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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 $(\hbar g^2)$, see [2]. It can be immediately seen if instead of the coordinate x the so-called classical coordinate $u = (g\,x)$ is introduced. This property implies that the action S in the path integral formalism becomes g-independent and the factor $\frac{1}{\hbar}$ in the exponent becomes $\frac{1}{\hbar g^2}$ [4]. 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 (4) 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 ϕ 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), $n = 0,1,2,\dots\ ,\ p = 0,1:$

$$\Psi^{(n,p)}_{(approximation)} \;=$$

$$\frac{u^p P_{n,p}(u^2)}{(B^2\;+\;u^2)^{\frac{1}{4}}\left(B\;+\;\sqrt{B^2\;+\;u^2}\right)^{2n+p+\frac{1}{2}}}$$

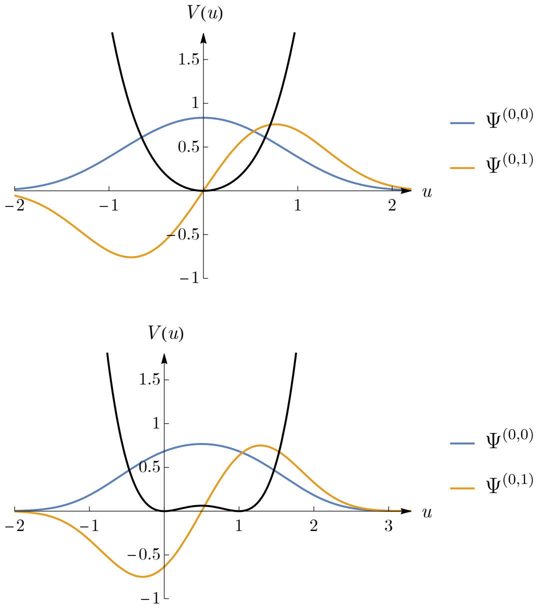

Figure 1. Two lowest, normalized to one eigenfunctions of positive/negative parity: for single-well potential (4), see (6) (top) and for double-well potential (5), see (9)(bottom). Potentials shown by black lines.

$$\times \exp\left(-\ \frac{A\ +\ (B^2+3)\,u^2/6\ +\ u^4/3}{\sqrt{B^2\ +\ u^2}}\ +\ \frac{A}{B}\right)\ , \tag{6}$$

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

$$A_{0,0}\ =\ -0.6244\ , B_{0,0}\ =\ 2.3667\ , \tag{7}$$

$$A_{0,1}\ =\ -1.9289\ , B_{0,1}\ =\ 2.5598\ , \tag{8}$$

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 $\sim 10^{-6}$.

3. Double-well potential: wavefunctions

Following the prescription, usually assigned in folklore to E. M. Lifschitz – one of the authors of the famous Course on Theoretical Physics by L. D. Landau and E. M. Lifschitz – when a wavefunction for single well potential with minimum at $u = 0$ is known, $\Psi(u)$, the wavefunction for double well potential with minima at $u = 0, 1$ can be written as $\Psi(u) \pm \Psi(u-1)$. This prescription was already checked successfully for the double-well potential (2) in [6] for somehow simplified version of (6), based on matching the small distances $u \to 0$ expansion and the large distances $u \to \infty$ expansion for the phase ϕ but ignoring subtleties emerging in semiclassical expansion. Taking the wavefunction (6) one can construct

$$\Psi^{(n,p)}_{(approximation)}\ =\ \frac{P_{n,p}(\tilde u^2)}{(B^2\ +\ \tilde u^2)^{\frac14}\left(\alpha B\ +\ \sqrt{B^2\ +\ \tilde u^2}\right)^{2n+\frac12}}$$

$$\exp\left(-\ \frac{A\ +\ (B^2+3)\,\tilde u^2/6\ +\ \tilde u^4/3}{\sqrt{B^2\ +\ \tilde u^2}}\ +\ \frac{A}{B}\right)\ D^{(p)}\ , \tag{9}$$

where $p = 0, 1$ and

$$D^{(0)}\ =\ \cosh\left(\frac{a_0\tilde u + b_0\tilde u^3}{\sqrt{B^2+\tilde u^2}}\right)\ ,$$

$$D^{(1)}\ =\ \sinh\left(\frac{a_1\tilde u + b_1\tilde u^3}{\sqrt{B^2+\tilde u^2}}\right)\ .$$

Here

$$\tilde u\ =\ u\ -\ \frac{1}{2}\ , \tag{10}$$

$\alpha = 1$ and $A, B, a_{0,1}, b_{0,1}$ are variational parameters. If $\alpha = 0$ as well as $b_{0,1} = 0$ the function (9) is reduced to ones which were explored in [6], see Eqs.(10)-(11) therein. The polynomial $P_{n,p}$ is found unambiguously after imposing the orthogonality conditions of $\Psi^{(n,p)}_{(approximation)}$ to $\Psi^{(k,p)}_{(approximation)}$ at $k = 0, 1, 2, \ldots, (n-1)$, here it is assumed that the polynomials $P_{k,p}$ at $k = 0, 1, 2, \ldots, (n-1)$ are found beforehand.

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,

$$E^{(0,0)}_{var}\ =\ 0.932\,517\,518\,401\ ,$$
$$E^{(0,0)}_{mesh}\ =\ 0.932\,517\,518\,372\ .$$

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

$$A\ =\ 2.3237\ ,$$
$$B\ =\ 3.2734\ ,$$
$$a_0\ =\ 2.3839\ ,$$
$$b_0\ =\ 0.0605\ ,$$

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,

$$E^{(0,1)}_{var} = 3.396\,279\,329\,936 \ ,$$
$$E^{(0,1)}_{mesh} = 3.396\,279\,329\,887 \ .$$

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

$$A = -2.2957 \ ,$$
$$B = 3.6991 \ ,$$
$$a_1 = 4.7096 \ ,$$
$$b_1 = 0.0590 \ ,$$

cf. (8). 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 (5). In Non-Linearization procedure [8] 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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