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A new method for the solution of the Schrödinger equation

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Abstract

We present a new method for the solution of the Schrödinger equation applicable to problems of a non-perturbative nature. The method works by identifying three different scales in the problem, which then are treated independently: an asymptotic scale, which depends uniquely on the form of the potential at large distances; an intermediate scale, still characterized by an exponential decay of the wavefunction; and, finally, a short distance scale, in which the wavefunction is sizable. The notion of optimized perturbation is then used in the last two regimes. We apply the method to the quantum anharmonic oscillator and find it suitable to treat both energy eigenvalues and wavefunctions, even for strong couplings.

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1. Introduction

It is well known that perturbation theory usually generates divergent asymptotic series [1]. Improving the convergence of the standard Rayleigh–Schrödinger perturbative expansion has been the subject of many studies in the past (see, e.g., [2–6] and references therein) and many variants of 'optimized expansions' have been proposed.

These efforts have been aimed to calculate either energy eigenvalues or wavefunctions and are limited in practice by the rapidly growing complexity of generating corrections beyond the first few orders in the perturbative expansion. In this paper, we present a method that works equally well for energy eigenvalues and wavefunctions and, furthermore, can be used to calculate these quantities to any given accuracy, since the generation of successive corrections in the perturbative expansion only requires the solution of algebraic equations.

The method can be placed within the general context of the multiple-scale perturbation theory (MSPT) [7–9], since it works by identifying different length scales in the problem,

which reflect in different behaviour of the wavefunction: we illustrate the method by applying it to the quantum anharmonic oscillator (AHO), which is the usual benchmark to test any non-perturbative method [3–6, 10–13].

A thorough analysis of the quantum AHO in the MSPT framework is given in [5]: here we follow a different path, by using the MSPT concept to write down a suitable ansatz for the AHO wavefunction and then by using it to generate an optimized perturbative expansion. This we do within the framework of the so-called linear delta expansion (LDE) [14–28]. The LDE has been extensively applied in many different settings with varying degrees of success. For example, in [29] it has been used to analyse disordered systems. In [30] it has been applied to study the slow roll potential in inflationary models. Pinto and collaborators have applied it to the Bose–Einstein condensation problem [31], the $O(N)(\phi^2)^2_{3d}$ model [32], the Walecka model [33] and to the ϕ^4 theory at high temperature [34]. More recently, the LDE has been applied with success to the study of classical nonlinear systems [35, 36].

The paper is organized as follows. In section 2 we introduce the method and apply it to the quantum AHO; in section 3 we present the numerical results and finally, in section 4 we draw our conclusions.

2. The method

Given a quantum system such as the anharmonic oscillator, a standard application of the LDE would involve a rearrangement of the Hamiltonian, e.g.

$$H = \frac{p^2}{2m} + V(q) \quad \longrightarrow \quad H_\delta = H_0 + \delta H' \tag{1}$$

with $H_0 = p^2/2m + m\Omega^2 q^2/2$ and $H' = V(q) - m\Omega^2 q^2/2$; so that $H_{\delta=1} \equiv H$, Ω being a trial frequency. Physical quantities are expanded in δ, which is then set to 1: although exact results should not depend upon Ω, at any finite order in δ one is left with Ω-dependent quantities. The value of Ω can then be fixed by invoking a *principle of minimal sensitivity* (PMS) [16] and minimizing the dependence upon Ω of a given observable, say the energy.

Here we would like to follow a different path, by introducing the trial parameter of the LDE not in the Hamiltonian, but into the wavefunction.

The first step of this approach consists in the identification of three different scales in the problem, which give rise to different behaviour of the wavefunction. Keeping in mind the standard separation of the Hamiltonian in an unperturbed piece (the harmonic oscillator) and a perturbative one (the anharmonic term), one can recognize that at very large distances the wavefunction assumes its asymptotic behaviour: this is completely determined by the anharmonic potential and it is the same for all (ground and excited) states; at intermediate distances the wavefunction still decays exponentially, but now governed by the harmonic term; finally, there is a short distance scale, in which the wavefunction is sizable.

Then, we introduce an arbitrary parameter in the last two scales, which is used, in the spirit of the LDE, to optimize a perturbative expansion in a suitable parameter.

Consider the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{m\omega^2}{2}x^2 + \frac{\mu}{4}x^4\right]\psi_n(x) = E_n\psi_n(x) \tag{2}$$

where μ is the anharmonic coupling. The asymptotic behaviour of $\psi_n(x)$ in the region of large x is determined by substituting the ansatz $\psi_n(x) \propto \mathrm{e}^{-\gamma|x|^p}$ into equation (2). One obtains $p = 3$ and $\gamma = \sqrt{\mu m/2}/3\hbar$.

In order to make the three scales explicit in the wavefunction, we write

$$\psi_n(x) = \mathrm{e}^{-\gamma|x|^3 - \beta x^2}\xi_n(x) \tag{3}$$

where the exponential takes care of the correct behaviour in the limit $|x| \to \infty$. Note that the quadratic term in the exponential does not affect the behaviour at large distances, but dominates at scales where $|x| < \beta/\gamma$. Here $\beta = m\sqrt{\omega^2+\Omega^2}/2\hbar$ is the coefficient of a harmonic oscillator of frequency $\widetilde{\Omega} \equiv \sqrt{\omega^2+\Omega^2}$, where Ω is an arbitrary parameter introduced by hand; ξ_n is a well-behaved function, which satisfies the equation[3]:

$$\xi_n''(x) - \left[\frac{\sqrt{2m\mu}}{\hbar}x^2 + \frac{2m\widetilde{\Omega}x}{\hbar}\right]\xi_n'(x) + \left[\frac{\sqrt{2\mu m^3\widetilde{\Omega}^2}}{\hbar^2}x^3 + \frac{m^2\Omega^2}{\hbar^2}x^2 - \frac{\sqrt{2m\mu}}{\hbar}x + \frac{2mE_n}{\hbar^2} - \frac{m\widetilde{\Omega}}{\hbar}\right]\xi_n(x) = 0. \qquad (4)$$

Equation (3) has been introduced in order to single out three different regimes in the wavefunction: the purely asymptotic regime ($|x| \to \infty$), where the cubic term in the exponential dominates; the intermediate regime, where $|x|$ is not yet asymptotic but large enough to expect the wavefunction to be exponentially damped; the regime of small $|x|$ where the physics is all contained in the ξ. The last two regimes will display a dependence upon the arbitrary frequency Ω, although in a quite different fashion (in fact, the intermediate regime displays a truly non-perturbative dependence upon Ω). In the limits $(\mu, \Omega) \to 0$ one obtains the equation for the harmonic oscillator of frequency ω, which admits polynomial solutions (the Hermite polynomials).

It is worth stressing that the energy E_n in equation (4) is still the true energy, since no approximation has been used to derive this equation.

We observe in equation (4) that both the wavefunction $\xi_n(x)$ and the energy E_n depend in some nontrivial way upon the anharmonic coefficient μ. On the other hand, the dependence of $\psi_n(x)$ and E_n upon the arbitrary frequency Ω is only fictitious, since this parameter does not appear in the original equation (2). Nonetheless, we will show that Ω can be used to generate an efficient expansion for the solution of equation (2).

Indeed we rewrite equation (4) as

$$\xi_n''(x) - \left[\frac{2m\widetilde{\Omega}x}{\hbar}\right]\xi_n'(x) + \left[\frac{2mE_n}{\hbar^2} - \frac{m\widetilde{\Omega}}{\hbar}\right]\xi_n(x) = \delta\left\{\frac{\sqrt{2m\mu}}{\hbar}x^2\xi_n'(x) - \left[\frac{\sqrt{2\mu m^3\widetilde{\Omega}^2}}{\hbar^2}x^3 + \frac{m^2\Omega^2}{\hbar^2}x^2 - \frac{\sqrt{2m\mu}}{\hbar}x\right]\xi_n(x)\right\} \qquad (5)$$

where the left-hand side of equation (5) corresponds to the equation for a harmonic oscillator of frequency $\widetilde{\Omega}$, with ansatz $\psi_n = \xi_n \exp[-(m\widetilde{\Omega}/2\hbar)x^2]$. Following the spirit of the LDE, we have introduced a parameter δ, which is going to be used as a power-counting device: when $\delta = 1$, equation (5) reduces exactly to equation (4).

Although δ is not a small parameter we will treat the right-hand side of equation (5) as a perturbation, writing down the following expansions:

$$\xi_n(x) = \sum_{j=0}^{\infty}\delta^j\xi_{nj}(x) \qquad E_n = \sum_{j=0}^{\infty}\delta^j E_{nj}. \qquad (6)$$

Combining equations (5) and (6), one can generate a hierarchy of equations, corresponding to the different orders in δ.

[3] We are considering only the region $x > 0$. The other region will be obtained by using the symmetry properties of the wavefunction.

Since we are doing perturbation theory, all the results, to any finite order in the expansion, will depend upon the arbitrary frequency Ω. Such dependence will therefore be minimized by applying the PMS, i.e. by requiring that a given observable O (the energy, for example) be locally independent of Ω:

$$\frac{\partial O}{\partial \Omega} = 0. \tag{7}$$

We will illustrate the method by explicitly showing the first two orders, although we have obtained results up to the fifteenth order. To lowest order equation (5) reduces to the equation of a harmonic oscillator of frequency $\widetilde{\Omega}$, whose solutions are the Hermite polynomials, $\xi_{n0}(x) = H_n(\sqrt{m\widetilde{\Omega}/\hbar}x)$, while the energy eigenvalues are given by $E_{n0} = \hbar\widetilde{\Omega}(n + 1/2)$, $n = 0, 1, \ldots$.

To first order we have the equation

$$\xi''_{n1}(x) - \left[\frac{2m\widetilde{\Omega}x}{\hbar}\right]\xi'_{n1}(x) + \frac{2m\widetilde{\Omega}}{\hbar}n\xi_{n1}(x) = \left\{-\frac{2mE_{n1}}{\hbar^2} + \frac{\sqrt{2m\mu}}{\hbar}x - \frac{m^2\Omega^2}{\hbar^2}x^2 - \frac{\sqrt{2\mu m^3\widetilde{\Omega}^2}}{\hbar^2}x^3\right\}\xi_{n0}(x). \tag{8}$$

Although such an equation is valid for any state of the AHO, for illustrative purposes we will now consider only the ground state, for which $\xi_{00}(x) = 1$. Then, for the case $n = 0$, the solution of equation (8) is a polynomial of order 3 and can be cast in terms of unknown coefficients as

$$\xi_{01}(x) = a_0 + a_1x + a_2x^2 + a_3x^3. \tag{9}$$

The coefficient a_0 is not determined by equation (8) and we impose $a_0 = 0$, since it corresponds to the same functional form of ξ_{00}.[4] By substituting this polynomial into equation (8) one gets the coefficients

$$a_1 = 0 \qquad a_2 = \frac{m\Omega^2}{4\hbar\widetilde{\Omega}} \qquad a_3 = \frac{1}{3\hbar}\sqrt{\frac{m\mu}{2}} \tag{10}$$

and the energy

$$E_{01} = -\frac{\hbar\Omega^2}{4\widetilde{\Omega}}. \tag{11}$$

Therefore, up to first order, we get the energy

$$E_0^{(1)} = \frac{\hbar\widetilde{\Omega}}{2} - \frac{\hbar\Omega^2}{4\widetilde{\Omega}}. \tag{12}$$

It is important to note that the wavefunction obtained up to first order does not have nodes, a desirable result for the wavefunction of the ground state.

The PMS to this order yields the solution $\Omega = 0$ and the corresponding energy

$$E_0^{(1)}\Big|_{\mathrm{PMS}} = \frac{\hbar\omega}{2}. \tag{13}$$

Here we would like to stress a point: we could have obtained a solution similar to that of equation (9) by direct application of the Rayleigh–Schrödinger perturbation theory to the wavefunctions of the harmonic oscillator. However, had we applied the LDE directly to the Rayleigh–Schrödinger expansion, we would not have been able to reproduce the correct asymptotic behaviour of the wavefunction [6].

[4] This is somewhat analogous to the procedure employed in the Lindstedt–Poincaré method to get rid of 'secular terms' in the solutions [35, 36].

The extension of the method to include higher orders is straightforward and the details will be presented elsewhere [37]. Here we just present the expression for the energy up to third order

$$E_0^{(3)} = \frac{\hbar}{32m^2\widetilde{\Omega}^5}[6\mu\hbar\widetilde{\Omega}(-\omega^2 + 2\widetilde{\Omega}^2) + m^2(\omega^6 - 5\omega^4\widetilde{\Omega}^2 + 15\omega^2\widetilde{\Omega}^4 + 5\widetilde{\Omega}^6)]. \tag{14}$$

The optimal value of Ω is then obtained by using the PMS. The expression for Ω in the general case is lengthy (see [37]) and we only write here its asymptotic value in the limit of large μ (from now on we assume $\hbar = m = \omega = 1$):

$$\Omega = 2\left(\frac{3\mu}{5}\right)^{1/3} + O[\mu^{-1/3}]. \tag{15}$$

We can then substitute this expression in equation (14) and extract the asymptotic behaviour of the energy of the ground state to third order:

$$E_0^{(3)} = \frac{3}{16}\left(\frac{75}{2}\right)^{1/3}\left(\frac{\mu}{4}\right)^{1/3} + O[\mu^{-1/3}]. \tag{16}$$

The asymptotic behaviour of the ground state energy of the AHO has been studied in [38], by using the exact Rayleigh–Schrödinger perturbation coefficients as an input. We use this calculation as a reference to compare to our results. Following the notation set in [38] we write the energy as

$$E_0 = \alpha_0\left(\frac{\mu}{4}\right)^{1/3} + O[\mu^{-1/3}] \tag{17}$$

and using this formula in equation (16) we obtain the coefficient α_0 to third order in our expansion to be

$$\alpha_0^{(3)} = \frac{3}{16}\left(\frac{75}{2}\right)^{1/3} \approx 0.627 \tag{18}$$

which falls within 6% of the true value. We present our results in the next section.

3. Results

In this section, we present the numerical results for both the ground and first excited states of the AHO. All the computations are carried out assuming $\hbar = m = \omega = 1$.

We begin by studying the dependence of the coefficient α_0 (the coefficient in the asymptotic expansion of the ground state energy) on the perturbative order. We show this dependence in figure 1, where the calculation has been carried out up to order 15. The horizontal line is the result of [38], calculated with 20 digit precision. We note that our approximation converges quickly towards this result, and in fact, the fifteenth order result falls within 0.01% of the true value. We also observe a change in the behaviour of the approximate α_0 in the passage from the tenth to the eleventh order. This is the result of the emergence of a new extremum fulfilling the PMS condition.

In figure 2 we plot the ground state energy of the AHO as a function of the anharmonic coefficient μ. The solid bold curve is the exact result obtained by numerically solving the Schrödinger equation for the AHO. The other five curves yield the energy at different perturbative orders, up to fifth order. We observe that the energies converge nicely to the exact result as the perturbative order is increased. We note from the plot that the perturbative results lie below the exact result. Unfortunately, this is not a general property of the method, as we have already observed in figure 1.

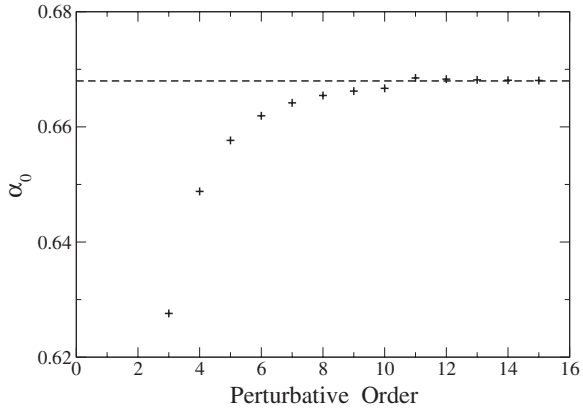

Figure 1. The coefficient α_0 in the asymptotic expansion of the ground state energy (see text) at different perturbative orders, up to order 15. The broken line is the exact result [38].

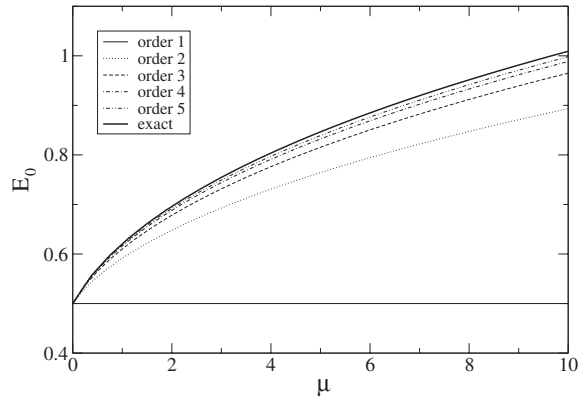

Figure 2. Ground state energy of the AHO as a function of μ to different perturbative orders, assuming $\hbar = m = \omega = 1$.

The ground state energy of the AHO as a function of the arbitrary parameter Ω is plotted in figure 3, for $\mu = 5$. The different curves correspond to different orders in perturbation theory (from second up to fifth order). We observe that the ground state energy develops local minima and maxima at different perturbative orders. In order to decide among the various extrema of the function one asks that the solution corresponds to the extrema around which the observable is flatter. We have noted that if another extremum is taken, the wavefunction can develop unphysical nodes.

In figure 4 we plot the wavefunction of the ground state of the AHO for a very large μ ($\mu = 200$). The solid line is the exact (numerical) result, whereas the other lines refer to the wavefunction obtained by applying our method to order 3, 10 and 15. From this plot we see that the approximation works very well, even for large values of μ, and that, by going to higher order, the wavefunction is approximated better and better.

This agreement is better appreciated by looking at figure 5, where we plot the ratio R of the approximate wavefunction to the exact one. We have used $\mu = 200$ and shown the results obtained to third, tenth and fifteenth order. This plot should be compared with the dashed curve in figure 2 of [6], the only one, to our knowledge, to provide a calculation of

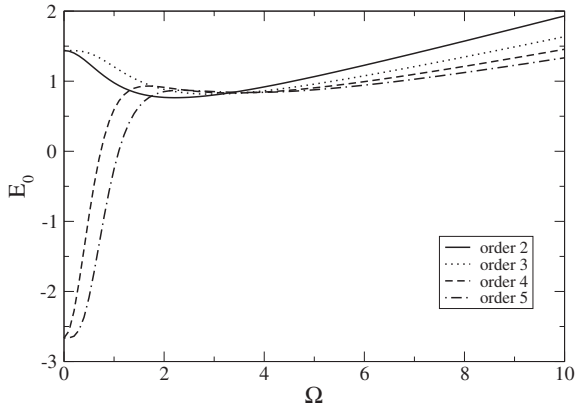

Figure 3. Energy of the AHO as a function of Ω, at different perturbative orders ($\hbar = m = \omega = 1$) and keeping μ fixed ($\mu = 5$).

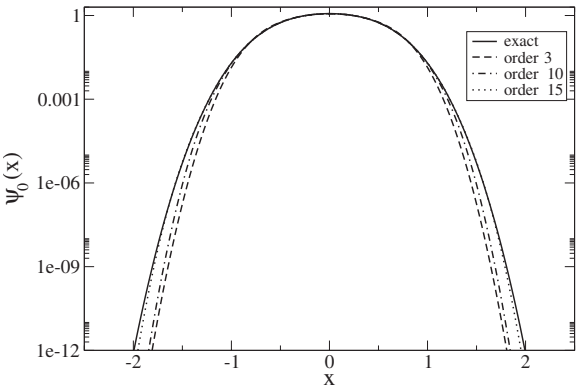

Figure 4. Wavefunction for the ground state of the anharmonic oscillator, assuming $m = \hbar = \omega = 1$ and $\mu = 200$.

the wavefunction of the AHO. Note, however, that the authors of [6] display results only for the ground state and only at first order.

This point is better illustrated in table 1, where we compare the results for the ground state wavefunction of the AHO, given in [6], with our results to various orders. For example, at $x = 1$ (which is already a rather large value), our method yields (at order 15) an error of 0.1%, compared with 4.7% of [6]. Only for $x = 2$, where, however, the wavefunction is exponentially small, does the method of [6] provide a better estimate. Moreover, the normalization of the wavefunction constrains the error in the region of large x.

In table 2 we also see that the expectation values of various quantities can be calculated with high precision using the method presented here.

A comparison of the AHO wavefunction to the same (high) perturbative order is not possible since the results of [6] are only available to first order. We would like to stress that with the technique described here, the calculation of the Nth order contribution requires the solution of $3N$ algebraic equations, which is quite straightforward using any computer algebra package.

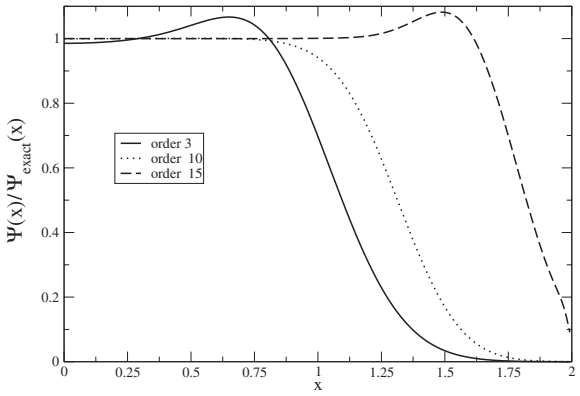

Figure 5. Ratio of the approximate wavefunction to the exact (numerical) result at different perturbative orders, assuming $\hbar = m = \omega = 1$ and $\mu = 200$.

Table 1. Ground state wavefunction for the AHO corresponding to $\mu = 200$. In the first three rows are the numerical results obtained by using our method to various orders; the fourth and fifth rows are taken from [6].

	$x = 0$	$x = 0.5$	$x = 1.0$	$x = 1.5$	$x = 2$
$\psi_{\rm us}(x)$ (order 3)	1.150	5.792×10^{-1}	1.379×10^{-2}	1.761×10^{-7}	5.752×10^{-17}
$\psi_{\rm us}(x)$ (order 10)	1.167	5.568×10^{-1}	1.863×10^{-2}	8.758×10^{-7}	2.128×10^{-16}
$\psi_{\rm us}(x)$ (order 15)	1.167	5.563×10^{-1}	1.981×10^{-2}	5.589×10^{-6}	1.043×10^{-13}
$\psi_{\rm Hatsuda}(x)$	1.170	5.519×10^{-1}	1.885×10^{-2}	3.925×10^{-6}	3.095×10^{-13}
$\psi_{\rm exact}(x)$	1.167	5.564×10^{-1}	1.979×10^{-2}	5.168×10^{-6}	7.982×10^{-13}

Table 2. Expectation values of p^2, x^2, x^4 and of the energy with our method to various orders, compared with the results of [6] for $\mu = 200$.

	$\langle p^2 \rangle$	$\langle x^2 \rangle$	$\langle x^4 \rangle$	$\langle H \rangle$
us (order 3)	3.212 412 23	0.080 885 49	0.017 237 22	2.508 510 06
us (order 10)	3.310 159 62	0.077 315 31	0.016 120 42	2.499 758 44
us (order 15)	3.307 231 35	0.077 309 03	0.016 148 77	2.499 708 80
Hatsuda	3.344 30	0.076 41	0.015 79	2.500 03
exact	3.307 174 23	0.077 312 37	0.016 149 31	2.499 708 77

In figure 6 we have tested the method by applying it to the calculation of the wavefunction of the first excited state. The solid line corresponds to the exact result, whereas the other lines correspond to the wavefunction obtained at different orders with our method. From the figure one can appreciate the fast convergence in the region where the wavefunction is large. The extension to study the full spectrum of the AHO is currently underway.

Finally, we have also applied our method to the problem of the double-well potential (DWP), $V(x) = -m\omega^2 x^2/2 + \mu x^4/4$. In this case, the ansatz for the wavefunction has been slightly modified in order to account for the different shape of the potential,

$$\psi_0^{(\rm dw)}(x) = \xi(x) \exp(-\gamma(x - x_0)^3 - \beta(x - x_0)^2) \tag{19}$$

where $x_0 = \sqrt{m/2\mu}\Omega$. In figure 7 we show the results of the application of our method to the DWP up to third order, using the values $\hbar = m = \omega = 1$ and $\mu = 0.1$. The main point of this figure is to show that the method that we are proposing here is viable even in this case,

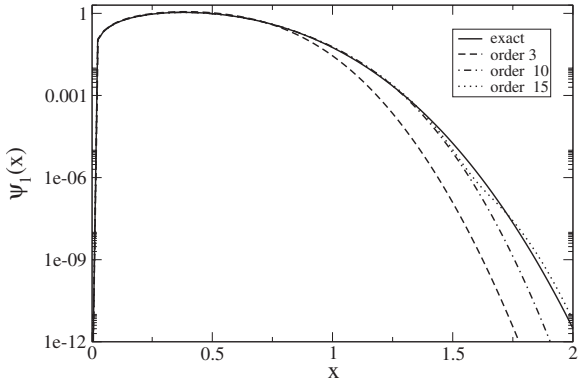

Figure 6. Wavefunction of the first excited state of the anharmonic oscillator, assuming $\hbar = m = \omega = 1$ and $\mu = 200$.

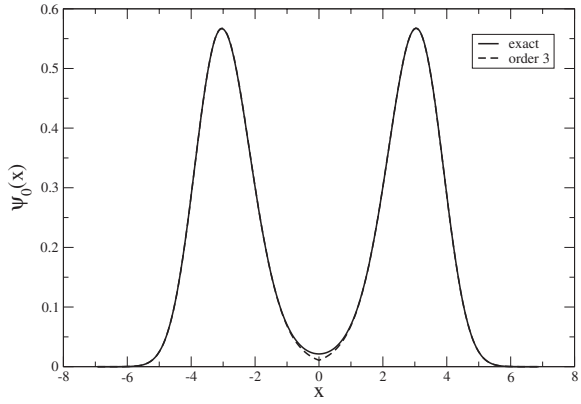

Figure 7. Wavefunction for the ground state of the double-well potential assuming $\hbar = m = \omega = 1$ and $\mu = 0.1$. The solid line is the exact (numerical) result, the dashed line is the wavefunction to third order.

although a detailed analysis is left for future work. We stress that already at third order the wavefunction of the DWP is well approximated by our method.

4. Conclusions

We have presented a method for the solution of the Schrödinger equation that can be applied to non-perturbative problems. It is based on a novel implementation of the LDE, realized through an ansatz for the wavefunction that takes into account its behaviour at different length scales: an arbitrary parameter *á la* LDE, which enables us to optimize a perturbative expansion, is then introduced directly *into the wavefunction* and not in the Hamiltonian as in a standard treatment of the LDE. Virtues of the method are that the generation of higher perturbative orders in the expansion can be accomplished with ease and that it can be used with no modifications to obtain results for both the ground and excited states.

We have presented the results of applying this new method to the quantum anharmonic oscillator. Specifically, we have computed the value for the ground state energy as a function of the anharmonic parameter for several perturbative orders (up to fifth order), the value

of the coefficient in the asymptotic expansion of the ground state energy up to perturbative order 15, the wavefunction of the ground state and its ratio to the exact (numerical) one, and the wavefunction of the first excited state. In all cases we found good agreement with the exact results. We have also shown results for the ground state wavefunction of the double-well potential, although a detailed analysis of this problem is left for future work.

Due to its simplicity and accuracy we believe this method to be competitive with the other methods developed to deal with the AHO: as a matter of fact, the degree of precision of the results can be drastically improved by raising the perturbative order in the expansion, a step which does not bear any technical difficulty. Of course, it would be interesting to give a formal proof of the convergence of this expansion, as already done in other approaches [10–13, 25–28]. Note however that, although we are also employing a LDE, we cannot directly apply in our case the procedure followed in these papers, since it is generally based on a standard perturbative series, modified to accommodate the LDE, whereas our ansatz already incorporates the exact asymptotic behaviour of the wavefunction, that is a non-perturbative contribution.

We are currently working on the application of this method to the calculation of the excited states of the AHO and to more general anharmonic potentials.

Acknowledgments

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