Solution of the Schrödinger equation for parabolic double-well potential

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The models with double-well potentials are used in various branches of physics and are investigated in numerous papers. For example, many references can be found in [1–4].

In the present paper, we consider a symmetric potential $V(q) = V(-q)$ which has two minima at points $\pm q_0$ and maximum $V_0 = V(0)$. Without loss of generality it is possible to equate minima to zero by means of choice of an additive constant.

1. L.V. Chebotarev, Am. J. Phys. **66**, 1086-1095 (1998).
2. Chang-Soo Park, J. of the Korean Phys. Soc. **42**, 830-834 (2003).
3. P. Pedram, M. Mirzaei, S.S. Gousheh, Mol. Phys. **108**, 1949-1955 (2010).
4. A.V. Turbiner, Int. J. Mod. Phys. A **25**, 647-658 (2010).

There is a small number of double-well potentials which permit the exact solutions to the Schrödinger equation

$$\frac{d^2\Psi(q)}{dq^2} = \frac{2m}{\hbar^2}\big(V(q) - E\big)\Psi(q). \tag{1}$$

The most studied smooth double-well potential is the quartic potential $V(q) = V_0\big(q^2 - q_0^2\big)^2/q_0^4$. For this potential, the validity of approximation methods is examined in [1–4] since the exact solution of the Schrödinger equation (1) is unknown in this case.

The double oscillator

$$V(q) = \frac{1}{2}m\omega^2(|q| - q_0)^2 \tag{2}$$

was considered in [5]. This quadratic potential consists of two parabolas which meet with discontinuous slope at the point $q = 0$. At the same time this model is exactly solvable. Models with quadratic and quartic double-well potentials are compared in [6].

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5. E. Merzbacher, Quantum Mechanics, 3rd Ed., John Willey and Sons, Inc., New York, 1998.
6. V. Jelic, F. Marsiglio, Eur. J. Phys. **33**, 1651-1666 (2012).

In the present paper, we propose the generalization of formula (2). The new potential

$$V(q) = \frac{1}{2} m\omega^2 \begin{cases} q_0^2 - \dfrac{q^2}{g}, & |q| < gq_0, \\ \dfrac{(|q| - q_0)^2}{(1-g)}, & |q| > gq_0, \end{cases} \tag{3}$$

consists of two parabolic wells and central parabolic barrier. Here $0 < g < 1$.

The points $q_{\mp} = \mp g q_0$ are the points of inflection where the second derivative is discontinuous. However, both the function $V(q)$ and its first derivative are continuous. In this case $V_0 = m\omega^2 q_0^2/2$.

The potential (3) coincides with (2) if $g = 0$.

If $q_0 = 0$, the potential (3) turns into the potential of single harmonic oscillator $m\omega^2(1-g)^{-1}q^2/2$.

By analogy with [5] it is convenient to introduce dimensionless quantities

$$x = \sqrt{\frac{2m\omega}{\hbar}}q, \quad x_0 = \sqrt{\frac{2m\omega}{\hbar}}q_0, \quad e = \frac{E}{\hbar\omega} \tag{4}$$

and to transform the initial Schrödinger equation to the form

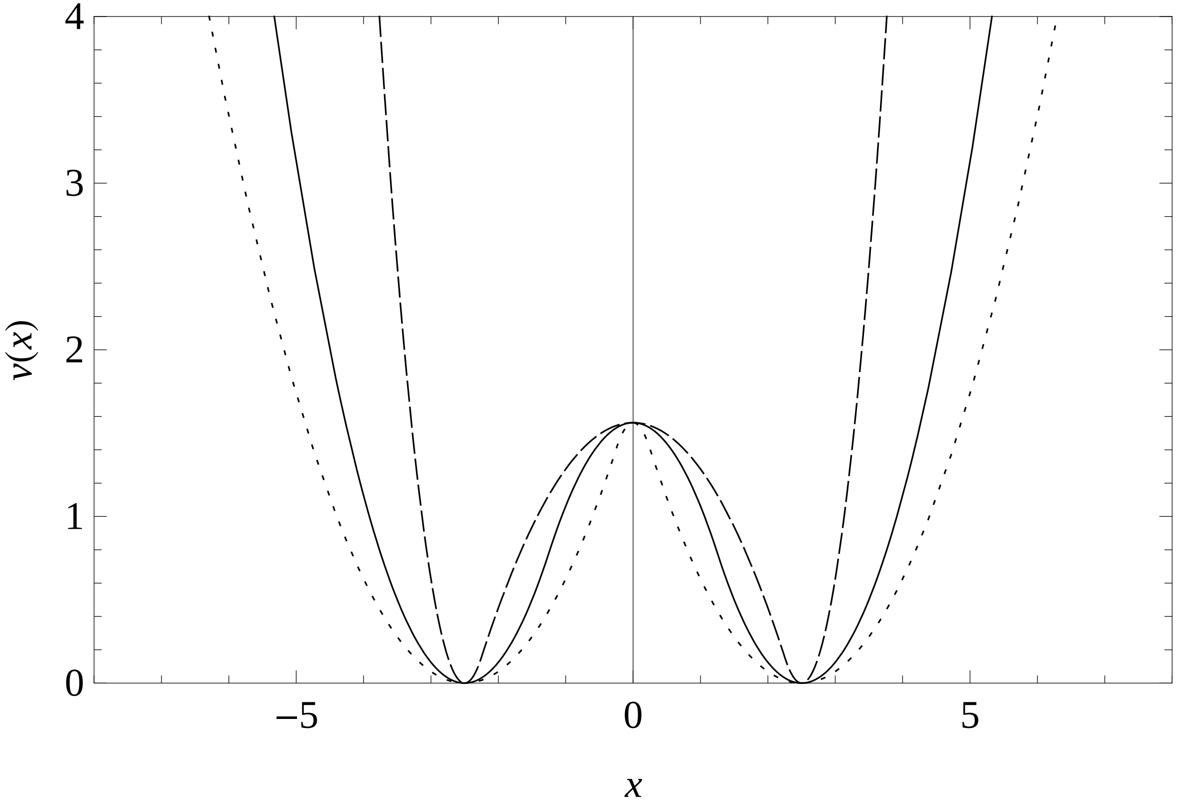
$$\frac{d^2\psi(x)}{dx^2} = \big(v(x) - e\big)\psi(x) \tag{5}$$

with reduced potential

$$v(x) = \frac{1}{4}\begin{cases} x_0^2 - \dfrac{x^2}{g}, & |x| < gx_0, \\ \dfrac{(|x| - x_0)^2}{(1-g)}, & |x| > gx_0. \end{cases} \tag{6}$$

Note that the value of the central maximum of the reduced potential is $v_0 = x_0^2/4$.

Fig. shows the behavior of the reduced potential for different values of g in the case of $x_0 = 2.5$. Here and in all subsequent figures, we use dotted lines for $g = 0.1$, solid lines for $g = 0.5$ and dashed lines for $g = 0.9$.



The reduced potential for different values of g

In the central region $|x| < gx_0$, the Schrödinger equation (5) for the potential (6) can be rewritten in the standard form [7]

$$\frac{d^2\psi_c}{dz_c^2} = \left(-\frac{z_c^2}{4} - d_c\right)\psi_c, \tag{7}$$

where

$$z_c = \frac{x}{g^{1/4}}, \quad d_c = g^{1/2}\left(e - \frac{1}{4}x_0^2\right). \tag{8}$$

The even $\psi_{c1}(x)$ and odd $\psi_{c2}(x)$ solutions of this equation are expressed through the confluent hypergeometric functions [7] with the help of formulas

$$\psi_{c1}(x_0, g, e, x) = e^{-iz_c^2/4} M\left(\frac{id_c}{2} + \frac{1}{4}, \frac{1}{2}, \frac{iz_c^2}{2}\right) + e^{iz_c^2/4} M\left(-\frac{id_c}{2} + \frac{1}{4}, \frac{1}{2}, -\frac{iz_c^2}{2}\right), \tag{9}$$

$$\psi_{c2}(x_0, g, e, x) = z_c e^{-iz_c^2/4} M\left(\frac{id_c}{2} + \frac{3}{4}, \frac{3}{2}, \frac{iz_c^2}{2}\right) + z_c e^{iz_c^2/4} M\left(-\frac{id_c}{2} + \frac{3}{4}, \frac{3}{2}, -\frac{iz_c^2}{2}\right). \tag{10}$$

It should be stressed that these solutions are real.

7. M. Abramovitz and I.A. Stegun (eds), Handbook of Mathematical Functions, Dover, New York, 1970.

In both side regions $x < -gx_0$ and $x > gx_0$ adjoining to the central region from the left and from the right, the wave functions satisfy another standard equation [7]

$$\frac{d^2\psi_s}{dz_s^2} = \left(\frac{z_s^2}{4} - d_s\right)\psi_s, \tag{11}$$

where

$$z_s = \frac{(|x| - x_0)}{(1-g)^{1/4}}, \quad d_s = (1-g)^{1/2}e. \tag{12}$$

The decreasing at $|x| \to \infty$ solution of this equation can be presented through the parabolic cylinder function [7] by means of the formula

$$\psi_s(x_0, g, e, x) = D_{d_s - 1/2}(z_s). \tag{13}$$

On the whole real axis $-\infty < x < \infty$, the continuous even $(i = 1)$ and odd $(i = 2)$ solutions of the Schrödinger equation with the symmetric smooth potential (6) can be written in the form

$$\psi_i(x_0, g, e, x) = N \begin{cases} \psi_{ci}(x_0, g, e, -gx_0)\psi_s(x_0, g, e, x), & x < -gx_0, \\ \psi_s(x_0, g, e, gx_0)\psi_{ci}(x_0, g, e, x), & -gx_0 < x < gx_0, \\ \psi_{ci}(x_0, g, e, gx_0)\psi_s(x_0, g, e, x), & x > gx_0. \end{cases} \tag{14}$$

The normalization coefficient N is determined by the condition

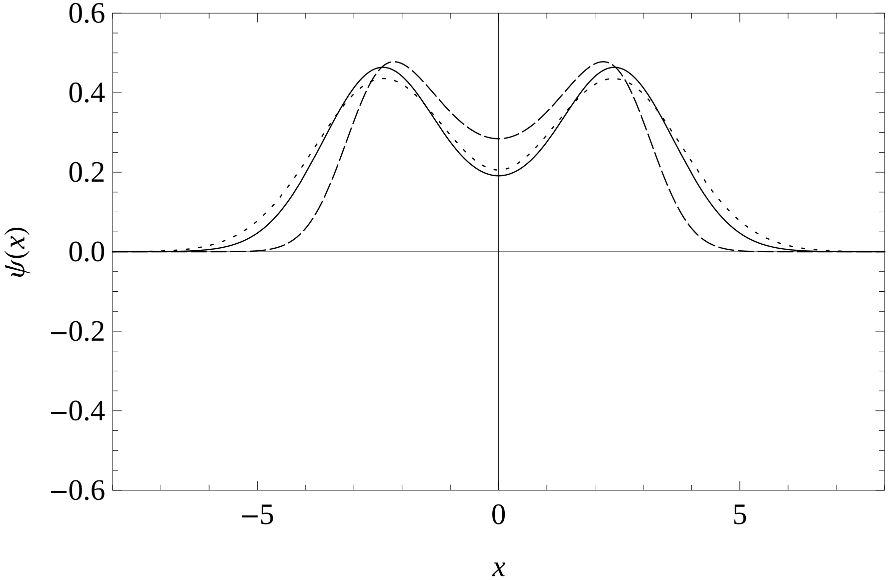
$$\int_{-\infty}^{\infty} \psi_i^2(x_0, g, e, x)\, dx = 1. \tag{15}$$

The additional requirement of continuity for the first derivative $\psi_i'(x_0, g, e, x) = d\psi_i(x_0, g, e, x)/dx$ at the point $x = gx_0$ leads to the energy quantization rule for even and odd states:

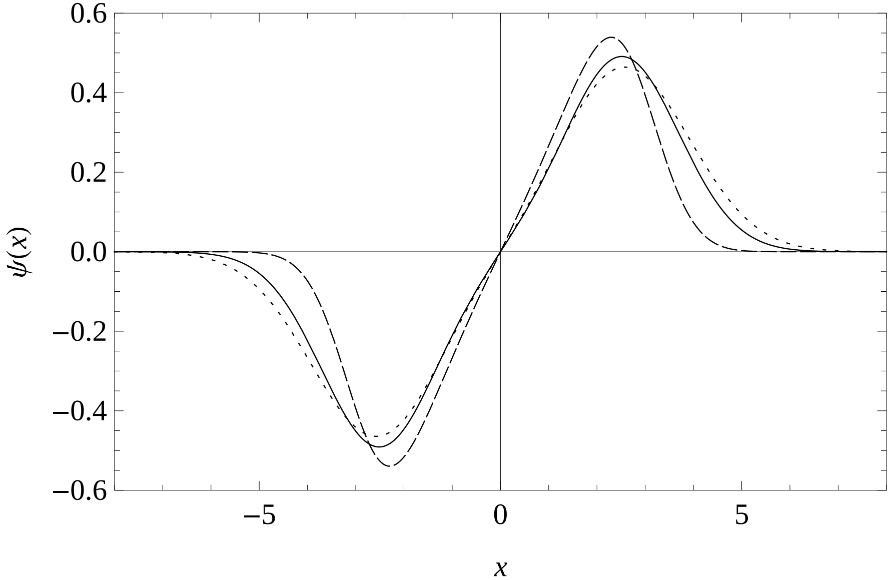
$$\psi_s(x_0, g, e, gx_0)\psi_{ci}'(x_0, g, e, gx_0) = \psi_{ci}(x_0, g, e, gx_0)\psi_s'(x_0, g, e, gx_0). \tag{16}$$

Due to the symmetry of potential this rule ensures continuity of the first derivative at the point $x = -gx_0$ too. The eigenvalues e of energy are easily found as the numerical solutions of the transcendental equation (16). Substituting obtained values of e into the formula (14) we get finally the eigenfunctions for the parabolic double-well potential.

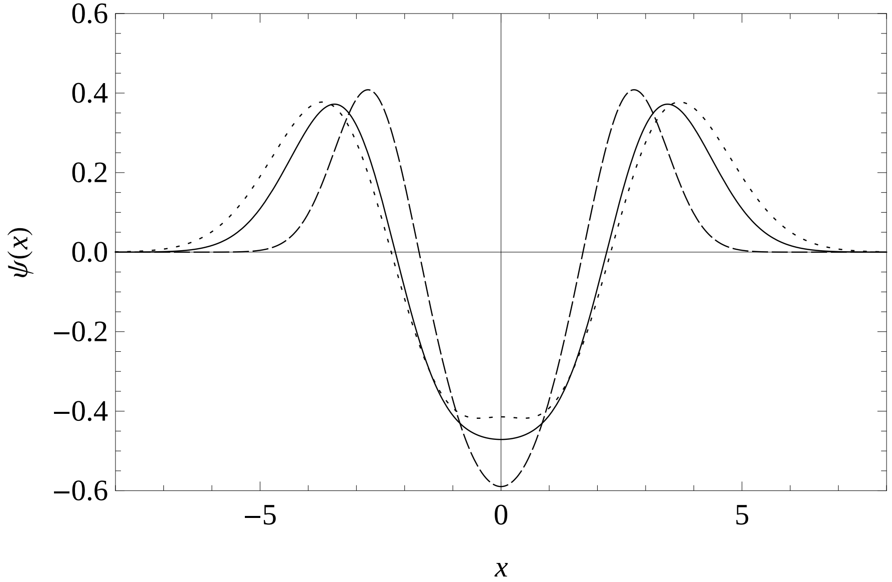
Figures show the normalized wave functions of the four lowest energy eigenstates for different values of g in the case of $x_0 = 2.5$.



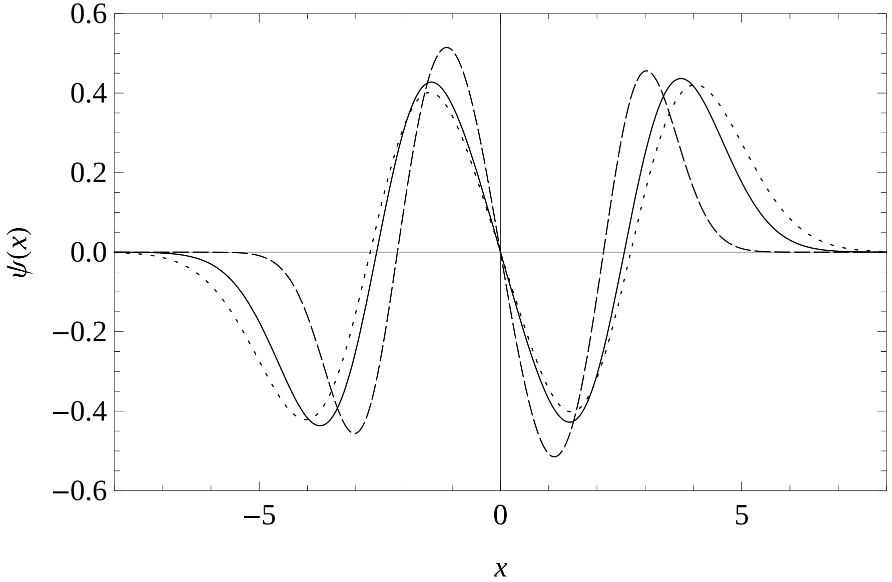
The ground state wave functions for different values of g



The first excited state wave functions for different values of g



The second excited state wave functions for different values of g



The third excited state wave functions for different values of g

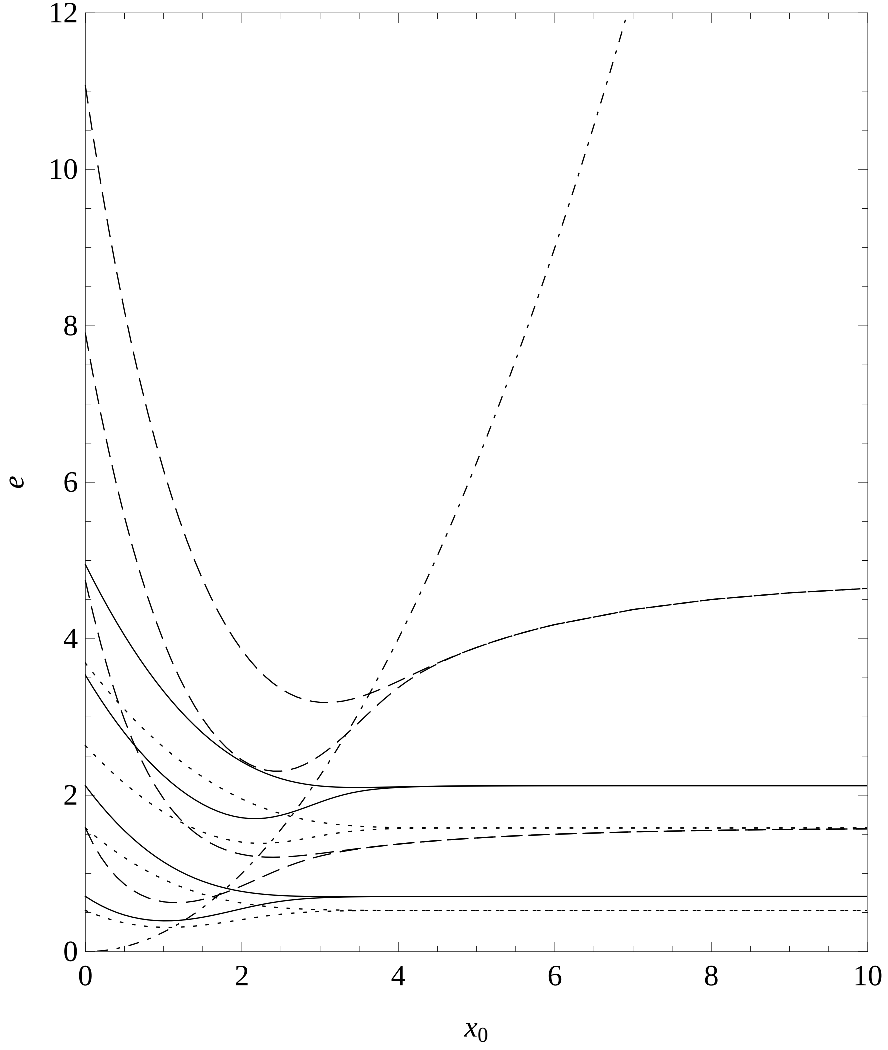


Fig. demonstrates dependence of the four lowest energy levels e on x_0 for different values of g. The dash-dot line reproduces the barrier height $x_0^2/4$ in the reduced potential.

There are pairs of lines which become indistinguishable at large values of x_0. This is the evidence of double degeneration of energy levels.

At $x_0 = 0$, in each pair, the values of nondegenerate lower (even) and upper (odd) levels are $(2n+1/2)/(1-g)^{1/2}$ and $(2n+1+1/2)/(1-g)^{1/2}$ respectively.

We see that at very large x_0, the indistinguishable levels tend to $(n+1/2)/(1-g)^{1/2}$.

References

[1] L.V. Chebotarev, Am. J. Phys. **66**, 1086-1095 (1998).

[2] Chang-Soo Park, J. of the Korean Phys. Soc. **42**, 830-834 (2003).

[3] P. Pedram, M. Mirzaei, S.S. Gousheh, Mol. Phys. **108**, 1949-1955 (2010).

[4] A.V. Turbiner, Int. J. Mod. Phys. A **25**, 647-658 (2010).

[5] E. Merzbacher, Quantum Mechanics, 3rd Ed., John Willey and Sons, Inc., New York, 1998

[6] V. Jelic, F. Marsiglio, Eur. J. Phys. **33**, 1651-1666 (2012).

[7] M. Abramovitz and I.A. Stegun (eds), Handbook of Mathematical Functions, Dover, New York, 1970.