analytical form explicitly.

The obtained solution analysis shows that the wave packet for this model has the same dispersion as the wave packet for a free particle. Moreover, this conclusion does not depend on the specific form of the time dependence or the choice of the wave function of the initial state and represents the general result of the behavior of a quantum-mechanical particle moving in the field of time-dependent linear potential.

Considering the fact that there are few examples of exactly solved problems in quantum mechanics, especially for the Schrödinger temporal equation, this approach could find practical application in solving more complicated applied problems of modern physics.

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