Periodic systems in time: double-well potential

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Abstract

Time analysis of oscillations of a particle between wells in the one-dimensional double-well potential with infinite high outside walls, based on wave packet use and energy spectrum analysis, is presented. For the double-well potential of the form $x^2 + 1/x^2$ in the external regions, an exact analytical solution of the energy spectrum is found (by standard QM approach), an analysis of oscillation periodicity is fulfilled, an approach for exact analytical calculation of the oscillation period is proposed (for the first time).

Key words: double-well potential, discrete spectrum, oscillation period, wave packet, exactly solvable model, periodic system, tunneling time, supersymmetry

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1 Introduction

A quantum system, representing a particle in the potential field in the form of two wells with a finite high barrier and infinite high outside walls, is used in many different tasks of physics and chemistry [1].

If the tunneling of the particle through the barrier in such system is possible then there are transitions of this particle between the wells, named as “oscillations”. In the general case, the oscillations are not periodic (and also harmonic) motion. For their description one can introduce the following characteristics:
the time duration, after which the system returns into its initial state (this time characteristic can be named as oscillation period of the particle between the wells [2]) or period of Poincare’s cycle;  
- the time duration, after which the system has passed into a state closed as much as possible with initial one.

Instanton methods [3,4] are powerful tools for realization of a time analysis of a behaviour of the particle in the double-well potential. An alternative and less widespread approach for the time analysis of the double-well system behaviour consists in use of wave packets in spite of the fact that such system has discrete energy spectrum only [5]. If to localize the packet in the initial time moment inside one well than one can suppose that a maximum of this packet has passed into another well after some time duration. One can define the oscillation period of the particle between wells for the systems with a periodic motion and also one can define the time duration of the most probable return into the initial state for the system, which motion is not periodic, on the basis of transition of the packet maximum or the center of mass of this packet between the wells. Note that the packet maximum and the center of mass of the packet describe the tunneling process of the packet through the barrier in different ways. Here, if in the tunneling the localization of the wave packet in the space region of the barrier is improbable (apparently, it is possible only in one case of essential contribution into the total packet of its component for sub-barrier energies), than a motion of the center of mass of the packet in the barrier region looks natural enough.

An approach for calculation of these time characteristics for the double-well systems on the basis of analysis of energy spectrum is presented in this paper.

2 An analysis of the time periodicity of wave function on the basis of the energy spectrum

Let’s consider a system with the discrete energy spectrum where energy levels are located one from another at such distances, for which one can calculate exactly the largest general divisor:

$$E_n = E_0 + \Delta \cdot n,$$

where $n \in 0, N$ ($N$ is a set of natural numbers). In particular, a harmonic oscillator, a particle inside box, a charged particle in the Coulomb field satisfy to this condition. Wave function of such system has a form [6]:

$$\Psi(x, t) = e^{-iE_0 t/\hbar} \sum_n g_n \psi_n(x)e^{-i(E_n-E_0)t/\hbar} = e^{-iE_0 t/\hbar} \sum_n g_n \psi_n(x)e^{-i\Delta nt/\hbar},$$

(2)
where $\psi_n(x)$ are the orthonormal functions of the stationary states of the system satisfied to equation $\hat{H} \psi_n(x) = E_n \psi_n(x)$; $\hat{H}$ is Hamiltonian of the system; $\sum_n |g_n|^2 = 1$. We choose the time moment $t = 0$ for time zero.

Consider the function

$$f(x, t) = \Psi(x, t)e^{iE_0t/\hbar}$$

(3)

in the time interval $[-\pi\hbar/\Delta, \pi\hbar/\Delta]$. It satisfy to Dirichle’s condition [7]: a) one can divide this interval into a finite number of intervals where the function $f(x, t)$ is continuous, monotonous and finite; b) if $t_0$ is a point of discontinuity of the function $f(x, t)$, then $f(x, t_0 + 0)$ and $f(x, t_0 - 0)$ exist. And the sum $\sum_n g_n \psi_n(x)e^{-i(E_n - E_0)t/\hbar}$ in (2) is an expansion of the function $f(x, t)$ into the Fourier trigonometric series (with constant coefficients $\Delta/\hbar$) by variable $t$. Such series is convergent at any point $t$ of the interval $[-\pi\hbar/\Delta, \pi\hbar/\Delta]$, where the function $f(x, t)$ is continuous in $t$. In any break point $t_0$ the Fourier series converges to $\frac{f(x, t_0 + 0) + f(x, t_0 - 0)}{2}$. Therefore, the function $f(x, t)$ is periodic by variable $t$ in the interval considered above. This periodic dependence can be extended into whole range of definition of this function by $t$. One can calculate the period by such a way:

$$T_f = \frac{2\pi\hbar}{\Delta}.$$  

(4)

An exact analytical dependence of the periodic function $f(x, t)$ on time variable $t$ is determined by the total set of eigenfunctions $\psi_n(x)$ with coefficients $g_n$ at any point $x$ and is changed in dependence on $x$.

We find out an influence of the ground state with the level $E_0$ on a periodicity of the function $\Psi(x, t)$ in time. Consider the following example. Let the function $f(x_0, t)$ at point $x = x_0$ be harmonic by variable $t$ (assume that this function can be written as $\text{const} \cdot e^{-i\Delta t/\hbar}$), then we obtain:

$$\Psi(x_0, t) = \text{const} \cdot e^{-iE_0t/\hbar}e^{-i\Delta t/\hbar} = \text{const} \cdot e^{-i(E_0 + \Delta)t/\hbar}.$$  

(5)

One can see that the function $\Psi(x_0, t)$ is harmonic and periodic by time variable $t$ also. We find an exact analytical solution for a period of the function $\Psi(x_0, t)$ with taking into account the first level $E_0$:

$$T_\Psi = \frac{2\pi\hbar}{E_0 + \Delta} = \frac{2\pi\hbar}{E_1}.$$  

(6)

Using (6), we can analyse a contribution of the first level $E_0$ in the period $T_\Psi$. 

In particular, if to use the parabolic function \( U(x) = \frac{mw^2x^2}{2} \) as the potential energy of the system (where \( m \) is a mass of the particle, \( w \) is an oscillation frequency of the particle in classical mechanics), then the energy spectrum of the system has a form:

\[
E_n = (n + \frac{1}{2})\hbar w, \ n = 0, 1, 2...
\]  (7)

If there is a coordinate \( x_0 \) where the function \( f(x_0, t) \) is harmonic by time variable \( t \) then the oscillation period relatively this coordinate decreases in 1.5 times with taking into account the first level \( E_0 = \frac{hw}{2} \) (i.e. the contribution of the first level is not small):

\[
T_{\text{old}} = \frac{2\pi \hbar}{\Delta} = \frac{2\pi \hbar}{\hbar w}, \ T_{\text{new}} = \frac{2\pi \hbar}{E_0 + \Delta} = \frac{2\pi \hbar}{(\frac{1}{2} + 1)\hbar w} = \frac{2}{3} \frac{2\pi \hbar}{\hbar w} = \frac{2}{3} T_{\text{old}}. \]  (8)

Therefore, the function \( \Psi(x, t) \) is harmonic in time at point \( x \) only in such case when at this point \( x \) the function \( f(x, t) \) is harmonic in time also.

If the function \( f(x, t) \) is not harmonic then one can consider the function \( \Psi(x, t) \) as periodic in time approximately and evaluate its period. Let \( f_1(t) \) and \( f_2(t) \) be two periodic functions with periods \( T_1 \) and \( T_2 \), accordingly. We assume that these functions are harmonic in enough small neighborhood of the point \( (x, t) \). The period \( T \) (i.e. the time duration, after which the system has passed into a state closed as much as possible with initial one) can be calculated from the following relation:

\[
\frac{1}{T} = \frac{1}{T_1} + \frac{1}{T_2}. \]  (9)

Taking into account that the functions \( f(x, t) \) and \( \exp(-iE_0t/\hbar) \) are periodic by variable \( t \), one can determine conditions of the periodicity of the function \( \Psi(x, t) \).

Any quantum system with discrete energy spectrum performs a finite motion. But if there is the largest divisor \( \Delta \) determined exactly for energy level of this system and the condition (1) is satisfied, then in general case one can consider the time behaviour of this system as periodic approximately and one can calculate the period more accurately by (6) or (9) (i.e. with taking into account of the first level) whereas the expression (4) (i.e. without taking into account the first level) is less accurate. The calculation accuracy of oscillation period can be estimated on the basis of the set of orthogonal functions \( \psi_n(x) \) with coefficients \( g_n \) at selected point \( x \). This method of the estimation of the periodicity of the wave function can be used for the time analysis of the
oscillations of the particle between wells in the double-well potential with infinite high outside walls.

3 Exactly solvable models with symmetric double-well potential

Apparently, the spectrum of the double-well potential with any form is not equidistant. Nevertheless, we find the double-well potential form, for which there is the exact analytical dependence of the wave function on time and one can analyse its periodicity on the basis of the energy spectrum.

Let’s consider a quantum system, representing a particle in the symmetric double-well potential field of a form:

\[
U(x) = \frac{mw^2}{2} \begin{cases} 
(x + x_0)^2 + \frac{B^2}{(x + x_0)^2}, & \text{for } x > a > 0; \\
C - Dx^2, & \text{for } -a < x < a; \\
(x - x_0)^2 + \frac{B^2}{(x - x_0)^2}, & \text{for } x < -a < 0;
\end{cases}
\]  

where \( m > 0, \ w > 0, \ B > 0, \ C > 0 \) and \( D > 0. \) \( C \) determines the barrier height. We assume that \( B, \ C \) and \( D \) have such values that \( U(x) \) is continuous at points \( x = \pm a. \) Minimums of two wells are located at points \( x_1 = -\sqrt{B} + x_0 \) and \( x_2 = \sqrt{B} - x_0. \)

The potential \( (10) \) is symmetric. In result of sub-barrier tunneling and above-barrier propagation there are transitions of the particle between wells, i.e. its oscillations. One can analyse the period of such oscillations on the basis of the energy spectrum. For finding the spectrum it is need to resolve the stationary Schrödinger equation and take into account all conditions, to which the wave function satisfies. In the calculation of the energy spectrum for the potential \( (10) \) the boundary conditions at \( x \to -\infty \) and \( x \to +\infty \) play the important role. According with analysis, the conditions of the continuity of the wave function and its derivative at points \( x = \pm a \) do not differ the localization of the energy levels. Therefore, the solution of the stationary Schrödinger equation in the external regions \( x < -a \) and \( x > a \) has caused the main interest in calculation of the energy spectrum.
3.1 Calculations of the energy spectrum

We use new parameters:

\[ G = \frac{2mE}{\hbar^2}, \quad F = -\frac{m^2w^2}{\hbar^2}, \quad K = -\frac{m^2w^2B^2}{\hbar^2}. \]  

(11)

Then the stationary Schrödinger equation in the external regions transforms into a form:

\[ \frac{d^2\psi}{d\bar{x}^2} + \left( G + F\bar{x}^2 + K\bar{x}^2 \right) \psi = 0, \]  

(12)

where

\[ \bar{x} = x - x_0, \text{ for } \bar{x} < -a; \]
\[ \bar{x} = x + x_0, \text{ for } \bar{x} > a. \]  

(13)

We find a solution of this equation. Fulfill the replacements:

\[ \xi = \alpha \bar{x}^2, \quad \alpha = \frac{mw}{\hbar} = \sqrt{-F}, \quad \psi(\xi) = \left( \frac{\xi}{\alpha} \right)^{-1/4} w(\xi). \]  

(14)

Then the equation (12) transforms into the standard Whittaker form [8]:

\[ \frac{d^2w}{d\xi^2} + \left[ -\frac{1}{4} + \frac{G}{4\sqrt{-F} \xi} + \left( \frac{3}{16} + \frac{K}{4} \right) \frac{1}{\xi^2} \right] w = 0. \]  

(15)

Include the following parameters

\[ k = \frac{G}{4\sqrt{-F}}, \quad \mu^2 = \frac{1}{16} - \frac{K}{4}, \quad a = \frac{1}{2} - k + \mu, \quad c = 1 + 2\mu \]  

(16)

and fulfill the following replacement

\[ y(\xi) = \xi^{-c/2} e^{\xi/2} w(\xi). \]  

(17)

Then the equation (15) transforms into the hypergeometric equation of the form:

\[ \xi \frac{d^2y}{d\xi^2} + (c - \xi) \frac{dy}{d\xi} - ay = 0. \]  

(18)
Its partial solutions can be presented using the hypergeometric function \( F(a, c; \xi) \) in a form:

\[
\begin{align*}
y_1(\xi) &= F(a, c; \xi), \\
y_2(\xi) &= \xi^{1-c} F(a - c + 1, 2 - c; \xi), \\
y_3(\xi) &= e^\xi F(c - a, c; -\xi), \\
y_4(\xi) &= \xi^{1-c} e^\xi F(1 - a, 2 - c; -\xi).
\end{align*}
\]  

(19)

Consider the case: \( c \notin \mathbb{Z} \). Here, the solutions \( y_3 \) and \( y_4 \) can be written through \( y_1 \) and \( y_2 \) by Kummer’s transformation \([8]\). Therefore, they depend linearly on \( y_1 \) and \( y_2 \). We obtain the first two solutions \( y_1 \) and \( y_2 \) with initial variables:

\[
\begin{align*}
\psi_1(\bar{x}) &= \alpha^{1/2 + \mu} \bar{x}^{-1 + 2\mu} e^{-\alpha \bar{x}^2/2} F(a, 1 + 2\mu; \alpha \bar{x}^2), \\
\psi_2(\bar{x}) &= \alpha^{1/2 + \mu} \bar{x}^{-1} e^{-\alpha \bar{x}^2/2} F(a - 2\mu, 1 - 2\mu; \alpha \bar{x}^2).
\end{align*}
\]  

(20)

In accordance with the finiteness condition of the wave function, one can write:

\[
\begin{align*}
&\text{for } \psi_1(x) : a < 0, -N; 2\mu \notin -N, \\
&\text{for } \psi_2(x) : -a + 2\mu \in 0, N; 2\mu \notin N.
\end{align*}
\]  

(21)

After satisfying of these conditions the series (which define the hypergeometric functions for the solutions \( \psi_1 \) and \( \psi_2 \)) transform into polynomial, and the energy spectrum becomes discrete. One can find from the expressions (21) that the solutions \( \psi_1 \) and \( \psi_2 \) cannot be used at the same time. But both \( \psi_1 \) and \( \psi_2 \) corresponds to the same energy spectrum. Write expressions for the energy spectrum and wave function (we point out the wave function in the external regions only):

\[
\begin{align*}
&\begin{cases}
E_n^- = 2\hbar w \left( \frac{1}{2} + n - \mu \right); \\
\psi_{1,n}(x) = \alpha^{1/2 - \mu} \bar{x}^{-1 - 2\mu} e^{-\alpha \bar{x}^2/2} F(-n, 1 - 2\mu; \alpha \bar{x}^2), \quad \text{for } x < -a \text{ and } x > a; \\
\psi_{2,n}(x) = \alpha^{1/2 + \mu} \bar{x}^{-1} e^{-\alpha \bar{x}^2/2} F(-n, 1 - 2\mu; \alpha \bar{x}^2), \quad \text{for } x < -a \text{ and } x > a;
\end{cases} \\
&\begin{cases}
E_n^+ = 2\hbar w \left( \frac{1}{2} + n + \mu \right); \\
\psi_{1,n}(x) = \alpha^{1/2 + \mu} \bar{x}^{-1 + 2\mu} e^{-\alpha \bar{x}^2/2} F(-n, 1 + 2\mu; \alpha \bar{x}^2), \quad \text{for } x < -a \text{ and } x > a; \\
\psi_{2,n}(x) = \alpha^{1/2 - \mu} \bar{x}^{-1} e^{-\alpha \bar{x}^2/2} F(-n, 1 + 2\mu; \alpha \bar{x}^2), \quad \text{for } x < -a \text{ and } x > a.
\end{cases}
\end{align*}
\]  

(22)  

(23)
Here
\[ \mu = \frac{1}{4} \sqrt{1 + \frac{4m^2w^2B^2}{\hbar^2}}, \quad \bar{x} = \begin{cases} |x - x_0|, & \text{for } x < -a; \\ |x + x_0|, & \text{for } x > a, \end{cases} \] (24)

\[ n \in 0, N \ (N \text{ is the natural number set}) \text{ and the total set of the levels } E_n \text{ consists from sets } E_n^+ \text{ and } E_n^- . \]

One can consider a co-existence of two eigenfunctions \( \psi_1 \) and \( \psi_2 \) (not dependent linearly one from another) for any level \( E_n \) as the doubly degeneracy of the energy spectrum. In similar cases, an additional quantum number is used for marking the difference between such states. Inclusion of the asymmetry in such double-well potential gives the double splitting of the energy spectrum and leads to degeneracy removal. Instanton methods give a similar result.

3.2 The time analysis of the particle oscillations between the wells

We write the expressions (22) and (23) for the energy spectrum by such a way:

\[ E_n^\pm = 2 \hbar w \left( \frac{1}{2} \pm \mu \right) + 2 \hbar w n = E_0^\pm + \Delta \cdot n, \]
\[ E_0^\pm = 2 \hbar w \left( \frac{1}{2} \pm \mu \right), \]
\[ \Delta = 2 \hbar w. \] (25)

From here one can conclude that two sets of the energy levels \( E_n^+ \) and \( E_n^- \) represent independently equidistant spectrum. One can study them separately, as described two independent waves with their periods. Without of taking into account the first levels \( E_0^+ \) and \( E_0^- \), the periods for these waves are equal:

\[ T_f = \frac{2\pi \hbar}{\Delta} = \frac{\pi}{w}. \] (26)

With taking into account the first levels \( E_0^+ \) and \( E_0^- \), a dependence of the wave function \( \Psi(x, t) \) on time is defined by such a way:

\[ \Psi(x, t) = e^{-iE_0^+ t/\hbar} f^+(x, t) + e^{-iE_0^- t/\hbar} f^-(x, t), \] (27)

where \( f^+(x, t) \) and \( f^-(x, t) \) are the wave functions of these waves without of consideration of the levels \( E_0^+ \) and \( E_0^- \). The expression (27) represents the exact analytical dependence of the wave function on time. One can consider
approximately these two items as periodic with the periods $T^+$ and $T^-$ calculated on the basis of (6):

$$T^+ = \frac{2\pi \hbar}{E_0^+ + \Delta}, \quad T^- = \frac{2\pi \hbar}{E_0^- + \Delta} = \frac{2\pi \hbar}{E_1^-}.$$

(28)

One can calculate approximately the period of the particle oscillation between the wells in the potential (10):

$$\frac{1}{T} = \frac{1}{T^+ + T^-} + \frac{1}{T^+ - T^-}. \quad (29)$$

In accordance with (25), a distance between two nearest levels $E_n^+$ and $E_n^-$ (considered in some tasks as a splitting value of energy spectrum $E_n$ in result of tunneling through the barrier) can be calculated by such a way:

$$\Delta E = E_n^+ - E_n^- = \hbar w \sqrt{1 + \frac{4m^2w^2}{\hbar^2}B^2}. \quad (30)$$

If the barrier form satisfies to conditions of use of semi-classical methods then one can find a dependence of the penetrability coefficient $D$ of the barrier on the oscillation period $T$ and on the largest divisor $\Delta$ [2]:

$$D \sim \pi^2 \left( 1 + \frac{4m^2w^2}{\hbar^2}B^2 \right) = \pi^2 \left( 1 + \frac{m^2B^2}{\hbar^4} \Delta^2 \right) = \pi^2 \left( 1 + \frac{\pi^216m^2B^2}{\hbar^2} \frac{1}{T^2} \right). \quad (31)$$

4 Conclusions and perspectives

The approach for the time analysis of the double-well systems on the basis of energy spectrum is presented in this paper. For the double-well symmetric potential with the form $x^2 + B^2/x^2$ in the external regions the energy spectrum is calculated exactly analytically and the analysis of the time periodicity is fulfilled. The approach to approximate calculation of the oscillation period is described. Similar potentials were studied in [9].

During last two decades an essential progress in study of quantum system properties has achieved after rapid development of methods of supersymmetry in their application to quantum mechanics (here, one can note a review [10], which should be the best SUSY QM review at opinion of the author).
Application of such methods (in particular, see last subsections in [11]) to the analysis of periodicity of the particle motion (oscillations) between two wells in the double-well potential looks perspective and interesting in future study of periodical systems. For example, a question about change of the periodicity characteristics of the particle oscillations after going to new isospectral potentials from the potential considered in this paper can be interesting.

For the double-well non-periodic quantum system one can select “quasi-cycles” (after which the system has passed into a state closed as much as possible with initial one) with needed accuracy [2]. The maximal values of wave function of such systems are localized inside a finite space region and one can calculate the oscillation period with needed accuracy (with taking into account the needed number of “quasi-cycles”). From the other side, it is interesting to use such approach in the generalization of the SUSY QM methods, developed for the analysis of the periodical quantum systems (i. e. for the analysis of quasi-periodical systems).

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