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Comment on: "Ground state energies from converging and diverging power series expansions", Ann. Phys. 373 (2016) 456–469

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ABSTRACT

We compare two alternative expansions for finite attractive wells. One of them is known from long ago and is given in terms of powers of the strength parameter. The other one is based on the solution of the equations of the Rayleigh–Schrödinger perturbation theory in a basis set of functions of period L. The analysis of exactly solvable models shows that although the exact solution of the problem with periodic boundary conditions yields the correct result when $L \to \infty$ the coefficients of the series for this same problem blow up and fail to produce the correct asymptotic expansion.

1. Introduction

In a recent paper Lisowski et al. [1] proposed the application of an approximate method for the treatment of the Schrödinger equation with finite attractive potentials. It consists of solving the secular equation for the matrix representation of the Hamiltonian operator in a basis set of functions of period L. The eigenvalues of this matrix are expected to approach the actual eigenvalues of the problem in the limit $L \to \infty$. The authors also applied the same approach to the equations given by perturbation theory thus obtaining approximate perturbation coefficients that depend on the box

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length L. They argued that this perturbation series is convergent when the width of the ground-state eigenfunction is larger than L and divergent when that width is smaller than L. The former case takes place when the potential strength $V_0 > 0$ is smaller than a critical value V_{crit} and the latter when $V_0 > V_{crit}$. In order to sum the perturbation series in both regimes the authors proposed the application of the well known Borel transformation with the substitution of a finite integral for the infinite one when carrying out the inverse transformation.

It is well known that there exists a perturbation series about $V_0 = 0$ in the case of a one-dimensional short-range potential and there are even explicit expressions for the first perturbation coefficients [2] (and references therein). However, Lisowski et al. [1] state that "It is often assumed that bound states of quantum mechanical systems are intrinsically non-perturbative in nature and therefore any power series expansion methods should be inapplicable to predict the energies for attractive potentials". The purpose of this paper is to discuss the connection between the approximate perturbation series proposed by Lisowski et al. [1] and the well known exact perturbation series [2].

In Section 2 we outline the application of the two perturbation methods just mentioned to a general finite attractive well. In Section 3 we discuss the perturbation series by means of simple, exactly solvable models. Finally, in Section 4 we summarize the main results and draw conclusions.

2. Short-range shallow wells

Throughout this paper we consider a particle of mass m that moves in one dimension under the effect of a short-range negative potential $-V_0 \leq V(x) \leq 0$ that we suppose to be of even parity $V(-x) = V(x)$. In order to simplify the calculations it is convenient to rewrite the Hamiltonian operator

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x), \tag{1}$$

in dimensionless form by means of the change of variables $x = \gamma x'$, where γ is a suitable length. In this way we obtain

$$H' = \frac{2m\gamma^2}{\hbar^2}H = -\frac{d^2}{dx'^2} + \lambda v(x'),$$
$$\lambda = \frac{2m\gamma^2 V_0}{\hbar^2}, \quad v(x') = \frac{V(\gamma x')}{V_0}. \tag{2}$$

Thus an eigenvalue E of H and the corresponding one ϵ of H' are related by

$$\epsilon = \frac{2m\gamma^2}{\hbar^2}E. \tag{3}$$

From now on we omit the prime on the dimensionless quantities and write the Hamiltonian operator as

$$H = -\frac{d^2}{dx^2} + \lambda v(x), \tag{4}$$

where $-1 \leq v(x) \leq 0$.

It is well known that in the case of a short-range potential the ground state energy can be expanded in a formal perturbation series of the form [2]:

$$-(-\epsilon)^{1/2} = \frac{\lambda}{2}\int v(x)\,dx + \frac{\lambda^2}{4}\int\int v(x)v(y)|x-y|\,dxdy$$
$$+ \frac{\lambda^3}{48}\int\int\int v(x)v(y)v(z)\,(|x-y|+|y-z|+|z-x|)^2\,dxdydz$$
$$+ \frac{\lambda^4}{96}\int\int\int\int v(x)v(y)v(z)v(t)\,\big(|x-y|^3$$

$$+ \; 6|x-y|^2|x-z| + 3|x-y|^2|z-t| + \; 6|x-y||x-z||z-t| \Big) \, dxdydzdt + \mathcal{O}\left(\lambda^5\right). \tag{5}$$

This expansion was derived from the zeros of a perturbative expansion for the inverse of the Noyes form of the T matrix. If we can calculate these integrals exactly then we obtain the first terms of the perturbation expansion for the dimensionless energy

$$\epsilon = \sum_{j=2}^{\infty} \epsilon^{(j)} \lambda^j, \tag{6}$$

exactly.

Alternatively, one can derive this last expression directly by means of the well known Rayleigh–Schrödinger perturbation theory when the unperturbed potential is $\beta v_0(x) = -\beta\delta(x)$, where $\delta(x)$ is the Dirac delta. One thus obtains

$$\hat{\epsilon} = \sum_{j=2}^{\infty} \hat{\epsilon}^{(j)}(\beta) \lambda^j, \tag{7}$$

and then recovers the actual λ-power series in the limit $\beta \to 0$ [3]. The perturbation expansions (5) and (6) are valid for sufficiently small values of λ and are based on the asymptotic boundary conditions $\lim_{|x|\to\infty} \psi(x) = 0$ for the eigenfunction $\psi(x)$.

On the other hand, the perturbation expansion proposed by Lisowski et al. [1] is based on periodic boundary conditions $\psi(x+L) = \psi(x)$. In this case the eigenfunctions and eigenvalues of the unperturbed problem ($\lambda = 0$) are

$$|n\rangle = \frac{1}{\sqrt{L}} \exp\left[\frac{2\pi i n x}{L}\right], \; n = 0, \pm 1, \pm 2, \ldots, \qquad e_n = \frac{4n^2\pi^2}{L^2}, \tag{8}$$

and the coefficients of the perturbation expansion

$$\tilde{\epsilon}(L) = \sum_{j=2}^{\infty} \tilde{\epsilon}^{(j)}(L) \lambda^j, \tag{9}$$

depend on the box length L. In principle, the exact solution of the problem with periodic boundary conditions should approach the exact solution of the problem with infinite boundary conditions in the limit $L \to \infty$. One of the questions that we investigate in what follows is if it is possible to recover the actual series (6) from the approximate one (9) when $L \to \infty$.

In order to facilitate the discussion in subsequent sections, from now on we call these three approaches the T-method, the β-method and the L-method, respectively.

In addition to the series for small λ we can also derive an expansion for large λ provided that we can expand $v(x)$ in a Taylor series about $x = 0$, $v(x) = v(0) + \frac{1}{2}v''(0)x^2 + \cdots$ [4]. The first two terms are

$$\epsilon_n = -\lambda + (2n+1)\sqrt{\frac{\lambda v''(0)}{2}} + \cdots, \; n = 0, 1, \ldots \tag{10}$$

3. Examples

In this section we analyze the perturbation series outlined above by means of some exactly solvable examples. The first one is given by $v(x) = -1/\cosh^2 x$ that supports the bound-state energies [5]

$$\epsilon_n = -\left(\xi - n - 1\right)^2, \; \xi = \frac{1 + \sqrt{1 + 4\lambda}}{2}, \tag{11}$$

where the quantum number is restricted to $n = 0, 1, \ldots, \xi - 1$. The perturbation series for all the eigenvalues has the same radius of convergence $R = 1/4$ that is determined by the branch-point singularity at $\lambda_c = -1/4$. For example, for the ground state we have

$$\epsilon_0 = \frac{\sqrt{1+4\lambda} - 1 - 2\lambda}{2} = -\lambda^2 + 2\lambda^3 - 5\lambda^4 + 14\lambda^5 + \cdots. \tag{12}$$

Here we obviously have a perturbation series for the eigenvalues of the quantum-mechanical problem valid at least for $\lambda < 1/4$. For larger values of the strength parameter we can resort to any suitable summation method, for example, Padé approximants [6,7] and, even better, quadratic Padé approximants [7]. Note that in the present case the quadratic Padé approximant $w^2 + w(2\lambda + 1) + \lambda^2 = 0$ yields the exact result $w(\lambda) = \epsilon_0(\lambda)$ for all values of λ. We can also build two-point Padé approximants [7] that match the small-λ and large-λ series mentioned in section 2.

The next example is given by the square potential

$$v(x) = \begin{cases} -1 \text{ if } |x| \le 1 \\ 0 \text{ if } |x| > 1. \end{cases} \tag{13}$$

The eigenvalues with even-parity eigenfunctions are solutions to the implicit equation

$$k_1 \tan k_1 - k = 0, \; k = \sqrt{-\epsilon}, \; k_1 = \sqrt{\epsilon + \lambda}, \tag{14}$$

from which we derive the perturbation expansion

$$\epsilon = -\lambda^2 + \frac{4\lambda^3}{3} - \frac{92\lambda^4}{45} + \frac{1072\lambda^5}{315} - \frac{84\,752}{14\,175}\lambda^6 + \cdots, \tag{15}$$

for the ground state. It agrees with the general expression (5) through the fourth term.

In order to obtain the branch points in this case we take into account that if $(d\lambda/d\epsilon)(\epsilon = \epsilon_c) = 0$ and $\left(d^2\lambda/d^2\epsilon\right)(\epsilon = \epsilon_c) \neq 0$ then $\lambda \approx \lambda_c + A(\epsilon - \epsilon_c)^2$, where $\lambda_c = \lambda(\epsilon_c)$, and $\epsilon \approx \epsilon_c + A^{-1/2}\sqrt{\lambda - \lambda_c}$. If the eigenvalues are determined by an implicit equation of the form $F(\epsilon, \lambda) = 0$, then it follows from $dF/d\epsilon = (\partial F/\partial\lambda) d\lambda/d\epsilon + \partial F/\partial\epsilon = 0$ that λ_c and ϵ_c are determined by the pair of equations $F(\epsilon, \lambda) = 0$, $\partial F(\epsilon, \lambda)/\partial\epsilon = 0$. In this way we obtain $\lambda_c = -0.4392288398$ and $\epsilon_c = -1$. As in the preceding case Padé and quadratic Padé approximants yield accurate results for the ground-state eigenvalue in a wide range of values of the strength parameter. In particular two-point Padé approximants (even of low order) yield considerably accurate results for all values of λ. This potential cannot be expanded in a Taylor series about origin but the ground-state eigenvalue behaves asymptotically as $\epsilon = -\lambda + \mathcal{O}(1)$ for large λ.

This model is suitable for illustrating the application of the β-method of Gat and Rosenstein [3]. To this end we solve the Schrödinger equation with the potential $\lambda v(x) - \beta\delta(x)$ and obtain the following quantization condition for the eigenvalues with eigenfunctions of even parity:

$$k = \frac{k_1 \left[\beta \cos(k_1) + 2k_1 \sin(k_1)\right]}{2k_1 \cos(k_1) - \beta \sin(k_1)}. \tag{16}$$

This expression becomes equation (14) when $\beta = 0$ as expected. If we expand ϵ in a Taylor series about $\lambda = 0$ we obtain the first terms of the expansion (7):

$$\begin{aligned}
\hat{\epsilon}^{(0)}(\beta) &= -\frac{\beta^2}{4}, \\
\hat{\epsilon}^{(1)}(\beta) &= e^{-\beta} - 1, \\
\hat{\epsilon}^{(2)}(\beta) &= \frac{2e^{-2\beta}\left(1 + \beta - e^{\beta}\right)}{\beta^2}, \\
\hat{\epsilon}^{(3)}(\beta) &= \frac{e^{-3\beta}\left(5e^{2\beta} - 8e^{\beta}(\beta + 2) + 6\beta^2 + 14\beta + 11\right)}{\beta^4}.
\end{aligned} \tag{17}$$

What is important here is that these perturbation coefficients tend to those in the expansion (15) when $\beta \to 0$.

The next example is the Dirac-delta-potential $v(x) = -\delta(x)$ already studied by Lisowski et al. [1]. Upon choosing the exact boundary conditions $\lim_{|x|\to\infty} \psi(x) = 0$ we obtain the dimensionless energy $\epsilon = -\lambda^2/4$ for the only bound-state eigenvalue. Note that both the T-method and the β-method discussed in Section 2 yield the exact result. On the other hand, if we solve the Schrödinger equation with the periodic boundary conditions $\psi(-L/2) = \psi(L/2)$ and $\psi'(-L/2) = \psi'(L/2)$ the eigenvalue is a root of

$$e^{-kL}(2k+\lambda) - 2k + \lambda = 0,\; k = \sqrt{-\epsilon}. \tag{18}$$

From this expression we obtain

$$\epsilon = -\frac{\lambda^2}{4}\frac{\left(1+e^{-kL}\right)^2}{\left(1-e^{-kL}\right)^2} = -\frac{\lambda^2}{4}\left(1 + 4e^{-kL} + 8e^{-2kL} + 12e^{-3kL} + \cdots\right), \tag{19}$$

which clearly shows that the error with respect to the exact result is of the order of e^{-kL} and, since k decreases with λ, we appreciate the necessity of increasing L as λ decreases as the authors concluded from numerical analysis.

If we expand the solution to Eq. (18) in a Taylor series about $\lambda = 0$ we obtain

$$\epsilon = -\frac{\lambda}{L} - \frac{\lambda^2}{12} - \frac{L\lambda^3}{180} - \frac{L^2\lambda^4}{3780} - \frac{L^3\lambda^5}{226\,800} + \cdots \tag{20}$$

that depends on both λ and L. The coefficients of this expansion can also be obtained by means of the well known Rayleigh–Schrödinger perturbation theory; for example:

$$\begin{aligned}\tilde{\epsilon}^{(1)} &= \langle 0|\, v\, |0\rangle = -\frac{1}{L},\\ \tilde{\epsilon}^{(2)} &= \sum_{n\neq 0}\frac{|\langle n|\, v\, |0\rangle|^2}{e_0 - e_n} = -\frac{1}{2\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2} = -\frac{1}{12}.\end{aligned} \tag{21}$$

While the T-method and β-method yield the exact result, the L-method gives rise to an infinite series. Furthermore, although Eq. (18) yields the exact result when $L \to \infty$ for fixed λ, the coefficients of the series (20) blow up. We conclude that the L-method perturbation series is not asymptotic to the eigenvalue of the actual quantum-mechanical problem but to the eigenvalue of the secular equation $\mathbf{HC} = \epsilon\mathbf{C}$, where $\mathbf{H}$ is the matrix representation of the Hamiltonian operator in the basis set of periodic functions (8) and $\mathbf{C}$ is a column vector with the expansion coefficients for the wavefunction. The eigenvalue of this matrix equation may be reasonably accurate provided that L is suitably chosen and the number of basis functions is sufficiently large. Besides, the approximate L-method perturbation series (i.e. obtained with a finite basis set) should approach the exact one (20) as the number of basis functions increases. What is clear from the results above is that the L-method perturbation series may bear no resemblance with the actual λ-series expansion given by either the T-method or the β-method discussed in Section 2. Both the β-method and the L-method resort to auxiliary parameters (β and L, respectively). However, while $\lim_{\beta\to 0}\hat{\epsilon}^{(j)}(\beta) = \epsilon^{(j)}$, $\lim_{L\to\infty}\tilde{\epsilon}^{(j)}(L)$ blows up.

It is worth noting that if instead of periodic boundary conditions we impose Neumann ones $\psi'(\pm L/2) = 0$ then we obtain exactly the same quantization condition (18).

Finally we consider the exponential potential $V(x) = -V_0 e^{-b|x|}$ also discussed by Lisowski et al. [1]. Upon choosing the length $\gamma = 1/b$ we obtain $v(x) = -e^{|x|}$, $\lambda = 2mV_0/(\hbar^2 b^2)$ and $\epsilon = 2mE/(\hbar^2 b^2)$. The solution to the Schrödinger equation can be expressed in terms of the Bessel function of the first kind $\psi(x) = AJ_\nu(z)$, where A is a normalization constant, $\nu = 2\sqrt{-\epsilon}$ and $z = 2\sqrt{\lambda}e^{-x/2}$. The boundary condition for even states at origin $\psi'(0) = 0$ leads to

$$z_0 J_{\nu+1}(z_0) - \nu J_\nu(z_0) = 0,\; z_0 = 2\sqrt{\lambda}. \tag{22}$$

From this equation we obtain the following expansion for the dimensionless ground-state energy

$$\epsilon = -\lambda^2 + 3\lambda^3 - \frac{143\lambda^4}{12} + \frac{3887\lambda^5}{72} - \frac{71\,303\lambda^6}{270} + \cdots, \tag{23}$$

that agrees with the general expression (5) through the fourth term. If we only keep the first term in the right-hand side we obtain $E \approx -2mV_0^2/(\hbar^2 b^2)$ that agrees with the result of Lisowski et al. [1] when $\hbar = 1$.

In this case we can also obtain reasonable results from the perturbation series by means of Padé approximants and quadratic Padé approximants. For example, the Padé approximant $[3, 3](\lambda)$ constructed from the expansion (23) yields acceptable results for $0 \leq \lambda < 1$.

4. Conclusions

It is known since long ago that one can apply perturbation theory to the Schrödinger equation with a short-range potential $\lambda v(x)$ and obtain a suitable λ-power series asymptotic to the ground-state eigenvalue [2] (and references therein). In Section 2 we mentioned two approaches for that purpose. Lisowski et al. [1] proposed the L-method for the construction of a perturbation series starting from an unperturbed model with periodic boundary conditions. Although the exact eigenvalue of the Schrödinger equation with periodic boundary conditions tends to the eigenvalue of the Schrödinger equation with boundary conditions at infinity as $L \to \infty$ the same does not occur in the case of the L-method perturbation series because its coefficients blow up when $L \to \infty$. Therefore, the L-method power series is asymptotic to the eigenvalue of the problem with periodic boundary conditions for a given L and never to the actual physical eigenvalue. Since the authors resorted to a matrix representation of the Hamiltonian operator they did not even obtain the exact L-method perturbation series because of a necessary truncation of the basis set. Their perturbation series is asymptotic to the eigenvalue of the matrix representation of the Hamiltonian operator. If L is sufficiently small the series exhibits good convergence properties but the result is far from the eigenvalue of the problem with infinite boundary conditions. On the other hand, if L is sufficiently large the convergence properties are poor and one is forced to resort to an efficient summation method. If possible one may prefer the straightforward diagonalization of the matrix representation of the Hamiltonian for a sufficiently large value of the box length L and a sufficiently large number of basis functions.

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