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ORIGINAL PAPER

Applications of the amplitude-phase method to symmetric double-well potentials

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Abstract An amplitude-phase method is used to derive general quantization conditions for energy levels in smooth double-well potentials. The resulting quantization condition is applied to symmetric double-well potentials, where the two types of symmetry levels are shown to be determined by separate quantization conditions.

Keywords Mathematical methods · Semiclassical methods · Amplitude-phase method · Double-well potentials

1 Introduction

The quantum mechanical aspect of smooth symmetric double-well potentials is a long-standing and well-known problem. Double-well potentials arise due to quite different physical mechanisms and occur in condensed matter physics, in chemistry, in spectroscopy, as well as in recent topics of Bose–Fermi mixtures [1].

Several methods have been adopted and applied to the computations of energy levels, e.g. time-independent perturbation theory [2], the WKB (Wentzel–Kramers–Brillouin) approximation [3–6], the variation method [2–7], the analytical transfer matrix method [8,9], the instanton method [10,11] and other numerical computations [5,12,13]. In this list the numerical performance of the so-called amplitude-phase method seems to have been neglected since an early attempt in reference [14].

The (semi-classical) WKB approximation is widely used for its simple approach and deep understanding of the relation between classical and quantal mechanics. However, the occurrence of classical turning points and the intricate quantal transitions involved

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as turning points come close to each other limits its use among nonspecialists of the WKB method.

In the present study an amplitude-phase approach is applied to derive a general quantization condition for double-well potentials, improving an early attempt of the present idea in [14]. The insights of quantal transitions are comparable with those of WKB results, but avoiding much of the analytical complexities of the WKB theory. The initial ideas of Milne, Young and Wheeler in the 1930s [15–19] has developed slowly over the years, with some later advances in references [14,20–23]. Applications using two amplitude functions were recently presented for barrier transmission problems [24] and for calculations of Regge poles [25].

Section 2 presents a non-relativistic Schrödinger equation for a general potential. The amplitude-phase method for single-well and double-well bound states is presented in Sect. 3. Details of computations and results are in Sect. 4, and conclusions are in Sect. 5.

2 Basic Schrödinger equation

The Schrödinger equation can be written in dimensionless units as

$$\Psi'' + R(x)\Psi = 0, \tag{2.1}$$

Ψ is the bound-state wave function, a prime ($'$) denotes a derivative along an x-axis in space. The coefficient function $R(x)$, given by

$$R(x) = 2m[E - V(x)], \tag{2.2}$$

contains parameters for mass (m) and energy (E), as well as the potential $V(x)$. Two potentials are used for numerical illustrations. One potential is given by

$$V(x) = x^4 - \lambda x^2, \quad m = 1/2, \tag{2.3}$$

where λ is a coupling parameter with values $\lambda = 0, 1, 6$ and 10. A second potential related to Bose-Fermi condensate mixtures, see references [1,6], is

$$V(x) = x^2/2 + 9\mathrm{e}^{-x^2}, \quad m = 1. \tag{2.4}$$

3 Amplitude phase method

3.1 Single well

The amplitude-phase method used here for computations is well known [14–19,22] and is only briefly rephrased here. Reference [14] is an excellent reading on the early and basic ideas of the method.

If there is a single classically allowed interval of the x-axis, where the coefficient function satisfies $R(x) > 0$, a bound state wave function $\Psi(x)$ can be represented in terms of an amplitude $u(x)$ and a phase $\phi(x)$ along the entire x-axis as [14–19]

$$\Psi(x) = Cu(x)\sin\phi(x). \tag{3.1}$$

The normalization constant C may be arbitrary in the present context, but the phase $\phi(x)$ is obtained from the amplitude function u by

$$\phi(x) = \int_{-\infty}^{x} u^{-2}(x)\mathrm{d}x, \quad \phi(-\infty) = 0. \tag{3.2}$$

For this representation to vanish as $|x| \to \infty$ the phase has to satisfy

$$\phi(+\infty) = (n+1)\pi, \tag{3.3}$$

where $\phi(+\infty)$ represents the total phase change of the wave function across the potential well. Equation (3.3) is a Bohr-Sommerfeld-type bound-state quantization condition, where n is the number of nodes of the wave function in the well.

As explained in references [14,25] the exact representation (3.1) is an oscillating function only in the classically allowed region, where $R(x) > 0$. In classically forbidden regions ($R(x) < 0$) the phase function $\phi(x)$ converges to a constant value, if integrated from the classically allowed region. In the present case the converged phase value is initially zero, by choice of the lower integration limit in (3.2). This convergence of the phase is a result of the rapid increase of the amplitude $u(x)$. However, the phase convergence is faster than the divergence of the amplitude as the wave penetrates in to a classically forbidden region.

The amplitude function u is a solution of a non-linear (Milne-type) differential equation [15–19]

$$u'' + R(x)u = u^{-3}, \tag{3.4}$$

where $R(x)$ is the coefficient function for any of the potentials given in Sect. 2. Equation (3.4) is solved numerically from certain initial conditions. The phase integral in (3.2) can be calculated along with u, i.e. along with the integration of (3.4). For potentials symmetric with respect to $x = 0$, and being finite there, it is convenient to use only the positive x-axis with the initial conditions at $x = 0$ (see [14])

$$u(0) = R^{-1/4}(0), \quad u'(0) = 0, \tag{3.5}$$

and integrating sufficiently far out towards $x \to +\infty$. The initial value $u(0)$ in (3.5), which is always strictly positive, does not generally affect the results. However, due to 'latent' oscillations in $u(x)$ by 'wrong' initial conditions, if conditions on $u(0)$ (3.5) are significantly perturbed, the speed of the computation is lost. In case the coefficient $R(x)$ being symmetric, one can use any symmetric amplitude solution $u(x)$ of (3.4) satisfying (3.5), so that

$$\phi(+\infty) = 2\int_{0}^{+\infty} u^{-2}\mathrm{d}x. \tag{3.6}$$

The initial value $u'(0) = 0$ guarantees the symmetry of the amplitude function $u(x)$ in that case. Since the amplitude function has no zeros on the real axis, all nodes in the wave function are due to zeros of the sine function in (3.1). If $n + 1$ in (3.3) is odd, there will not be a zero at the midpoint $x = 0$, only so if $n + 1$ is even.

Note that this outline is applicable also to double-well potentials as long as the energies are above the top of the barrier.

3.2 Double well

The present subsection contains a generalization of the original method of Milne, containing a single amplitude function, to an amplitude-phase method using two real-valued amplitude functions; a complex method with two amplitudes for Regge pole calculations is presented in reference [25]. In reference [14] the use of two amplitude functions is applied for the first time to obtain energy levels in double-well potential. This reference refers to another reference [20,21] as the origin of the idea of using two amplitude functions. Since the numerical results presented in [14] agree with those of the present approach, there should be some close relations between the two approaches. Reference [20,21] uses a method referred to as a 'quantum momentum method', also based on the original ideas of Milne 1930 [15–19].

Initially there is no restriction to symmetric double-well potentials. Two asymmetric wells are assumed with a single hump between them. The left-hand well is assumed deeper then the right-hand well. We use one amplitude function for each well, here u_L and u_R, the ones defined by initial conditions at the potential minima $x = x_L < 0$ and $x = x_R > 0$, respectively, i.e. from

$$u_{L,R}(x_{L,R}) = R^{-1/4}(x_{L,R}), \quad u'_{L,R}(0) = 0. \tag{3.7}$$

The two amplitude-phase representations of the wave are typically matched at the location of the top of the barrier, assumed here to be at $x = 0$.

3.2.1 Left well

The bound state wave function vanishes at $x = -\infty$ and can be represented by the amplitude-phase solution

$$\Psi = u_L \sin\phi, \quad \phi(-\infty) = 0, \tag{3.8}$$

where the lower limit of the phase integral is at $x = -\infty$, as in (3.2). This solution is evaluated at a matching point, here taken at $x = 0$, where the same solution is expressed in terms of a phase-shifted (only) amplitude-phase representation (the matching representation):

$$\Psi = u_L \left[a_L \cos\phi_m + b_L \sin\phi_m\right], \quad \phi_m(0) = 0. \tag{3.9}$$

The lower limit of the phase integral ϕ_m is thus taken at $x = 0$. At $x = 0$, both representations (3.8) and (3.9) provide equivalent expressions for Ψ and Ψ', yielding

$$a_L = \sin\phi_L, \quad b_L = \cos\phi_L, \quad \phi_L = \phi(0). \tag{3.10}$$

Hence, at the matching point one has (with any of the two representations)

$$\Psi(0) = U_L a_L, \quad \Psi'(0) = U'_L a_L + U_L^{-1} b_L, \tag{3.11}$$

where the notations $U_L = u_L(0)$ and $U'_L = u'_L(0)$ are introduced.

3.2.2 Right well

In the right well the solution is represented in terms of the amplitude function u_R in (3.7) as a linear combination

$$\Psi = u_R \left[a_R \cos\phi_m + b_R \sin\phi_m\right], \quad \phi_m(0) = 0. \tag{3.12}$$

The phase ϕ_m is here ($x > 0$) computed in terms of u_R and at the matching point we have

$$\Psi(0) = U_R a_R, \quad \Psi'(0) = U'_R a_R + U_R^{-1} b_R, \tag{3.13}$$

with $U_R = u_R(0)$ and $U'_R = u'_R(0)$. By equating Ψ and Ψ' from both sides at $x = 0$, we obtain

$$a_R = \left(\frac{U_L}{U_R}\right) \sin\phi_L, \quad b_R = \left(\frac{U_R}{U_L}\right) \cos\phi_L + \left(U_R U'_L - U_L U'_R\right) \sin\phi_L. \tag{3.14}$$

3.2.3 Quantization condition

Finally the right-well wave has to vanish as $x \to +\infty$, which requires

$$a_R \cos\phi_R + b_R \sin\phi_R = 0, \quad \phi_R = \phi_m(+\infty). \tag{3.15}$$

More explicitly, we find the condition

$$\left(\frac{U_L}{U_R}\right) \sin\phi_L \cos\phi_R + \left(\frac{U_R}{U_L}\right) \cos\phi_L \sin\phi_R + \left(U_R U'_L - U_L U'_R\right) \sin\phi_L \sin\phi_R = 0. \tag{3.16}$$

This quantization condition is not a previously published formula, but should relate to formulas (4a, b) in [20,21]. Their 'quantum momentum' method originates in the same ideas of Milne [15–19], but results are formulated with other notions and in an apparently different way. No numerical applications are presented in [20,21].

3.3 Symmetric double well

A closer look at the symmetric case simplifies the general double-well quantization condition (3.16). We find that the phases and amplitudes in (3.16) satisfy

$$U_L = U_R, \quad U'_L = -U'_R, \quad \phi_L = \phi_R. \tag{3.17}$$

As a result of (3.17) the quantization condition can be expressed in terms of quantities from the right half of the double well as

$$\sin\phi_R \cos\phi_R - U_R U'_R \sin^2\phi_R = 0. \tag{3.18}$$

The last condition splits into two separate conditions:

$$\sin\phi_R = 0, \quad (-) \tag{3.19}$$

and

$$\cos\phi_R - U_R U'_R \sin\phi_R = 0. \quad (+) \tag{3.20}$$

In the single-well limit, with a common potential minimum at $x = 0$, the two conditions represent odd $(-)$ and even $(+)$ states, respectively. These representations of quantizing the two level symmetries are similar to Eqs. (6)-(9) of the quantum momentum method in [20,21].

The general ordering is that $(+)/(-)$-states alternate as the energy increases from a ground state, which is a $(+)$-state. Their separations are very small if the two wells are well separated, but become more and more like separations of levels in a single well.

4 Computations and results

For symmetric double-well potentials it is sufficient to use only one half of the potential (here the right half) in the calculations. Firstly, the minimum of the potential in this range is localized. The value of the Schrödinger coefficient $R(x)$ at this point is then used to initiate the integration of the Milne's equation in two directions: from the minimum to some distant point in the direction of $x = +\infty$, and from the minimum to $x = 0$. As the phase contributions are integrated simultaneously with the amplitude functions, one can add appropriately the two phase contributions to obtain ϕ_R. The values of u_R and u'_R at the boundary $x = 0$ are also saved for evaluating the quantization condition. The quantization condition is iterated using a Newton algorithm until it is smaller than a certain tolerance. In this process an estimate of the energy derivatives of ϕ_R, u_R and u'_R are needed.

To keep track of the number of nodes in the quantal wave it is instructive to rewrite the condition (3.19) as

$$\phi_R = (n+1)\pi, \quad n = 0, 1, \ldots, \quad (-) \tag{4.1}$$

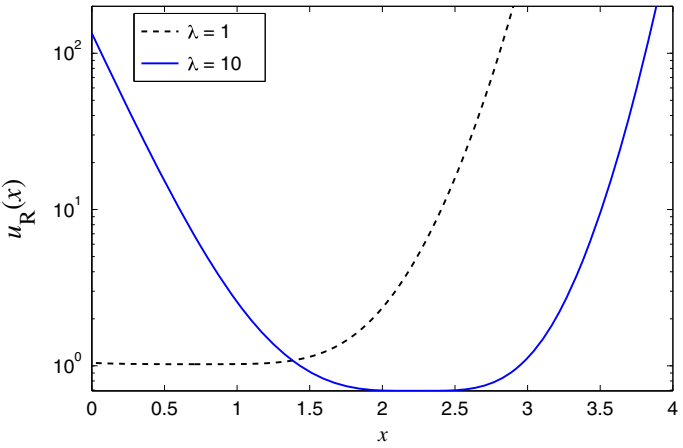

Fig. 1 The amplitude function $u_R(x)$ computed for two ground states 0(+) of $V(x) = x^4 - \lambda x^2$ corresponding to $\lambda = 1$ and 10

recalling the fact that only half the double well potential is used when the nodes are counted. The (+)-levels always appere in between the (−)-levels, and the (+)-level with the same quantum number n as that in (4.1) is the one next below this (−)-level.

4.1 $V(x) = x^4 - \lambda x^2$

This symmetric potential, with a variable parameter λ, was considered in reference [26] in another context related to energy levels. The potential minimum at $x = \sqrt{\lambda/2}$ has the value $V(\sqrt{\lambda/2}) = -\lambda^2/4$, and at this minimum the initial value of the amplitude function $u_R(\sqrt{\lambda/2}) = \left(E + \lambda^2/4\right)^{-1/4}$ is also a minimum of $u_R(x)$.

As $u_R(x)$ is computed, it increases indefinitely as $x \to +\infty$ and increases in various degrees to a finite value as $x \to +0$; see Fig. 1. In Fig. 1 one observes that the value $u_R(0)$ generally increases exponentially for a ground state as the local well becomes deeper (larger λ). If the barrier is small and no tunneling is expected (the case $\lambda = 1$ in Fig. 1) the amplitude function $u_R(x)$ remains approximately constant.

Table 1 presents some low-lying energy levels, more or less influenced by the barrier. For $\lambda = 0$ there is no barrier and the single-well condition (3.3) would be equivalent to the two conditions based on half the potential. Therefore, the quantum numbers $n = 0$ and 1 in (3.3) correspond to $n = 0(+)$ and $n = 0(-)$ from (3.20) respectively (3.19), recalling (4.1). For $\lambda = 1$ the barrier is present, but the energy levels are above the barrier top ($E > 0$). Hence, the energy levels are similar to most single-well potentials, only slightly perturbed levels.

Table 1 shows also results for $\lambda = 10$, where ($\pm$)-levels are very close. The ground levels $n = 0$ would hardly be correctly obtained by approximate methods without difficulties. The amplitude-phase method barely yields acceptable results with a numerical tolerance of 2.3×10^{-7}. Sharpening of the tolerance to 2.3×10^{-10} and 2.3×10^{-14} shows that the results are consistent and that the method is rather efficient with respect

Table 1 Bound state energies as functions of λ, $n(\pm)$. To illustrate the effectiveness of the method, we do the calculations with tolerances $2.3\times$: 10^{-7}, 10^{-10} and 10^{-14} resulting in E_7, E_{10} and E_{14}, respectively

λ	$n(\pm)$	E_7	E_{10}	E_{14}
0	0(+)	1.060362	1.0603620905	1.06036209048419
0	0(−)	3.799673	3.7996730299	3.79967302980142
1	0(+)	0.657653	0.6576530052	0.65765300518072
1	0(−)	2.834536	2.8345362022	2.83453620211933
10	0(+)	−20.633576	−20.6335767026	−20.6335767029477
10	0(−)	−20.633546	−20.6335468841	−20.6335468844048
10	1(+)	−12.379543	−12.3795437857	−12.3795437860132
10	1(−)	−12.375673	−12.3756737204	−12.3756737207055
10	2(+)	−5.1328375	−5.1328379615	−5.13283796180837
10	2(−)	−4.9648698	−4.9648702733	−4.96487027361538

Table 2 Bound state energies as functions of $n(\pm)$ of the potential $V(x) = x^2/2 + 9\mathrm{e}^{-x^2}$ with mass $m = 1$

$n(\pm)$	E_7	E_{10}	E_{14}
0(+)	3.0753948	3.0753946678	3.07539466774414
0(−)	3.0785072	3.0785072384	3.07850723837740
1(+)	5.1383003	5.13830027735	5.13830027732138
1(−)	5.1643731	5.16437304859	5.16437304855738
2(+)	6.97139622	6.97139619594	6.97139619593572
2(−)	7.09839760	7.09839758348	7.09839758347426
15(+)	31.1833984	31.18339831956	31.1833983195843
15(−)	32.1714206	32.17142076313	32.1714207631386

Calculations are done with tolerances $2.3\times$: 10^{-7}, 10^{-10} and 10^{-14} resulting in E_7, E_{10} and E_{14}, respectively

to the numerical tolerance. However, the last two decimal digits may be insignificant because of the lack of exact results to compare with. They differ with those of reference [26].

4.2 $V(x) = x^2/2 + 9\mathrm{e}^{-x^2}$

This potential was studied in modified form in reference [1] studying mixed spin-1/2 and spin-0 condensates, and in reference [6] studying higher-order phase-integral (WKB) approximations. A local minimum is at $x = \ln 18 > 0$. In a similar way as described in the previous subsection, one initiates the integrations in two directions to collect phases and the values $u_R(0)$ and $u'_R(0)$.

Amplitude-phase results for various numerical tolerances are reported in Table 2. The lower levels are significantly influenced by the barrier and the higher levels are sim-

ilar to those of single-well potentials. The present results agree with the exact quantal results of reference [6] to the latter's full (limited) 8-decimal precision. Amplitude-phase results in Table 2 again shows a consistency and efficiency, as those in Table 1, as the numerical tolerance is varied. Note, however, that the close-lying ground states of this double-well potential are less close compared to those of the the previous potential with $\lambda = 10$.

5 Conclusions and discussions

Two symmetrical double-well potential models are studied numerically by an amplitude-phase approach. Quantization conditions are obtained for arbitrary double-well potentials, but applied here to the symmetric case. In this case the quantization conditions are of two types, according to different odd and even symmetries of wave functions. Numerical results are accurate in comparison with existing 'exact' methods. Energy splittings of low-lying levels are well described by the amplitude-phase method.

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