Variational Perturbation Theory for the Ground-State Wave Function

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We evaluate perturbatively the density matrix in the low-temperature limit and thus the ground-state wave function of the anharmonic oscillator up to second order in the coupling constant. We then employ Kleinert’s variational perturbation theory to determine the ground-state wave function for all coupling strengths.

I. INTRODUCTION

Variational perturbation theory as developed by Kleinert [1] provides a systematic algorithm to evaluate perturbation series at all coupling strengths including the strong-coupling limit \( g \to \infty \). It was thoroughly investigated for the ground-state energy of the anharmonic oscillator up to the 150th order [2,3], and its convergence was found to be exponentially fast and uniform. A similar systematic study has not yet been performed for the ground-state wave function. A first-order variational approach was set up by Kunihiro [4]. However, his method did not satisfactorily deal with certain problems in the variational procedure which will be discussed in detail below.

In this work we improve Kunihiro’s first-order calculation and extend the treatment to the second order in the coupling strength. The ground-state wave function of the anharmonic oscillator is calculated from the low-temperature limit of the diagonal elements of the density matrix. A variational evaluation of the density matrix for the double-well potential has already been performed for finite temperatures in Ref. [5].

II. PERTURBATION THEORY

Consider a quantum-mechanical point particle of mass \( M \) moving in the one-dimensional anharmonic oscillator potential

\[
V(x) = \frac{M}{2} \omega^2 x^2 + gx^4 ,
\]

(2.1)

where \( \omega \) denotes the frequency and \( g \) the coupling constant. We determine its ground-state wave function \( \Psi(x) \) by evaluating the low-temperature limit of the diagonal elements of the density matrix

\[
\Psi(x) = \lim_{\beta \to \infty} \sqrt{\rho(x,x)} ,
\]

(2.2)

which is defined by

\[
\rho(x_b,x_a) = \frac{(x_b \hbar \beta | x_a 0)}{Z} .
\]

(2.3)

Here \( (x_b \hbar \beta | x_a 0) \) denotes the imaginary-time evolution amplitude with the path integral representation [1]

\[
(x_b \hbar \beta | x_a 0) = \int_{x(0)=x_a}^{x(h \beta)=x_b} D x \exp \left\{ -\frac{1}{\hbar} \int_0^{h \beta} d \tau \left[ \frac{M}{2} \dot{x}^2(\tau) + \frac{M}{2} \omega^2 x^2(\tau) + gx^4(\tau) \right] \right\} ,
\]

(2.4)

and \( Z \) denotes the partition function

\[
Z = \int_{-\infty}^{+\infty} dx (x \hbar \beta | x 0) .
\]

(2.5)

By expanding Eq. (2.4) in powers of the coupling constant \( g \) we obtain the perturbation series

\[
(x_b \hbar \beta | x_a 0) = (x_b \hbar \beta | x_a 0)_\omega \left[ 1 - \frac{g}{\hbar} \int_0^{h \beta} d \tau_1 (x^4(\tau_1))_\omega + \frac{g^2}{2\hbar^2} \int_0^{h \beta} d \tau_1 \int_0^{h \beta} d \tau_2 (x^4(\tau_1) x^4(\tau_2))_\omega + \ldots \right] ,
\]

(2.6)

1
where we have introduced the harmonic imaginary-time evolution amplitude

\[ (x_h \beta | x_0) = \int_{x(0)=x_0}^{x(\beta)=x_h} \mathcal{D}x \exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar \beta} d\tau \left[ \frac{M}{2} \dot{x}^2(\tau) + \frac{M}{2} \omega^2 x^2(\tau) \right] \right\}, \quad (2.7) \]

and the harmonic expectation value for an arbitrary functional \( F[x] \) of the path \( x(\tau) \):

\[ \langle F[x] \rangle_\omega = \int_{x(0)=x_0}^{x(\beta)=x_h} \mathcal{D}x F[x] \exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar \beta} d\tau \left[ \frac{M}{2} \dot{x}^2(\tau) + \frac{M}{2} \omega^2 x^2(\tau) \right] \right\}. \quad (2.8) \]

The latter is evaluated with the help of the generating functional for the harmonic oscillator, whose path integral representation reads

\[ (x_h \beta | x_0)[j] = \int_{x(0)=x_0}^{x(\beta)=x_h} \mathcal{D}x \exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar \beta} d\tau \left[ \frac{M}{2} \dot{x}^2(\tau) + \frac{M}{2} \omega^2 x^2(\tau) - j(\tau) x(\tau) \right] \right\}, \quad (2.9) \]

leading to

\[ (x_h \beta | x_0)[j] = (x_h \beta | x_0) \exp \left[ \frac{1}{\hbar} \int_0^{\hbar \beta} d\tau_1 x_{cl}(\tau_1) j(\tau_1) + \frac{1}{2\hbar} \int_0^{\hbar \beta} d\tau_1 \int_0^{\hbar \beta} d\tau_2 G(\tau_1, \tau_2) j(\tau_1) j(\tau_2) \right]. \quad (2.10) \]

with

\[ (x_h \beta | x_0) = \sqrt{\frac{M \omega}{2\pi \hbar \sinh \hbar \beta \omega}} \exp \left\{ -\frac{M \omega}{2\hbar \sinh \hbar \beta \omega} \left[ (x_a^2 + x_b^2) \cosh \hbar \beta \omega - 2x_a x_b \right] \right\}. \quad (2.11) \]

In Eq. (2.10) we have introduced the classical path

\[ x_{cl}(\tau) = x_a \frac{\sinh(h \beta - \tau) \omega + x_b \sinh \omega \tau}{\sinh h \beta \omega}, \quad (2.12) \]

and the Green function

\[ G(\tau_1, \tau_2) = \frac{1}{2M \omega \sinh h \beta \omega} \left[ \theta(\tau_2 - \tau_1) \sinh(h \beta - \tau_1) \omega \sinh \omega \tau_2 + \theta(\tau_2 - \tau_1) \sinh(h \beta - \tau_2) \omega \sinh \omega \tau_1 \right]. \quad (2.13) \]

We follow Ref. [6] and evaluate harmonic expectation values of polynomials in \( x \) arising from the generating functional (2.10) according to Wick’s theorem. Let us illustrate the procedure to reduce the power of the polynomial by the example of the harmonic expectation value

\[ \langle x^n(\tau_1) x^m(\tau_2) \rangle_\omega. \quad (2.14) \]

(i) Contracting \( x(\tau_1) \) with \( x^{n-1}(\tau_1) \) and \( x^{m}(\tau_2) \) leads to a Green function \( G(\tau_1, \tau_1) \) and \( G(\tau_1, \tau_2) \) with multiplicity \( n - 1 \) and \( m \), respectively. The rest of the polynomial remains within the harmonic expectation value, leading to \( \langle x^{n-2}(\tau_1) x^{m}(\tau_2) \rangle_\omega \) and \( \langle x^{n-1}(\tau_1) x^{m-1}(\tau_2) \rangle_\omega \).

(ii) If \( n > 1 \), extract one \( x(\tau_1) \) from the expectation value giving \( x_{cl}(\tau_1) \) multiplied by \( \langle x^{n-1}(\tau_1) x^{m}(\tau_2) \rangle_\omega \).

(iii) Add the terms (i) and (ii).

(iv) Repeat the previous steps until only products of expectation values \( \langle x(\tau_1) \rangle_\omega = x_{cl}(\tau_1) \) remain.

With the help of this procedure, the first-order harmonic expectation value \( \langle x^4(\tau_1) \rangle_\omega \) is reduced to

\[ \langle x^4(\tau_1) \rangle_\omega = x_{cl}(\tau_1) \langle x^3(\tau_1) \rangle_\omega + 3 G(\tau_1, \tau_1) \langle x^2(\tau_1) \rangle_\omega. \quad (2.15) \]

Furthermore, we find

\[ \langle x^3(\tau_1) \rangle_\omega = x_{cl}(\tau_1) \langle x^2(\tau_1) \rangle_\omega + 2G(\tau_1, \tau_1) x_{cl}(\tau_1), \quad (2.16) \]
\[
\langle x^2(\tau_1) \rangle_\omega = x_{cl}^2(\tau_1) + G(\tau_1, \tau_1). \tag{2.17}
\]

Combining Eqs. (2.15)–(2.17) we obtain in first order
\[
\langle x^4(\tau_1) \rangle_\omega = x_{cl}^4(\tau_1) + 6 x_{cl}^2(\tau_1) G(\tau_1, \tau_1) + 3 G^2(\tau_1, \tau_1). \tag{2.18}
\]

The second-order harmonic expectation value requires considerably more effort and finally leads to
\[
\langle x^4(\tau_1) x^4(\tau_2) \rangle_\omega = x_{cl}^4(\tau_1) x_{cl}^4(\tau_2) + 16 x_{cl}^3(\tau_1) G(\tau_1, \tau_2) x_{cl}^3(\tau_2) + 12 x_{cl}^2(\tau_1) G(\tau_1, \tau_1) x_{cl}^2(\tau_2) \\
+ 72 x_{cl}^2(\tau_1) G^2(\tau_1, \tau_2) x_{cl}(\tau_2) + 36 x_{cl}(\tau_1) G(\tau_1, \tau_1) G(\tau_2, \tau_2) x_{cl}(\tau_2) + 9 G^2(\tau_1, \tau_1) G^2(\tau_2, \tau_2) \\
+ 96 x_{cl}(\tau_1) G(\tau_1, \tau_2) G(\tau_2, \tau_2) x_{cl}(\tau_2) + 6 G^2(\tau_1, \tau_1) x_{cl}^4(\tau_2) + 96 x_{cl}(\tau_1) G^3(\tau_1, \tau_1) x_{cl}(\tau_2) \\
+ 144 x_{cl}(\tau_1) G(\tau_1, \tau_1) G(\tau_1, \tau_2) G(\tau_2, \tau_2) x_{cl}(\tau_2) + 36 G^2(\tau_1, \tau_1) x_{cl}^2(\tau_2) G(\tau_2, \tau_2) \\
+ 144 x_{cl}(\tau_1) G^2(\tau_1, \tau_2) G(\tau_2, \tau_2) + 72 G(\tau_1, \tau_1) G^2(\tau_1, \tau_2) G(\tau_2, \tau_2) + 24 G^4(\tau_1, \tau_2). \tag{2.19}
\]

The contractions can be illustrated by Feynman diagrams with the following rules. A vertex represents the integration over \( \tau \)
\[
\times = \int_0^{h\beta} d\tau, \tag{2.20}
\]
a line denotes the Green function
\[
\begin{array}{c}
1 \\
\hline
2
\end{array} = G(\tau_1, \tau_2), \tag{2.21}
\]
and a cross pictures a classical path
\[
\times = x_{cl}(\tau_1). \tag{2.22}
\]

Inserting the harmonic expectation values (2.18) and (2.19) into the perturbation expansion (2.7) leads in first order to the diagrams
\[
\int_0^{h\beta} d\tau_1 \langle x^4(\tau_1) \rangle_\omega = \begin{array}{c}
\times \times \times + 6 \bigcirc \bigcirc \bigcirc + 3 \bigcirc \bigcirc \bigcirc ,
\end{array}\tag{2.23}
\]
whereas the second-order terms are
\[
\int_0^{h\beta} d\tau_1 \int_0^{h\beta} d\tau_2 \langle x^4(\tau_1) x^4(\tau_2) \rangle_\omega = \begin{array}{c}
\times \times \times \times \times + 16 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc + 144 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc + 96 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc + 72 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc + 24 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc + 36 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc + 144 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc + 96 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc + 96 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc + 144 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc + 36 \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc ,
\end{array}. \tag{2.24}
\]

We observe that contributions from both connected and disconnected Feynman diagrams appear. The disconnected diagrams vanish once we rewrite the imaginary-time evolution amplitude in the form
\[
(x_b h\beta|x_{a}, 0) = (x_b h\beta|x_{a}, 0)_\omega \exp\{W(x_b, h\beta; x_{a}, 0)\}, \tag{2.25}
\]
where the exponent \( W(x_b, h\beta; x_{a}, 0) \) contains only the connected Feynman diagrams. We obtain from (2.6) and (2.23)–(2.24) the expansion
\[ W(x_\beta, h\beta; x_\alpha, 0) = -\frac{g}{\hbar} \left( x + 6 \times 3 \right) + \frac{g^2}{2\hbar^2} \left( 8 \times + 36 \right) + 48 \times + 48 \times + 72 \times + 72 \times + 36 \times + 12 \times + \ldots, \]  

(2.26)

where disconnected diagrams are indeed no longer present. As mentioned above, we restrict ourselves to the low-temperature limit of the diagonal elements of the density matrix which determine the ground-state wave function. In order to evaluate the various contributions in (2.26), we need the classical path (2.12) and the Green function (2.13) in the low-temperature limit:

\[ \lim_{\beta \to \infty} x_{cl}(\tau) = x \left( e^{-\omega \tau} + e^{-\omega (h\beta - \tau)} \right), \]  

(2.27)

\[ \lim_{\beta \to \infty} G(\tau_1, \tau_2) = \frac{\hbar}{2M\omega} \left[ \theta(\tau_1 - \tau_2) e^{-\omega(\tau_1 - \tau_2)} + \theta(\tau_2 - \tau_1) e^{-\omega(\tau_2 - \tau_1)} - e^{-\omega(\tau_1 + \tau_2)} - e^{-2h\beta \omega + \omega(\tau_1 + \tau_2)} \right]. \]  

(2.28)

Computing with these expressions the Feynman diagrams in (2.26), the low-temperature limit of the imaginary-time evolution amplitude (2.25) reads together with (2.11)

\[ \lim_{\beta \to \infty} (x h \beta | x \rangle = \lim_{\beta \to \infty} \sqrt{\frac{M\omega}{h\pi}} \exp \left[ -\frac{\hbar\beta \omega}{2} - \frac{M\omega}{h} x^2 + \frac{g}{\hbar} \left( \frac{9h^2}{8M^2\omega^3} - \frac{3h^2}{2M^2\omega^2} - \frac{3h}{2M\omega^2} x^2 - \frac{1}{2\omega} x^4 \right) \right] \]  

\[ + \frac{g^2}{2\hbar^2} \left( \frac{21h^5\beta}{4M^4\omega^5} - \frac{205h^4}{16M^4\omega^6} + \frac{21h^3}{2M^3\omega^5} x^2 + \frac{11h^2}{4M^4\omega^6} x^4 + \frac{3h}{4M^4\omega^7} x^6 \right) + \ldots. \]  

(2.29)

According to (2.3), the partition function \( Z \) follows from (2.29) by performing an integration with respect to \( x \). This results in

\[ \lim_{\beta \to \infty} Z = \lim_{\beta \to \infty} \exp \left[ -\frac{\hbar\beta \omega}{2} - \frac{3gh^2\beta}{4M^2\omega^2} + \frac{21g^2h^3\beta}{8M^4\omega^3} + \ldots \right]. \]  

(2.30)

Inserting (2.29) and (2.30) into (2.3) we observe a cancellation of all terms which would diverge in the low-temperature limit \( \beta \to \infty \). Thus the diagonal elements of the density matrix read in this limit

\[ \lim_{\beta \to \infty} \rho(x, x) = \sqrt{\frac{M\omega}{h\pi}} \exp \left[ -\frac{M\omega}{h} x^2 + \frac{g}{\hbar} \left( \frac{9h^2}{8M^2\omega^3} - \frac{3h^2}{2M^2\omega^2} - \frac{1}{2\omega} x^4 \right) \right] \]  

\[ + \frac{g^2}{2\hbar^2} \left( -\frac{205h^4}{16M^4\omega^6} + \frac{21h^4}{2M^3\omega^5} x^2 + \frac{11h^2}{4M^4\omega^6} x^4 + \frac{h}{3M^4\omega^7} x^6 \right) + \ldots. \]  

(2.31)

By taking the square root and expanding the exponential term up to second order in the coupling strength \( g \), we derive the second-order ground-state wave function (2.2):

\[ \Psi(x) = \left( \frac{M\omega}{h\pi} \right)^{1/4} \exp \left[ -\frac{M\omega}{h} x^2 \right] \left[ 1 - \frac{g}{\hbar} \left( \frac{9h^2}{16M^2\omega^3} + \frac{3h}{4M^2\omega^2} x^2 + \frac{1}{4\omega} x^4 \right) \right] \]  

\[ + \frac{g^2}{2\hbar^2} \left( -\frac{1559h^4}{256M^4\omega^6} + \frac{141h^3}{32M^3\omega^5} x^2 + \frac{53h^2}{32M^2\omega^4} x^4 + \frac{13h}{24M\omega^3} x^6 + \frac{1}{16\omega^2} x^8 \right) + \ldots. \]  

(2.32)

This result corresponds to the solution of the Bender-Wu recursion relation [I] for the ground-state wave function which is normalized such that

\[ \int_{-\infty}^{+\infty} dx \Psi^2(x) = 1 \]  

(2.33)

holds up to second order in the coupling strength \( g \).
III. VARIATIONAL PERTURBATION THEORY

Variational perturbation theory enables us to evaluate the ground-state wave function for all values of the coupling constant \( g \) and even in the strong-coupling limit \( g \to \infty \). To this end we simply add and subtract a harmonic oscillator of trial frequency \( \Omega \) to the anharmonic oscillator potential \((2.1)\):

\[
V(x) = \frac{M}{2} \Omega^2 x^2 + \frac{g M \omega^2 - \Omega^2}{g} x^2 + g x^4. \tag{3.1}
\]

We now treat the second term as if it was of the order of the coupling constant \( g \). The result is obtained most simply by substituting the frequency \( \omega \) in the original anharmonic oscillator potential \((2.1)\) according to Kleinert’s trick \[1\] where we have

\[
\omega \to \Omega \sqrt{1 + gr}, \tag{3.2}
\]

\[
r \equiv \frac{\omega^2 - \Omega^2}{g \Omega^2}. \tag{3.3}
\]

Writing the ground-state wave function \((2.32)\) in the form \(\Psi(x) = \exp[W(x)]\) with the cumulant expansion

\[
W(x) = \exp \left[ \frac{1}{4} \log \left( \frac{M \omega}{\hbar \pi} \right) - \frac{M \omega^2}{2 \hbar} x^2 + \frac{g}{\hbar} \left( \frac{9h^2}{16M^2\omega^3} - \frac{3h}{4M\omega^2} x^2 - \frac{1}{16} \right) \right.
\]
\[
+ \frac{g^2}{2\hbar^2} \left( -\frac{205h^4}{32M^4\omega^6} + \frac{21h^4}{4M^2\omega^6} x^2 + \frac{11h^2}{8M^2\omega^4} x^4 + \frac{h}{6M\omega^3} x^6 \right) + \left. \ldots \right], \tag{3.4}
\]

we apply the trick \((3.2)\) to \(W(x)\), and reexpand in powers of \(g\) at fixed \(r\). Afterwards \(r\) is substituted according to \((3.3)\). Thus we obtain in the first order

\[
\Psi^{(1)}(x, \Omega) = \exp \left[ \frac{1}{4} \log \left( \frac{M \Omega}{\hbar \pi} \right) - \frac{1}{8} + \frac{\omega^2}{8\Omega^2} - \frac{M \Omega}{4h} \left( \frac{1}{4} + \frac{\omega^2}{\Omega^2} \right) x^2 \right.
\]
\[
+ \frac{g}{\hbar} \left( \frac{9h^2}{16M^2\Omega^3} - \frac{3h}{4M\Omega^2} x^2 - \frac{1}{4\Omega} \right) x^4 \right], \tag{3.5}
\]

whereas the second-order expansion reads

\[
\Psi^{(2)}(x, \Omega) = \exp \left[ \frac{1}{4} \log \left( \frac{M \Omega}{\hbar \pi} \right) - \frac{1}{16} + \frac{\omega^2}{4\Omega^2} - \frac{\omega^4}{16\Omega^4} - \frac{M \Omega}{2h} \left( \frac{3}{8} + \frac{3\omega^2}{4\Omega^2} - \frac{\omega^4}{8\Omega^4} \right) x^2 \right.
\]
\[
+ \frac{g}{\hbar} \left[ \frac{9h^2}{16M^2\Omega^3} \left( \frac{5}{2} - \frac{3\omega^2}{4\Omega^2} \right) - \frac{3h}{4M\Omega^2} \left( 2 - \frac{\omega^2}{\Omega^2} \right) x^2 - \frac{1}{4\Omega} \left( \frac{3}{2} - \frac{\omega^2}{2\Omega^2} \right) x^4 \right]
\]
\[
+ \frac{g^2}{2h^2} \left[ -\frac{205h^4}{32M^4\Omega^6} + \frac{21h^4}{2M^2\Omega^6} x^2 + \frac{11h^2}{8M^2\Omega^4} x^4 + \frac{h}{6M\Omega^3} x^6 \right] \right] \} \right]. \tag{3.6}
\]

Both in first and in second order, the ground-state wave function depends on the artificially introduced frequency parameter \(\Omega\). According to the principle of minimal sensitivity \[8\] we minimize its influence on \(\Psi^{(n)}(x, \Omega)\) by searching for local extrema of \(\Psi^{(n)}(x, \Omega)\) with respect to \(\Omega\). As we have written the wave function in the form \(\Psi^{(n)}(x, \Omega) = \exp[W^{(n)}(x, \Omega)]\), it is sufficient to take into account just the inner derivative of \(\Psi^{(n)}(x, \Omega)\), i.e. we obtain the condition \(\partial W^{(n)}(x, \Omega)/\partial \Omega = 0\).

It turns out in the first order \(n = 1\) that this equation has two solutions for \(x < 0.684\) and for \(x > 0.780\), however in the interval \(0.684 < x < 0.780\), \(\Psi^{(1)}(x, \Omega)\) does not have any extremum \[8\]. In accordance with the principle of minimal sensitivity we look for turning points on that interval instead, i.e. we solve \(\partial^2 W^{(1)}(x, \Omega)/\partial \Omega^2 = 0\). Fig. \[8\] shows how the curve for the turning points links the extremal branches. Now we have to choose which one of the branches of \(\Omega^1(x)\) we take into account. Inserting the lower branch for \(x > 0.780\) into the wave function \((3.3)\) leads to unphysical results as the ground-state wave function explodes dramatically. Thus we choose the upper branch for \(x > 0.780\). For \(x < 0.684\) the wave function becomes rather independent of the choice of \(\Omega\). As we are looking for a function \(\Omega^{(1)}(x)\) which is as smooth as possible, we choose the lower branch for \(x < 0.684\). Fig. \[8\] shows all branches of \(\Omega\) and highlights our final choice by a solid line.
FIG. 1. First-order results for the variational parameter $\Omega$ at the intermediate coupling $g = 1/2$. The extremal branches for $x < 0.684$ and for $x > 0.780$ (solid lines and dashed lines) are obtained from the equation $\partial W^{(1)}(x, \Omega)/\partial \Omega = 0$. For $0.684 < x < 0.780$ there are no real positive solutions of this equation. Thus we look in this interval also for turning points, i.e. we determine real positive solutions of the equation $\partial^2 W^{(1)}(x, \Omega)/\partial \Omega^2 = 0$. The curve for the turning points on the entire interval lies between the two other branches (dot-dashed line) and fills the gap. Thus we can take those branches into account which provide us with the most continuous function $\Omega^{(1)}(x)$, i.e. the solid line.

FIG. 2. The two positive branches of $\Omega^{(2)}(x)$ on the interval $[0, 4]$ for intermediate coupling $g = 1/2$ obtained by solving the turning point equation $\partial^2 W^{(2)}(x, \Omega)/\partial \Omega^2 = 0$. In order to achieve the smoothest function we choose the lower branch for $x < 0.8$ and the upper branch for $x > 0.8$. This choice is justified by the results of our first-order calculation (see Fig. 1).

For the second order $n = 2$ there are no real positive solutions of the equation $\partial W^{(2)}(x, \Omega)/\partial \Omega = 0$ on the interval $x = [0, 4]$. Once more we have to look for turning points instead and solve $\partial^2 W^{(2)}(x, \Omega)/\partial \Omega^2 = 0$. This equation has two positive solutions on this interval, so we get two branches for the solution $\Omega^{(2)}(x)$ (see Fig. 2). Again we have to choose one of these two branches. Relying on a similar argument as for the first-order we choose the upper branch for $x > 0.8$ and the lower one for $x < 0.8$. The perturbation series converges so quickly that the curves for the first and second order as well as the exact ground-state wave function are not distinguishable on the plots. To see the difference we determine the mean square deviation from the exact numerical solution

$$D^{(n)} = 2 \int_0^\infty dx \left[ \Psi^{(n)}(x) - \Psi^{ex}(x) \right]^2,$$

where the index $n$ denotes the order. The integration is performed numerically. The factor 2 is introduced for symmetry reasons, since we restrict our calculations to the positive $x$-axis. It turns out that the mean square deviation $D^{(2)} = 6.8 \times 10^{-7}$ is smaller than $D^{(1)} = 1.1 \times 10^{-5}$ by a factor of 0.063, which indicates that variational perturbation theory converges very quickly also for the ground-state wave function. The same applies to both weak
FIG. 3. The normalized second-order ground-state wave function for weak coupling (dashed, $g = 0.1$), for intermediate coupling (solid, $g = 1/2$), and for strong coupling (dotted, $g = 50$).

and strong coupling as is illustrated in Fig. 3 which shows the second-order ground-state wave function $\Psi^{(2)}(x)$ for $g = 0.1$, $g = 1/2$, and $g = 50$, respectively.

Note that variational perturbation theory does not preserve the normalization of the wave function. Although the perturbative ground-state wave function $\Psi(x, \Omega)$ is still normalized in the usual sense, this normalization is spoilt by extremizing $\Psi(x, \Omega)$ with respect to the frequency parameter $\Omega$. Thus we have to normalize the variational ground-state wave function at the end.

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