Bound states for systems with quartic energy-momentum dispersion

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Bound states and its energies for systems with the quartic energy-momentum dispersion $E(p) \sim p^4$ and polynomial potentials are studied using the Wentzel-Kramers-Brillouin (WKB) semiclassical approximation and the Wentzel complex method taking into account higher order WKB corrections. The obtained energies are compared with numerical values found by applying the variational approach utilizing the universal Gaussian basis. It is found that the wave functions of the ground and higher-energy states for systems with quartic dispersion have nodes in the classically forbidden region. Thus, the well-known oscillation theorem for the one-dimensional Schrödinger equation is not, in general, applicable for systems with quartic dispersion. Still it is observed that the oscillation theorem holds in the classically allowed region in all considered examples. The properties of bound state wave functions are compared with the solutions of the exactly solvable problem of a square well potential.

I. INTRODUCTION

Quantum mechanical systems in which interactions or potential energy dominates over the kinetic energy attract a significant interest because they often exhibit strongly correlated behavior and give rise to novel quantum phases of matter which are not well described by traditional perturbative or mean-field approaches [1, 2]. These systems are central to many open questions in modern physics including entanglement, the simulation of strongly interacting gauge theories in condensed matter analogs, and the realization of quantum criticality and emergent symmetries. The relevant condensed matter systems include high-temperature superconductors (cuprates), heavy fermion systems, transition metal oxides, twisted bilayer graphene which exhibit such interaction dominant phases as correlated insulating phases, Wigner crystal, unconventional superconductivity, and non-Fermi liquid behavior [3–6].

Quasiparticles with the dispersion relation $E(p) \sim p^{2n}$, $n \geq 2$, refer to emergent excitations in quantum many-body systems whose energy-momentum dispersion is soft, meaning that their energy increases slowly with momentum near zero momentum. Such systems naturally realize the regime of dominance of potential energy over the kinetic energy and for large n describe and model weakly dispersing flat bands. Flat bands are especially prone to strong correlation effects as electrons' kinetic energy is quenched and interactions dominate. Theoretical studies explore how even weakly dispersing flat bands can lead to enhanced susceptibilities, magnetism, superconductivity, or localization [7].

The problem of localization is related to the study of disorder and impurity induced bound states. The latter problem provides us with motivation for the investigation of bound states in systems with quartic dispersion performed in this paper. Mathematically, finding eigenvalues and eigenfunctions of bound states for quasiparticles with soft dispersion implies solving higher order Schrödinger-like equation in the presence of an interaction potential which is not an easy task.

The semiclassical Wentzel-Kramers-Brillouin (WKB) approach is an efficient method for determining approximate solutions to linear differential equations with spatially varying coefficients [8–10]. In the last decades, the WKB method for the one-dimensional second-order Schrödinger equation has showed a significant progress. One should mention such achievements as the method of the Maslov canonical operator [11], the summation of asymptotic series in the Planck constant $\hbar$ (the exact (complex) WKB method [12, 13]), the finding of "instanton-like" non-perturbative in $\hbar$ corrections to the Bohr-Sommerfeld quantization condition [14, 15]. The method has been extended to higher spatial dimensions and multi-component Hamiltonians [16] and used to study such physical systems as graphene (see, e.g., Refs.[17–19]).

Two of us applied recently the WKB method to determine bound state energies for quasiparticles with quartic dispersion [20]. It should be noted that for fourth-order ordinary differential equations with generic potential $V(x)$ only local WKB solutions in low orders in the Planck constant $\hbar$ are available in the literature (see, e.g., [21–23]), but their global properties, related to quantization, only begin to be investigated [24].

Since the WKB method is not applicable in vicinity of turning points, to determine energies of bound states requires matching semiclassical wave functions in the classically allowed and forbidden regions and finding the connection formulas. The latter could be derived by using solutions to the equation with linearised potential in vicinity of turning points. For the quartic dispersion, such solutions are given by the higher-order Airy functions [25, 26]. Studying its asymptotics on the real axis as $x \to \pm\infty$ by using the method of steepest descents [27, 28] and determining the leading asymptotics as well as the exponentially suppressed terms (hyperasymptotics) necessary for matching the

WKB solutions in vicinity of the turning points, the corresponding Bohr-Sommerfeld quantization condition was obtained in [20]. It contains a non-perturbative in $\hbar$ term which is relevant for low-energy states.

Here we extend the study performed in [20] aiming to account for higher order WKB corrections in powers of $\hbar$ that provides an important information on energy levels. In addition, since the WKB expansion is the asymptotic one and the series in $\hbar$ does not capture non-analytic in $\hbar$ contributions, we include non-perturbative contributions due to hyperasymptotics in our analysis. Since, to the best of our knowledge, there are no exact solutions to the double quartic problem (with the Hamiltonian $H = a^4\hat{p}^4 + b^4x^4$) and to check the validity of our results, we determine the bound state energies numerically by applying the variational approach utilizing the universal Gaussian basis. However, since it is always instructive to have an exact solvable example, we find bound state energies and their wave functions for the exactly solvable problem of a square potential well. One of our main findings is that in the case of quartic dispersion, although the wave functions of bound states in the classically forbidden region exponentially decay, they have nodes in all considered examples. This invalidates the oscillation theorem characteristic for the one-dimensional second-order Schrödinger equation. Still it is observed that the oscillation theorem holds in the classically allowed region.

The paper is organized as follows. The WKB method is formulated in Sec. II. The Wentzel complex method is considered in Sec. III. In Sec.IV, numerical analysis for the bound state energies and wave functions is performed. Bound states for the square well potential are found in Sec.V. The results are summarized in Sec.VI.

II. WKB SOLUTIONS FOR QUARTIC ENERGY-MOMENTUM DISPERSION

The Hamiltonian of one-dimensional quasiparticles with quartic energy-momentum dispersion is given by

$$H = a^4p^4 + V(x), \tag{1}$$

where $p = -i\hbar\partial_x$ is the momentum operator, a^4 is parameter whose dimension is v^4/W^3, where v is velocity and W is energy (cf. with the energy dispersion in ABC-stacked tetra-layer graphene where $E(p) = (v_Fp)^4/\gamma_1^3$).

To solve the stationary Schrödinger-like equation $H\psi = E\psi$ we use the WKB ansatz for the wave function

$$\psi(x) = \exp[iS(x)/\hbar] \tag{2}$$

and obtain the following equation:

$$a^4\left[(S')^4 - 6i\hbar S''(S')^2 - \hbar^2(4S'S''' + 3(S'')^2) - i\hbar^3S^{IV}\right] + V(x) = E, \tag{3}$$

where primes denote derivatives with respect to x. Expanding S in powers of $\hbar$, $S = \sum_{n=0}^{\infty}\hbar^nS_n$, one can get recursive relations for S_n. For example, in the zero order, we find the classical momentum

$$p(x) = S_0'(x) = (E - V(x))^{1/4}/a, \tag{4}$$

which gives $S_0(x) = \int^x dx(E - V(x))^{1/4}/a$. Notice that terms in the expansion $S' = \sum_{n=0}^{\infty}\hbar^nS_n'$ with odd $n \geq 3$ are total derivatives like in the case of the Schrödinger equation and vanish after integrating over the closed contour in the complex plane encircling turning points [24].

For the first and second order corrections, we have the following equations:

$$4(S_0')^3S_1' - 6iS_0''(S_0')^2 = 0, \tag{5}$$

$$6(S_0')^2(S_1')^2 + 4(S_0')^3S_2' - 12iS_0'S_1'S_0'' - 3(S_0'')^2 - 6i(S_0')^2S_1'' - 4S_0'S_0''' = 0, \tag{6}$$

which give

$$S_1' = \frac{3iS_0''}{2S_0'} = \frac{3i}{2}\left(\ln S_0'\right)' = \frac{3i}{2}\left(\ln p(x)\right)', \tag{7}$$

$$S_2' = \frac{5}{4}\left(\frac{3(p')^2}{2p^3} - \frac{p''}{p^2}\right) = -\frac{5}{4}\left(\frac{(p')^2}{2p^3} + \left(\frac{p'}{p^2}\right)'\right), \tag{8}$$

where we used $S_0'(x) = p(x)$. Integrating the equation for S_1', we obtain $S_1 = i\ln p^{3/2}$.

The fourth order correction S_4' is given in Ref.[24] (up to total derivatives) and has the following form:

$$S_4' = \frac{35(p'')^2}{256\,p^5} - \frac{21p^{IV}}{1024\,p^4}. \tag{9}$$

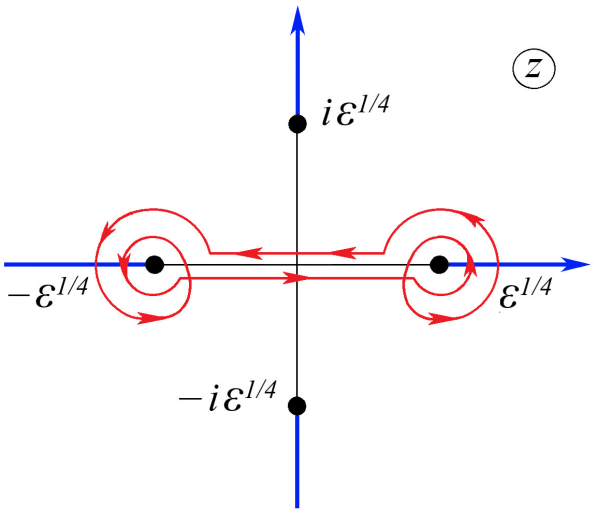

FIG. 1. Contour enclosing two turning points.

The higher order terms with $n \geq 6$ can be also obtained recursively and expressed through $p(x)$ and its derivatives (for terms S_6', S_8', see Ref.[24]). However, in this paper, we restrict ourselves to the corrections up to the 4th order. In the next section, we use the obtained results and apply the Wentzel complex method to determine the bound state energies for the system with the quartic dispersion and the quartic potential $V(x) = b^4x^4$.

III. QUANTIZATION CONDITION FOR DOUBLE QUARTIC PROBLEM

The Wentzel complex method uses the single-valuedness of a wave function ψ in the region containing turning points. The argument principle then leads to the condition

$$\oint_\gamma \frac{\psi'(z)}{\psi(z)}dz = \frac{i}{\hbar}\oint_\gamma S'(z)dz = 2\pi i n, \tag{10}$$

where n is an integer number and the contour γ encloses the classical turning points anticlockwise in the complex z-plane. For quartic dispersion and in the fourth order in $\hbar$, we have

$$\frac{1}{\hbar}\oint_\gamma S(z)dz = \frac{1}{\hbar}\oint_\gamma p(z)dz + \frac{3i}{2}\oint_\gamma \frac{p'(z)dz}{p(z)} - \frac{5\hbar}{4}\oint_\gamma \frac{(p')^2}{2p^3}dz + \frac{7\hbar^3}{256}\oint_\gamma \left(\frac{5(p'')^2}{p^5} - \frac{3p^{IV}}{4p^4}\right)dz = 2\pi n. \tag{11}$$

To determine bound state energies for the double quartic problem (quartic dispersion and quartic potential)

$$\left(a^4\hbar^4\partial_x^4 + b^4x^4\right)\psi(x) = E\psi(x), \tag{12}$$

it is convenient to use dimensionless quantities $z = x\sqrt{b/(a\hbar)}$, $\varepsilon = E/(\hbar^2a^2b^2)$, and $p(z) = (\varepsilon - z^4)^{1/4}$. Then we set the branch cuts to be the half-lines $(-\infty, -\varepsilon^{1/4}]$, $[\varepsilon^{1/4}, \infty)$, $(-i\infty, -i\varepsilon^{1/4}]$, and $[i\varepsilon^{1/4}, i\infty)$ so that $p(z) = (\varepsilon - z^4)^{1/4}$ takes positive real values on the real axis between the turning points $-\varepsilon^{1/4}$ and $\varepsilon^{1/4}$ ($\varepsilon > 0$). Further, $p(z)$ is a single-valued function on the four-sheeted Riemann surface $p^4 + z^4 = \varepsilon$ of genus 3. The closed contour γ is 1-cycle on this surface which runs twice around the turning point $\varepsilon^{1/4}$, then twice around the point $-\varepsilon^{1/4}$ as shown schematically in Fig.1. Therefore, calculating higher order WKB corrections we could omit terms with total derivatives which give zero.

For the double quartic problem, to determine higher order WKB corrections we need to calculate the contour

integrals

$$\oint_\gamma p(z)dz = 2\int\limits_{-\varepsilon^{1/4}}^{\varepsilon^{1/4}} (\varepsilon - y^4)^{1/4} dy = 2\frac{\sqrt{\varepsilon}\Gamma^2(1/4)}{4\sqrt{\pi}}, \tag{13}$$

$$\oint_\gamma \frac{p'(z)dz}{p(z)} = \oint_\gamma \frac{dp^4(z)}{4p^4(z)} = 2\pi i, \tag{14}$$

where we took into account in the last integral that each pole due to zeros of $p^4(z)$ is enclosed twice. For corrections with $n \geq 2$, after calculating derivatives $\partial_z^k p(z)$, reducing the integer powers of z which are multiples of z^4, and using $z^4 = \varepsilon - p^4$, we obtain an expression which is given as a sum of terms with negative powers of $p(z)$. Representing negative powers of $p(z)$ as derivatives with respect to ε, we can write, e.g., the first term in the second order WKB correction (8) in the form of the Picard-Fuchs differential operator acting on the period integrals of $p(z)$

$$\oint_\gamma \frac{(p')^2}{p^3}dz = \oint_\gamma \frac{z^6 dz}{p^9(z)} = \oint_\gamma \left(\frac{\varepsilon z^2}{p^9(z)} - \frac{z^2}{p^5(z)}\right) dz = \left(\frac{16}{5}\varepsilon\partial_\varepsilon^2 + 4\partial_\varepsilon\right) \oint_\gamma \frac{z^2 dz}{p(z)} = 2\frac{6\Gamma^2(3/4)}{5\sqrt{\pi}}\frac{1}{\sqrt{\varepsilon}}. \tag{15}$$

Similarly, for the fourth order correction integral, we get

$$\begin{aligned} &\frac{7}{256}\oint_\gamma \left(\frac{5(p'')^2}{p^5} - \frac{3p^{IV}}{4p^4}\right) dz = \frac{7}{256}\oint_\gamma \left(\frac{135\varepsilon}{2p^{11}} - \frac{1125\varepsilon^2}{4p^{15}} + \frac{873\varepsilon^3}{4p^{19}}\right) dz \\ &= \left[\frac{45}{8}\varepsilon\partial_\varepsilon^3 + \frac{375}{44}\varepsilon^2\partial_\varepsilon^4 + \frac{97}{55}\varepsilon^3\partial_\varepsilon^5\right] \oint_\gamma p(z)dz = -2\frac{3\Gamma^2(1/4)}{128\sqrt{\pi}\varepsilon^{3/2}}. \end{aligned} \tag{16}$$

Finally, we obtain the following equation for the WKB energy levels of the double quartic problem:

$$\frac{\Gamma^2(1/4)\sqrt{\varepsilon}}{4\sqrt{\pi}} - \frac{3\Gamma^2(3/4)}{4\sqrt{\pi}}\frac{1}{\sqrt{\varepsilon}} - \frac{3\Gamma^2(1/4)}{128\sqrt{\pi}\varepsilon^{3/2}} = \pi\left(n + \frac{1}{2}\right), \qquad n = 0, 1, \ldots . \tag{17}$$

Adding non-perturbative contribution due to hyperasymptotics derived in Ref.[20], we obtain the quantization condition

$$\frac{\Gamma^2(1/4)\sqrt{\varepsilon}}{4\sqrt{\pi}} - \frac{3\Gamma^2(3/4)}{4\sqrt{\pi}}\frac{1}{\sqrt{\varepsilon}} - \frac{3\Gamma^2(1/4)}{128\sqrt{\pi}\varepsilon^{3/2}} - 2(-1)^n \arctan\left[\frac{1}{2}\exp\left(-\frac{\Gamma^2(1/4)\sqrt{\varepsilon}}{4\sqrt{\pi}}\right)\right] = \pi\left(n + \frac{1}{2}\right), \qquad n = 0, 1, \ldots . \tag{18}$$

$\varepsilon \setminus n$	0	1	2	3	4	5	6
$\varepsilon_{2ndcorr}$	1.3138	7.1289	18.6234	35.8529	58.8228	87.5342	121.9876
ε_{2hyper}	1.4241	7.1093	18.6249	35.8528	58.8228	87.5342	121.9876
$\varepsilon_{4thcorr}$	1.4175	7.1539	18.6332	35.8581	58.8260	87.5364	121.9891
ε_{4hyper}	1.5151	7.1345	18.6348	35.8580	58.8260	87.5364	121.9891
ε_{var}	1.3967	7.1315	18.6404	35.8590	58.8263	87.5365	121.9892

TABLE I. Numerical values of the bound state energy ε for the one-dimensional system with quartic dispersion and quartic potential for $n = 0, 1, \ldots, 6$ taking into account the WKB corrections of the second $\varepsilon_{2ndcorr}$ and fourth $\varepsilon_{4thcorr}$ order, as well as the non-perturbative correction due to hyperasymptotics.

Numerical computation of the WKB energies for the double quartic system defined by Eqs.(17) and (18) are presented in Table I for the states with $n = 0, 1, ..., 6$. The second and fourth rows of the table show the WKB energies with the second and fourth order WKB corrections taken into account, respectively. To quantify the role of the non-perturbative contribution, we include in the third and fifth rows the non-perturbative in $\hbar$ contribution given by the last term on the left-hand side of Eq.(18). The last row presents variational estimates which are derived in the next section.

Comparing these numerical values, we conclude that both WKB corrections and the non-perturbative contribution are indeed relevant for the lowest bound state energies. Note also that the non-perturbative correction due to hyperasymptotics in the Bohr-Sommerfeld quantization condition is always smaller than $\pi/2$ in accordance with similar results obtained for the Schrödinger equation [29]. It can be seen also that the deviation of ε_{4hyper} from the variational value ε_{var} is around 8 per cent for the lowest state and then quickly decreases.

IV. NUMERICAL RESULTS FOR THE LOWEST ENERGY LEVELS

To check the validity and accuracy of the results obtained in the previous section, we determine bound state energies for the harmonic $V(x) = x^2$ and quartic $V(x) = x^4$ potentials using the variational method with the universal Gaussian basis [30].

In the universal Gaussian basis and dimensionless variables, the trial wave functions are represented as a series expansion of basic Gaussian functions

$$\psi(x) = \sum_{k=1}^{\mathcal{K}} C_k \chi_k(x) \equiv \sum_{k=1}^{\mathcal{K}} C_k \exp\left(-a_k (x - x_k)^2\right), \tag{19}$$

where C_k, a_k, and x_k are variational parameters. Note that this basis enables one to consider both symmetric (even parity) and antisymmetric (odd parity) states within the same variational procedure, while if $x_k = 0$, then we need to deal with symmetric states and antisymmetric states separately. To find C_k, it is suitable to use the Galerkin method and solve the algebraic system of equations

$$\sum_{k=1}^{\mathcal{K}} C_k \langle \varphi_n | H - E | \varphi_k \rangle = 0, \;\; n = 1, ..., \mathcal{K}, \tag{20}$$

which is equivalent to the Schrödinger equation for $\mathcal{K} \to \infty$. Parameters x_k and a_k can be found within different schemes of variational procedures or chosen randomly using the stochastic variational method [31, 32]. For the matrix elements of powers of x and $\hat{p}$ (where $\hat{p} = -i\partial_x$), we have

$$\langle \chi_n | \hat{p}^2 | \chi_k \rangle = \frac{2\sqrt{\pi}\, a_k a_n}{u_{nk}^{3/2}} (1 - 2\omega_{nk}) \exp(-\omega_{nk}), \quad \langle \chi_n | \hat{p}^4 | \chi_k \rangle = \frac{4\sqrt{\pi}\, a_k^2 a_n^2}{u_{nk}^{5/2}} \left(3 - 12\omega_{nk} + 4\omega_{nk}^2\right) \exp(-\omega_{nk}),$$

$$\langle \chi_n | x^2 | \chi_k \rangle = \frac{\sqrt{\pi}}{2u_{nk}^{3/2}} \left(1 + 2\lambda_{nk}^2 u_{nk}\right) \exp(-\omega_{nk}), \langle \chi_n | x^4 | \chi_k \rangle = \frac{3\sqrt{\pi}}{4u_{nk}^{5/2}} \left(1 + 4\lambda_{nk}^2 u_{nk} + \frac{4}{3}\lambda_{nk}^4 u_{nk}^2\right) \exp(-\omega_{nk}), \tag{21}$$

where

$$\lambda_{nk} \equiv \frac{a_n x_n + a_k x_k}{u_{nk}}, \quad \omega_{nk} \equiv \frac{a_n a_k}{u_{nk}} (x_n - x_k)^2, \quad u_{nk} = a_n + a_k.$$

Finally, for the normalization of matrix elements, we find

$$\langle \chi_n | \chi_k \rangle = \frac{\sqrt{\pi}}{\sqrt{u_{nk}}} \exp(-\omega_{nk}).$$

In Table II, we present the variational estimations for a few lowest energy levels obtained using the universal basis (19) for the Hamiltonian $H = \hat{p}^4 + x^4$. These energy levels lies higher then those obtained for the Hamiltonian $H = \hat{p}^4 + x^2$ and the convergence of the consequent variational estimations at $\mathcal{K} \to \infty$ is noticeably more slow. This may be connected with the fact that the wave functions of the problem with quartic dispersion have nontrivial asymptotics containing oscillations in the classically forbidden regions [20]. This means that nontrivial kinetic energy $\sim \hat{p}^4$, generally speaking, violates the well-known oscillation theorem for the quadratic dispersion $E \sim \hat{p}^2$ (see, e.g, [33]) which relates the number of nodes of a bound state wave function with its quantum number n. According to [20], eigenfunctions of the Hamiltonian $H = \hat{p}^4 + x^4$ have the following behaviour in the classically forbidden region at $x \to +\infty$:

$$\psi_n(x) \to C_n \cdot \exp\left(-\frac{x^2}{2\sqrt{2}}\right) \cos\left(\frac{x^2}{2\sqrt{2}} + \theta_n\right), \tag{22}$$

where C_n and θ_n are constants. At $x \to -\infty$, symmetric states have the same asymptotics (22), while antisymmetric states change their overall sign. This asymptotics is valid for the ground state too and leads to an infinite number of nodes of the ground state wave function. In addition, such a nontrivial oscillating asymptotics of wave functions requires a large number of basic functions to reproduce accurately the wave functions under study in the whole interval of x.

n	$\mathcal{K}=1$	$\mathcal{K}=2$	$\mathcal{K}=3$	$\mathcal{K}=4$	$\mathcal{K}=5$	$\mathcal{K}=6$	$\mathcal{K}=7$	$\mathcal{K}=8$	$\mathcal{K}=12$	$\mathcal{K}=16$	$\mathcal{K}=20$
0	1.500000	1.429335	1.396878	1.396797	1.396767	1.396736	1.396733	1.396732	1.396729	1.396728	1.396728
1		7.230771	7.182810	7.136187	7.132385	7.132262	7.132011	7.131535	7.131530	7.131529	7.131529
2			18.738913	18.664837	18.643336	18.641597	18.641059	18.640460	18.640388	18.640383	18.640383
3				35.902068	35.879689	35.869507	35.863001	35.859417	35.859226	35.859024	35.859024
4					58.956623	58.846621	58.831935	58.827747	58.826352	58.826330	58.826330
5						88.826155	87.661908	87.604080	87.536543	87.536528	87.536528
6							122.042196	122.010137	121.989268	121.989198	121.989193

TABLE II. Successive approximations for the energy levels for the Hamiltonian $H=\hat{p}^4+x^4$ calculated within the variational procedure using the variational basis (19) for different number $\mathcal{K}$ of the Gaussian functions. Empty cells in the left lower part of the table are present because to determine $\mathcal{K}$ energy levels one should use not less than $\mathcal{K}$ basis functions in the variational ansatz.

Finally, we wish to stress that all presented numbers in Table II are only the variational estimations from above, and we do not present here the "exact" values which, to the best of our knowledge, are not available in the literature. Still, due to the convergence of our results as we extend the number of basis functions, we think that our values found for $\mathcal{K}=20$ provide the correct results with accuracy in the last decimal digit.

Let us consider now the wave functions of the bound states. Using Eq.(19) and the determined coefficients C_k and parameters a_k, x_k, we depict the bound state wave functions of the ground and first excited states for the Hamiltonian $H=p^4+x^4$ in the left and middle panels of Fig.2 (red solid lines). For comparison, we show in the same figure the wave functions for the harmonic potential $V(x)=x^2$ (blue dashed lines). Energies of the ground and first excited states for the Hamiltonian $H=p^4+x^4$ are $E=1.3967$ and $E=7.1315$, respectively. For the Hamiltonian with quadratic potential $H=p^4+x^2$, the corresponding energies are lower and equal $E=1.0603$ and $E=3.7996$. Vertical red solid and blue dashed lines in the left and middle panels show boundaries of the classically allowed region for the ground and first excited states, respectively. While for the ground state of the Hamiltonian $H=p^4+x^4$ the classically allowed region is defined by $-1.0871<x<1.0871$ for the ground state, it is given by $-1.6341<x<1.6341$ for the first excited state. As to the classically allowed region for the Hamiltonian $H=p^4+x^2$, it is $-1.0297<x<1.0297$ and $-1.94927<x<1.94927$ for the ground and first excited states, respectively. The wave functions are normalized to the unity, i.e., $\int|\psi(x)|^2dx=1$. Oscillations of the wave functions of the ground and first excited states for the potential $V(x)=x^4$ in the classically forbidden region are shown in insets of all panels of Fig.2. It is instructive to compare the wave functions of the ground and first excited states of the double quartic problem with the familiar case of the quadratic energy-momentum dispersion. The wave functions of the later problem are plotted in the right panel of Fig.2.

The wave functions of the 2nd, 3rd, and 4th excited states are shown in Fig.3, where vertical red solid and blue dashed lines show boundaries of the classically allowed region for the potentials $V(x)=x^4$ and $V(x)=x^2$, respectively. Note that the number of nodes equals n for the nth energy level in the classically allowed region. Certainly, the presence of nodes in the wave functions in the classically forbidden region clearly distinguishes the bound state problem for quasiparticles with quartic dispersion from that with the conventional quadratic dispersion. This result is definitely worth checking and illustrating by analysing an exactly solvable problem. As such a problem, we consider in the next section a square well potential, which has not been discussed in detail in the literature. We determine the bound state energy spectrum and the wave functions which show explicitly the presence of oscillations in the classically forbidden region, thus, confirming the violation of the oscillation theorem for systems with quartic dispersion.

V. FINITE SQUARE WELL POTENTIAL

Let us determine bound state energies and the corresponding wave functions for an exactly solvable problem of quasiparticles with quartic dispersion in a square well potential. We consider the one-dimensional Hamiltonian (1) with potential

$$V(x)=\begin{cases} V_0>0, & \text{for} \quad |x|>L, \\ 0, & \text{for} \quad -L<x<L. \end{cases} \tag{23}$$

Energy levels and wave functions of bound states are defined by the equation

$$\psi^{IV}(x)+\frac{V(x)-E}{\hbar^4a^4}\psi(x)=0. \tag{24}$$

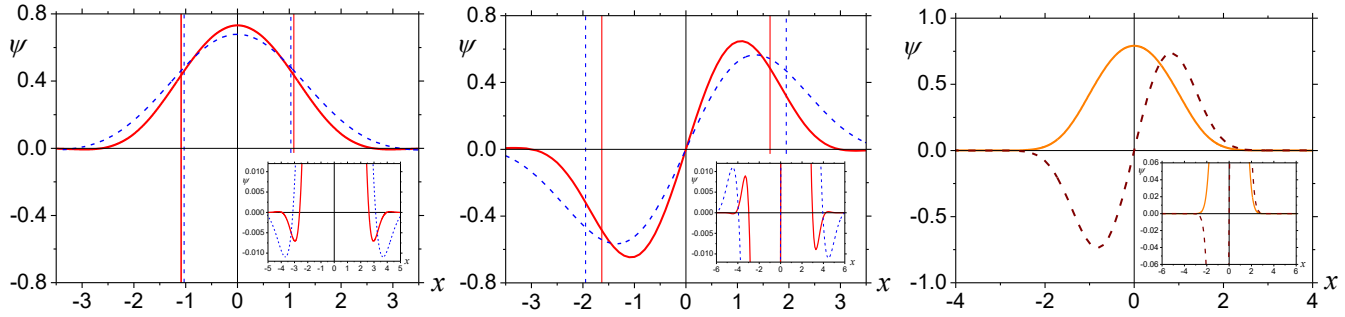

FIG. 2. Left panel: The ground state wave function for the $H = \hat{p}^4 + x^4$ (red solid line) and $H = \hat{p}^4 + x^2$ Hamiltonians (blue dashed line). Middle panel: The wave functions of the first excited state for the $H = \hat{p}^4 + x^4$ (red solid line) and $H = \hat{p}^4 + x^2$ Hamiltonians (blue dashed line). Vertical red solid and blue dashed lines in the left and middle panels show boundaries of the classically allowed region for the ground and first excited states, respectively. Right panel: The wave function of the ground state (orange solid line) and the first excited state (brown dashed line) for the quartic oscillator with the Hamiltonian $H = \hat{p}^2 + x^4$.

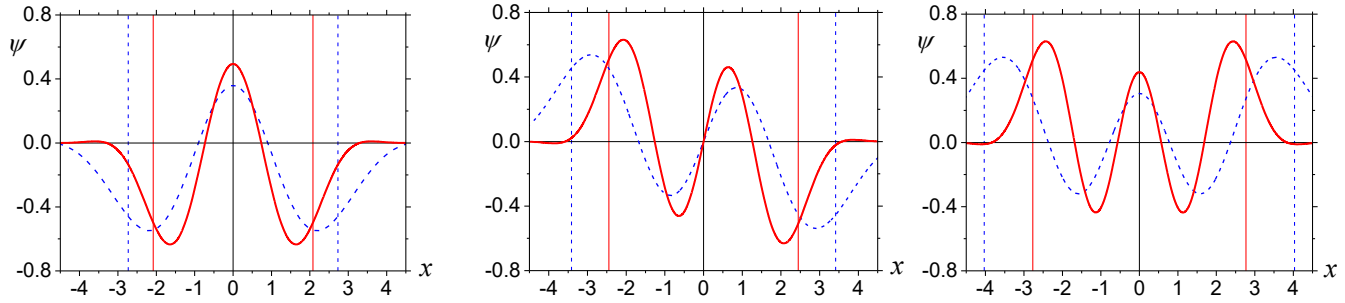

FIG. 3. The wave functions of the second (left panel), third (middle panel), and fourth excited state (right panel) for the potentials $V(x) = x^4$ (red solid lines) and $V(x) = x^2$ (blue dashed lines). Vertical red solid and blue dashed lines show boundaries of the corresponding classically allowed regions.

We seek for bound state solutions which can exist for energies $0 < E < V_0$. In the regions $x < -L$ and $x > L$, the corresponding solutions decreasing for $x \to \mp\infty$, respectively, are

$$\psi_I(x) = A_1 e^{\kappa_1 x} + A_2 e^{\kappa_2 x}, \qquad x < -L, \tag{25}$$

$$\psi_{III}(x) = B_1 e^{-\kappa_1 x} + B_2 e^{-\kappa_2 x}, \qquad x > L, \tag{26}$$

where

$$\kappa_{1,2} = \frac{1 \pm i}{\sqrt{2}} \frac{(V_0 - E)^{1/4}}{\hbar a}. \tag{27}$$

In the region $-L < x < L$, we have four independent solutions

$$\psi_{II}(x) = \sum_{k=1}^{4} C_k e^{i p_k x}, \quad p_k = e^{\frac{i\pi k}{2}} \frac{E^{1/4}}{\hbar a}, \qquad -L < x < L. \tag{28}$$

Matching these functions and their three derivatives at $x = -L$ and $x = L$ we get the system of eight homogeneous linear equations for eight constants $A_1, A_2, B_1, B_2, C_1, C_2, C_3, C_4$. By setting the determinant of this system equal to zero, we obtain the characteristic equation for the energy levels.

Actually, it is quite helpful in the case under consideration to simplify our task by using the symmetry of the Hamiltonian under the inversion transformation $x \to -x$ which separates all eigenstates in states of either positive or negative parity. Then it suffices to find solutions only for positive x using the basis of real functions. We begin our analysis with states of positive parity. The corresponding solution ψ_{III} finite at $x \to +\infty$ can be written in the form

$$\psi_{III}(x) = B_1 e^{-kx} \cos(kx) + B_2 e^{-kx} \mathrm{sgn}(x) \sin(kx), \qquad k = \frac{(V_0 - E)^{1/4}}{\sqrt{2}\hbar a}, \qquad x > L. \tag{29}$$

The general solution ψ_{II} of positive parity in the classically allowed region $-L < x < L$ is

$$\psi_{II}(x) = C_1 \cos(px) + C_2 \cosh(px), \qquad p = \frac{E^{1/4}}{\hbar a}, \qquad 0 < x < L. \tag{30}$$

The wave function ψ_I in the classically forbidden region $x < -L$ is obtained by changing the sign of x in $\psi_{III}(x)$. As mentioned above, in view of the inversion symmetry, it suffices to match solutions $\psi_{II}(x)$ and $\psi_{III}(x)$ and their first, second, and third derivatives at $x = L$. Then we get a system of four homogeneous linear equations for four real constants C_1, C_2, B_1, B_2 with the matrix

$$M = \begin{pmatrix} \cos(pL) & \cosh(pL) & -e^{-kL}\cos(kL) & -e^{-kL}\sin(kL) \\ -p\sin(pL) & p\sinh(pL) & ke^{-kL}(\cos(kL)+\sin(kL)) & ke^{-kL}(-\cos(kL)+\sin(kL)) \\ -p^2\cos(pL) & p^2\cosh(pL) & -2k^2e^{-kL}\sin(kL) & 2k^2e^{-kL}\cos(kL) \\ p^3\sin(pL) & p^3\sinh(pL) & 2k^3e^{-kL}(-\cos(kL)+\sin(kL)) & -2k^3e^{-kL}(\cos(kL)+\sin(kL)) \end{pmatrix}. \tag{31}$$

Equating the determinant of this matrix to zero, we obtain the following equation for energies of positive parity states in the potential well:

$$2\sqrt{2}k^3p + (k^4 - 2k^2p^2 - p^4)\tan(pL) + (k^4 + 2k^2p^2 - p^4 - 2\sqrt{2}kp^3\tan(pL))\tanh(pL) = 0, \tag{32}$$

where

$$p = \varepsilon^{1/4}, \qquad k = (v-\varepsilon)^{1/4}, \qquad \varepsilon = \frac{E}{\hbar^4 a^4}, \qquad v = \frac{V_0}{\hbar^4 a^4} \tag{33}$$

[note that we redefined k compared to Eq. (29) omitting $1/\sqrt{2}$].

Equation (32) can be written in another form

$$e^{-2pL}\frac{p^2 - \sqrt{2}pk + k^2}{p^2 + \sqrt{2}pk + k^2} = -\frac{B\tan(pL) + A}{A\tan(pL) - B}, \quad A = p^2 - \sqrt{2}pk - k^2, \quad B = p^2 + \sqrt{2}pk - k^2. \tag{34}$$

For negative parity states, general solutions are

$$\psi_{II}(x) = C_1 \sin(px) + C_2 \sinh(px), \qquad 0 < x < L, \tag{35}$$

$$\psi_{III}(x) = B_1 e^{-kx}\mathrm{sgn}(x)\cos(kx) + B_2 e^{-kx}\sin(kx), \qquad x > L. \tag{36}$$

Matching solutions $\psi_{II}(x)$ and $\psi_{III}(x)$ and their three derivatives at the point $x = L$ we get a system of four homogeneous linear equations for four real constants C_1, C_2, B_1, B_2 with the matrix

$$M = \begin{pmatrix} \sin(pL) & \sinh(pL) & -e^{-kL}\cos(kL) & -e^{-kL}\sin(kL) \\ p\cos(pL) & p\cosh(pL) & ke^{-kL}(\cos(kL)+\sin(kL)) & ke^{-kL}(-\cos(kL)+\sin(kL)) \\ -p^2\sin(pL) & p^2\sinh(pL) & -2k^2e^{-kL}\sin(kL) & 2k^2e^{-kL}\cos(kL) \\ -p^3\cos(pL) & p^3\cosh(pL) & 2k^3e^{-kL}(-\cos(kL)+\sin(kL)) & -2k^3e^{-kL}(\cos(kL)+\sin(kL)) \end{pmatrix}. \tag{37}$$

Equating the determinant of this matrix to zero we obtain the eigenvalue equation

$$\left[2\sqrt{2}kp^3 + (k^4 + 2k^2p^2 - p^4)\tan(pL)\right]\cosh(pL) - \left[k^4 - 2k^2p^2 - p^4 - 2\sqrt{2}k^3p\tan(pL))\right]\sinh(pL) = 0. \tag{38}$$

The last equation can be written in the form

$$e^{-2pL}\frac{p^2 - \sqrt{2}pk + k^2}{p^2 + \sqrt{2}pk + k^2} = -\frac{A\tan(pL) - B}{B\tan(pL) + A}, \quad A = p^2 - \sqrt{2}pk - k^2, \quad B = p^2 + \sqrt{2}pk - k^2, \tag{39}$$

where p and k are defined in Eq.(33).

Equation (39) agrees with the corresponding equation for negative parity states in Example 4 of Ref.[34] (modulo some misprints in the expressions for A and B). The behaviour of energy levels given by Eqs.(34) and (39) as a function of $\lambda = v^{1/4}L$ is shown in the left panel of Fig.4. The energies of states with negative parity lie between neighbouring states of positive parity and the ground state has positive parity.

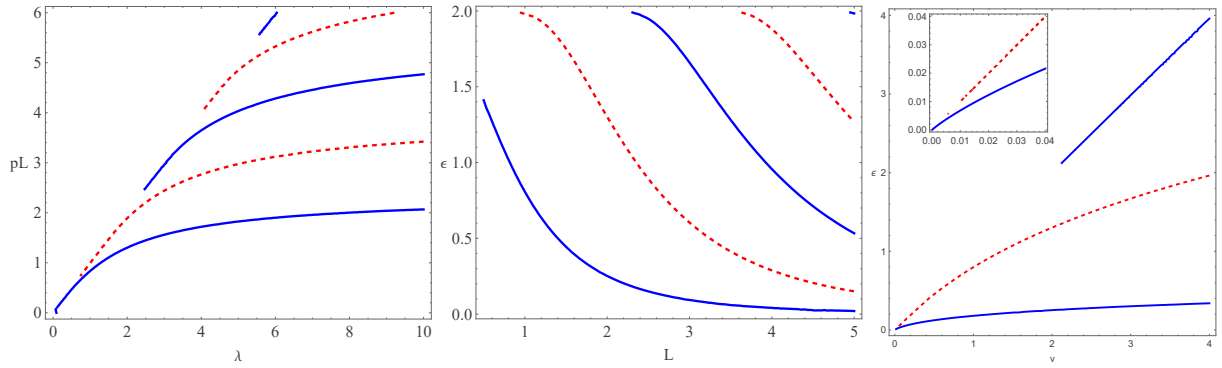

FIG. 4. Left panel: Energy levels pL for positive and negative parity bound states as a function of $\lambda = v^{1/4}L$ (blue and red lines, respectively). Middle panel: energy levels as a function of the well width L for the fixed well depth $v = 2$. Right panel: energy levels as a function of the well depth v for the fixed well width $L = 1$.

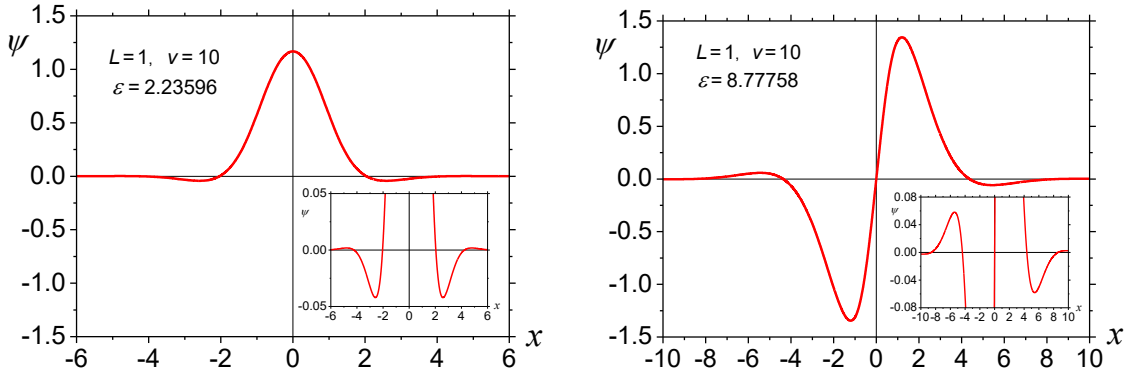

FIG. 5. The wave function of the ground state (left panel) and the first excited state (right panel) for the potential well.

Note that in the limit $v \to \infty$ (infinite square well), Eqs.(32) and (38) reduce in view of $k \to \infty$ to the following simple equation:

$$\tan(pL) = \mp \tanh(pL) \tag{40}$$

for states of positive and negative parity, respectively. In contrast to the Schrödinger equation in the infinite well limit, Eq.(40) is transcendental and corresponds to the infinite well problem with the boundary conditions $\psi(\pm L) = 0$ and $\psi'(\pm L) = 0$. As in the case of Schrödinger's equation, the energy levels in an infinite well potential are higher than the corresponding values for a finite well potential because the wave function in the latter case penetrates into a classically forbidden region. Further, the wave function of the ground state is nodeless. In fact, for systems with quartic dispersion, it was proved [35, 36] that the node theorem is valid for infinite well $v \to \infty$. However, the wave function for a finite potential well problem has infinite number of oscillations in the classically forbidden region confirming our conclusion made in Sec.IV. It is worth mentioning also that, for a finite width barrier, oscillations of wave functions may lead to the appearance of oscillating tunneling current [37, 38].

Equations (32) and (38) (or, equivalently, Eqs.(34) and 39) are eigenvalue equations for $pL = \varepsilon^{1/4}L$ defining it as a function of a dimensionless combination vL^4 of the depth v and width L of the potential well because $kL = (vL^4 - (pL)^4)^{1/4}$. The behaviour of pL as a function of $\lambda = v^{1/4}L$ for states of both parities is shown in Fig.4. It is not difficult to show that the number of eigenvalues $N(v, L)$ of both parities grows asymptotically as $\simeq \lambda/\pi$ for $\lambda \to \infty$. It is clearly seen that all levels, except the ground state, start with some threshold value λ_{th}. The ground state is of positive parity and exists for arbitrary shallow potential well, i.e., for any $v > 0$ like in the case of the one-dimensional Schrödinger's equation.

It is interesting to look at the behaviour of energy levels as a function of the width or the depth of the well when one of these parameters is fixed. Such a behaviour is shown in the middle and right panels of Fig.4. The energies of states with negative parity lie between neighbouring states of positive parity. The deeper and wider the potential well, the greater the number of eigenvalues in the well, provided that the maximal energy level does not exceed v, i.e., $\varepsilon_{max} < v$. The ground state exists at any finite depth or width of the potential well, whereas other levels begin at a

certain threshold value of these parameters in accordance with the above-mentioned dependence of levels on λ.

The wave functions of the ground and first excited states of the considered potential well problem are shown in the left and right panels of Fig.5, respectively. Obviously, the ground state wave function is even in the coordinate x (i.e., of positive parity) and the wave function of the first excited state is odd (negative parity). To demonstrate more clearly the presence of oscillations of wave functions in the classically forbidden region, we add inset to the left panel (ground state) and the right panel (first excited state).

VI. SUMMARY

To investigate bound states for quasiparticles in weakly dispersing energy bands, we studied 1D systems with the quartic energy-momentum dispersion and the quartic potential (the double quartic problem). To determine bound state energies, we applied the WKB semiclassical method formulated for systems with quartic dispersion in [20]. Since the connection formulas in the vicinity of turning points require the use of hyperasymptotics of higher-order Airy functions for fourth order differential equations, the Bohr-Sommerfeld quantization rule for systems with quartic dispersion contains non-perturbative in the Planck constant contribution.

To analyse the role of higher order WKB corrections, we calculated the second and fourth WKB corrections and found that like the non-perturbative contribution these higher order WKB corrections are mostly relevant for the lowest bound states energies with their contributions quickly decreasing for states with higher energy. To quantify the accuracy of the energy levels found using the WKB approach, we computed the bound state energy numerically by using the variational method with the universal Gaussian basis. Quantitatively, we found that the WKB corrections notably improve the accuracy of WKB results and the deviation of the energy obtained in the WKB approach from the numerically calculated energy is around 8 percent for the lowest energy state. For states with higher energy this deviation quickly decreases.

As to wave functions of bound states, they provide important information also. Our main principal finding is the result that the wave function of the bound states have nodes (in fact, infinitely many) in the classically forbidden region for systems with quartic dispersion unlike the Schrödinger equation where the bound state wave functions do not have such nodes. On the other hand, the number of nodes in the classically allowed region coincides with the quantum number n of the corresponding bound state. To check this observation, we considered an exactly solvable potential well problem and found that the wave function of the ground state indeed does not have nodes in the classically allowed region and oscillates producing nodes in regions beyond the potential well. The higher energy states also have nodes in the classically forbidden region.

Interestingly, although our findings show that the oscillation theorem is not valid for systems with quartic dispersion, this theorem holds in the classically allowed region where the number of nodes of the wave function coincides with the quantum number n of the corresponding bound state. The mathematical reason for the presence of nodes of the ground state wave function in the classically forbidden region is the existence of both real and imaginary parts in all four semiclassical momenta defining the asymptotics of the wave function in the classically forbidden region. This is in contrast to the case of Schrödinger‘s equation where the semiclassical momentum is purely imaginary in the classically forbidden region which gives non-oscillating exponentially decreasing asymptotics. Oscillations in the classically forbidden region may have important physical consequences, for example, lead to oscillating tunneling current [37, 38].

Since the quartic energy-momentum dispersion is obviously only the first step beyond the conventional quadratic dispersion, to fully address the properties of bound states in weakly dispersing energy bands it is important to extend the study performed here to the case of sextic and more high order dispersion. The extension to the two-dimensional case is also of interest due to the growth of the number of planar physical systems with dispersion higher than quadratic.

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