FROM QUARTIC ANHARMONIC OSCILLATOR TO DOUBLE WELL POTENTIAL

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ABSTRACT. Quantum quartic single-well anharmonic oscillator \( V_{ao}(x) = x^2 + g^2x^4 \) and double-well anharmonic oscillator \( V_{dw}(x) = x^2(1-gx)^2 \) are essentially one-parametric, they depend on a combination \((g^2\hbar)\). Hence, these problems are reduced to study the potentials \( V_{ao} = u^2 + u^4 \) and \( V_{dw} = u^2(1-u)^2 \), respectively. It is shown that by taking uniformly-accurate approximation for anharmonic oscillator eigenfunction \( \Psi_{ao}(u) \), obtained recently, see JPA 54 (2021) 295204 [1] and arXiv 2102.04623 [2], and then forming the function \( \Psi_{dw}(u) = \Psi_{ao}(u) \pm \Psi_{ao}(u-1) \) allows to get the highly accurate approximation for both the eigenfunctions of the double-well potential and its eigenvalues.

KEYWORDS: Anharmonic oscillator, double-well potential, perturbation theory, semiclassical expansion.

1. INTRODUCTION

It is already known that for the one-dimensional quantum quartic single-well anharmonic oscillator \( V_{ao}(x) = x^2 + g^2x^4 \) and double-well anharmonic oscillator with potential \( V_{dw}(x) = x^2(1-gx)^2 \) the (trans)series in \( g \) (which is the Perturbation Theory in powers of \( g \) (the Taylor expansion) in the former case \( V_{ao}(x) \) supplemented by exponentially-small terms in \( g \) in the latter case \( V_{dw}(x) \)) and the semiclassical expansion in \( \hbar \) (the Taylor expansion for \( V_{ao}(x) \) supplemented by the exponentially small terms in \( \hbar \) for \( V_{dw}(x) \)) for energies coincide [3]. This property plays crucially important role in our consideration.

Both the quartic anharmonic oscillator
\[
V = x^2 + g^2x^4 , \tag{1}
\]
with a single harmonic well at \( x = 0 \) and the double-well potential
\[
V = x^2(1-gx)^2 , \tag{2}
\]
with two symmetric harmonic wells at \( x = 0 \) and \( x = 1/g \), respectively, are two particular cases of the quartic polynomial potential
\[
V = x^2 + agx^3 + g^2x^4 , \tag{3}
\]
where \( g \) is the coupling constant and \( a \) is a parameter. Interestingly, the potential (3) is symmetric for three particular values of the parameter \( a \): \( a = 0 \) and \( a = \pm 2 \). All three potentials (1), (2), (3) belong to the family of potentials of the form
\[
V = \frac{1}{g^2} \tilde{V}(gx) ,
\]
for which there exists a remarkable property: the Schrödinger equation becomes one-parametric, both the Planck constant \( \hbar \) and the coupling constant \( g \) appear in the combination \((g^2\hbar)\), see [2]. It can be immediately seen if instead of the coordinate \( x \) the so-called classical coordinate \( u = (gx) \) is introduced. This property implies that the action \( S \) in the path integral formalism becomes \( g \)-independent and the factor \( \frac{1}{g^2} \) in the exponent becomes \( \frac{1}{g^2} \). Formally, the potentials (1)-(2), which enter to the action, appear at \( g = 1 \), hence, in the form
\[
V = u^2 + u^4 , \tag{4}
\]
\[
V = u^2(1-u)^2 , \tag{5}
\]
respectively. Both potentials (4), (5) are symmetric with respect to \( u = 0 \) and \( u = 1/2 \), respectively.

Namely, this form of the potentials will be used in this short Note. This Note is the extended version of a part of presentation in AAMP-18 given by the first author [5].

2. SINGLE-WELL POTENTIAL

In [1] for the potential (1) matching the small distances \( u \to 0 \) expansion and the large distances \( u \to \infty \) expansion (in the form of semiclassical expansion) for the phase \( \phi \) in the representation
\[
\Psi = P(u) e^{-\phi(u)} ,
\]
of the wave function, where \( P \) is a polynomial, it was constructed the following function for the \((2n+p)\)-excited state with quantum numbers \((n,p)\), \( n = 0,1,2,\ldots \), \( p = 0,1 \):
\[
\Psi_{(n,p)\text{approximation}}^{(n,p)} = \frac{u^p P_{np}(u^2)}{(B^2 + u^2)^{\frac{p}{2}} (B + \sqrt{B^2 + u^2})^{2n+p+\frac{1}{2}}}
\]

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208
This prescription was already checked successfully for
where

The double-well potential (2) in [6] for somehow sim-
ima at

eigenstates. Furthermore, the func-

Figure 1. Two lowest, normalized to one eigenfunc-
tions of positive/negative parity: for single-well potential (1), see (3) (top) and for double-well potential (5), see (7) (bottom). Potentials shown by black lines.

\[ V(u) = \begin{cases} \frac{u^2}{2} & \text{for } u^2 < 1 \\ \frac{u^2}{2} + u^4/3 + \frac{A}{B} & \text{for } u^2 > 1 \end{cases} \]

where \( P_{n,p} \) is some polynomial of degree \( n \) in \( u^2 \) with positive roots. Here \( A = a_{n,p}, B = b_{n,p} \) are two parameters of interpolation. These parameters \((-A), B\) are slow-growing with quantum number \( n \) at fixed \( p \) taking, in particular, the values

\[ A_{0,0} = -0.6244, B_{0,0} = 2.3667 \]

\[ A_{0,1} = -1.9289, B_{0,1} = 2.5598 \]

for the ground state and the first excited state, respectively. This remarkably simple function (6), see Figure 1 (top), provides 10-11 exact figures in energies for the first 100 eigenstates. Furthermore, the function (6) deviates uniformly for \( u \in (-\infty, +\infty) \) from the exact function in \( \sim 10^{-6} \).

4. DOUBLE-WELL POTENTIAL: RESULTS

In this section we present concrete results for energies of the ground state \((0,0)\) and of the first excited state \((0,1)\) obtained with the function (9) at \( p = 0, 1 \), respectively, see Figure 1 (bottom). The results are compared with the Lagrange-Mesh Method (LMM) [7].

4.1. Ground State \((0,0)\)

The ground state energy for (5) obtained variationally using the function (9) at \( p = 0 \) and compared with LMM results [7], where all printed digits (in the second line) are correct,

\[ E^{(0,0)}_{\text{var}} = 0.932517518401 \]

\[ E^{(0,0)}_{\text{mesh}} = 0.932517518372 \]

Note that ten decimal digits in \( E^{(0,0)}_{\text{var}} \) coincide with ones in \( E^{(0,0)}_{\text{mesh}} \) (after rounding). Variational parameters in (9) take values,

\[ A = 2.3237, \quad B = 3.2734, \quad a_0 = 2.3839, \quad b_0 = 0.0605 \]

cf. (7). Note that \( b_0 \) takes a very small value.
4.2. FIRST EXCITED STATE (0,1)

The first excited state energy for (5) obtained variationally using the function (9) at \( p = 1 \) and compared with LMM results [7], where all printed digits (in the second line) are correct,

\[
E_{\text{var}}^{(0,1)} = 3.396 279 329 936 , \quad E_{\text{mesh}}^{(0,1)} = 3.396 279 329 887 .
\]

Note that ten decimal digits in \( E_{\text{var}}^{(0,1)} \) coincide with ones in \( E_{\text{mesh}}^{(0,1)} \). Variational parameters in (9) take values,

\[
A = -2.2957 , \quad B = 3.6991 , \quad a_1 = 4.7096 , \quad b_1 = 0.0590 ,
\]

cf. (5). Note that \( b_1 \) takes a very small value similar to \( b_0 \).

5. CONCLUSIONS

It is presented the approximate expression (9) for the eigenfunctions in the double-well potential [6]. In Non-Linearization procedure [5], it can be calculated the first correction (the first order deviation) to the function (9). It can be shown that for any \( u \in (-\infty, +\infty) \) the functions (9) deviate uniformly from the exact eigenfunctions, beyond the sixth significant figure similarly to the function (6) for the single-well case. It increases the accuracy of the simplified function, proposed in [5] with \( \alpha = 0 \) and \( b_{0,1} = 0 \), in the domain under the barrier \( u \in (0.25, 0.75) \) from 4 to 6 significant figures leaving the accuracy outside of this domain practically unchanged.

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