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Rapid Communication

Iterative solutions for low lying excited states of a class of Schrödinger equation*

R. Friedberg[a], T. D. Lee(李政道)[a)b)], and Zhao Wei-Qin(赵维勤)[b)c)]

[a)] *Physics Department, Columbia University, New York, NY 10027, USA*
[b)] *China Center of Advanced Science and Technology (CCAST/World Laboratory), Beijing 100080, China*
[c)] *Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100039, China*

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The convergent iterative procedure for solving the groundstate Schrödinger equation is extended to derive the excitation energy and the wavefunction of the low-lying excited states. The method is applied to the one-dimensional quartic potential problem. The results show that the iterative solution converges rapidly when the coupling g is not too small.

Keywords: iterative solution, low-lying excited state, convergence
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1. Introduction

Consider the N-dimensional Schrödinger equation

$$\Big(-\frac{1}{2}\nabla^2 + V(q) - E\Big)\psi(q) = 0 \tag{1}$$

with

$$q = (q_1,\ q_2,\ \ldots,\ q_N),$$

and

$$\nabla^2 = \sum_{i=1}^{N} \frac{\partial^2}{\partial q_i^2}. \tag{2}$$

Through a linear transformation of the coordinates $q_1,\ q_2,\ \ldots,\ q_N$, Eq.(1) can be applied to most of the nonrelativistic many body problems. Similarly, in the limit $N \to \infty$, the same equation can also be extended to relativistic bosonic field theories. However, except in a few special cases, it is difficult to derive analytical solutions. Recently, for a class of Schrödinger equations we have succeeded in deriving a convergent iterative series solution for the groundstate.[1−4] These include the Sombrero shaped potential in any space dimension and arbitrary angular momentum.[5] In this paper, we discuss possible extension to low lying excited states.

Let

$$\psi_{\rm gd}(q) = {\rm e}^{-S(q)} \tag{3}$$

and $E_{\rm gd}$ be the ground state wavefunction and the ground state energy. Denote the corresponding ones for the first excited state as

$$\psi_{\rm ex} = {\rm e}^{-S}\chi \quad \text{and} \quad E = E_{\rm gd} + \epsilon. \tag{4}$$

We assume the potential $V(q)$ to have high barriers and low valleys, so that the excitation energy ϵ is very small. As an example, take q to be a one-dimensional space x and

$$V(x) = \frac{g^2}{2}(x^2-1)^2 \tag{5}$$

with g large. The first excited state would have an excitation energy

$$\epsilon \sim {\rm e}^{-\frac{4}{3}g} \ll 1. \tag{6}$$

For clarity, we shall also assume that, in the general case of $V(q)$, there is only one such low-lying state, as in the example of the one-dimensional quartic potential.

Let the Schrödinger equations for $\psi_{\rm gd} = {\rm e}^{-S}$ and $\psi_{\rm ex} = {\rm e}^{-S}\chi$ be

$$\Big(-\frac{1}{2}\nabla^2 + V - E_{\rm gd}\Big){\rm e}^{-S} = 0 \tag{7}$$

and

$$\Big(-\frac{1}{2}\nabla^2 + V - E_{\rm gd}\Big){\rm e}^{-S}\chi = \epsilon{\rm e}^{-S}\chi. \tag{8}$$

Multiplying Eq.(7) by ${\rm e}^{-S}\chi$ and Eq.(8) by ${\rm e}^{-S}$, we obtain from their difference,

$$-\frac{1}{2}\nabla\cdot({\rm e}^{-2S}\nabla\chi) = \epsilon{\rm e}^{-2S}\chi. \tag{9}$$

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Replace Eq.(9) by a series of iterative equations: for $n \geq 1$

$$-\frac{1}{2}\nabla \cdot (\mathrm{e}^{-2S}\nabla\chi_n) = \epsilon_n \mathrm{e}^{-2S}\chi_{n-1} \tag{10}$$

and when $n = 0$,

$$\mathrm{e}^{-S}\chi_0 = \psi_{\mathrm{trial}} \quad \text{(a trial function)}, \tag{11}$$

which satisfies the orthogonality condition between ψ_{gd} and ψ_{trial}; i.e.

$$\int \mathrm{e}^{-2S}\chi_0 \mathrm{d}^N q = 0. \tag{12}$$

When χ_{n-1} is known, the iteration of Eq.(10) gives only the ratio χ_n/ϵ_n. To perform the next order iteration it is necessary to separate ϵ_n and χ_n. For this purpose, we may choose a fixed point q^0 and set

$$\chi_n(q^0) = \chi_0(q^0). \tag{13}$$

Clearly, different choices of q^0 will yield different sequences of $\chi_n(q)$ and ϵ_n, as we shall discuss.

For given e^{-S} and χ_{n-1}, Eq.(10) can be viewed as an analogous problem in electrostatics with a dielectric constant κ and an external electric charge σ_n given by

$$\kappa = \mathrm{e}^{-2S} \quad \text{and} \quad \sigma_n = \epsilon_n \mathrm{e}^{-2S}\chi_{n-1}. \tag{14}$$

Let $\boldsymbol{E}_n$ be the corresponding electrostatic field and $\boldsymbol{D}_n$ the displacement field. We write

$$\boldsymbol{E}_n = -\frac{1}{2}\nabla\chi_n \tag{15}$$

and

$$\boldsymbol{D}_n = \kappa \boldsymbol{E}_n. \tag{16}$$

Thus, Eq.(10) becomes

$$\nabla \cdot \boldsymbol{D}_n = \sigma_n. \tag{17}$$

At ∞, $\psi_{\mathrm{gd}} = \mathrm{e}^{-S} = 0$. Therefore $\kappa(\infty) = 0$, $\sigma_n(\infty) = 0$ and

$$\boldsymbol{D}_n(\infty) = 0. \tag{18}$$

Integrating Eq.(17) over all space we find, on account of Eq.(18),

$$\int \sigma_n \mathrm{d}^N q = \int \mathrm{e}^{-2S}\chi_n \mathrm{d}^N q = 0. \tag{19}$$

Hence, the orthogonality condition (12) is now carried over to all $n \geq 1$.

Expand $\mathrm{e}^{-S}\chi_n$ in terms of the set of all eigenstates $\{\psi_a\}$ of Eq.(1). We have, because of Eq.(19),

$$\mathrm{e}^{-S}\chi_n = \sum_{a \neq \mathrm{gd}} c_a(n)\psi_a \tag{20}$$

with

$$c_a(n) = \frac{1}{E_a - E_{\mathrm{gd}}}\epsilon_n \cdot c_a(n-1). \tag{21}$$

For problems like the one-dimensional quartic potential (5), when the coupling g^2 is large, only the first excited state $a = 1$ has an excitation energy $\epsilon = E_1 - E_{\mathrm{gd}}$ that is exponentially smaller than all other $E_a - E_{\mathrm{gd}}$. Thus, the corresponding $c_1(n)$ becomes exponentially large compared with all other $c_{a\neq 1}(n)$, in accordance with Eq.(21). Hence the iteration process (10) becomes rapidly convergent.

For a large class of problems in which $V(q)$ has high barriers and low valleys, there are often only a finite number of low-lying excited states:

$$a = 1,\ 2,\ \ldots,\ m \tag{22}$$

with excitation energies $\epsilon_a = E_a - E_{\mathrm{gd}}$ comparable to each other, but exponentially smaller than those of $a > m$ states. By maintaining the orthogonality relations between these m low-lying excited states, the iteration process (10) can be readily generalized to such problems.

2. One dimensional problem

In one dimension, we replace $\{q_i\}$ by a single x. For simplicity, consider the special case

$$V(x) = V(-x). \tag{23}$$

Thus, the groundstate wavefunction $\mathrm{e}^{-S(x)}$ is an even function of x and the first excited state $\mathrm{e}^{-S(x)}\chi(x)$ an odd function. We assume that $\mathrm{e}^{-S(x)}$ is already known, e.g. by following the method discussed in Refs.[1–4]. We further assume that the first excited state has an excitation energy

$$\epsilon \ll 1, \tag{24}$$

as would be the case if $V(x)$ is like the quartic potential (5) with large g. In one-dimension, Eq.(9) becomes

$$-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}(\mathrm{e}^{-2S}\frac{\mathrm{d}\chi}{\mathrm{d}x}) = \epsilon \mathrm{e}^{-2S}\chi. \tag{25}$$

The corresponding series of iterative equations (10) for $n \geq 1$ is

$$-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{e}^{-2S}\frac{\mathrm{d}\chi_n}{\mathrm{d}x}\right) = \epsilon_n \mathrm{e}^{-2S}\chi_{n-1} \tag{26}$$

with χ_0 a properly chosen trial function. As in Eq.(13), in order to separate χ_n and ϵ_n from the ratio χ_n/ϵ_n we choose a fixed point x^0 and set

$$\chi_n(x^0) = \chi_0(x^0) \tag{27}$$

for all n.

In terms of the electrostatic analogue (14)–(16), write

$$\kappa = \mathrm{e}^{-2S}, \qquad \sigma_n = \epsilon_n \mathrm{e}^{-2S}\chi_{n-1},$$
$$E_n = -\frac{1}{2}\chi_n' \quad \text{and} \quad D_n = \kappa E_n \tag{28}$$

with $'$ denoting $\mathrm{d}/\mathrm{d}x$. Thus, Eqs.(17) and (18) become

$$D_n'(x) = \sigma_n(x), \tag{29}$$

$$D_n(\pm\infty) = 0 \ \text{ and } \ \sigma_n(\pm\infty) = 0. \tag{30}$$

From Eqs.(29) and (30), we have

$$D_n(x) = -\epsilon_n \int_x^\infty \mathrm{e}^{-2S(z)}\chi_{n-1}(z)\mathrm{d}z, \tag{31}$$

and therefore

$$E_n(x) = \mathrm{e}^{2S(x)} D_n(x) \tag{32}$$

can also be readily expressed in terms of χ_{n-1}. Since $\chi_n(x)$ is odd in x, we need only to consider $x \geq 0$. From Eqs.(28) and (32), we find

$$\chi_n(x) = 2\epsilon_n \int_0^x \mathrm{e}^{2S(y)}\mathrm{d}y \int_y^\infty \mathrm{e}^{-2S(z)}\chi_{n-1}(z)\mathrm{d}z. \tag{33}$$

Since $\mathrm{e}^{-S(x)}$ is the groundstate, it has no zero at finite x. Thus, the factor $\mathrm{e}^{2S(y)}$ in the y-integration of Eq.(33) is always finite. This is an important fact that enables us to extend the effectiveness of the iterative procedures of Refs.[1–5] for the groundstate to the low-lying excited state.

3. An analytically soluble example

As an analytically soluble example, we consider the following simple one-dimensional example:

$$V(x) = \lambda\delta(x) + \begin{cases} 0, & |x| < 1, \\ \infty, & |x| > 1. \end{cases} \tag{34}$$

The unnormalized groundstate solution is

$$\mathrm{e}^{-S(x)} = \begin{cases} \sin p(1-x), & \text{for} \quad 0 < x < 1, \\ 0, & \text{for} \quad |x| > 1, \\ \sin p(1+x), & \text{for} \quad -1 < x < 0 \end{cases} \tag{35}$$

with

$$p \equiv \pi - \delta,$$
$$\lambda = -p\cot p = (\pi - \delta)\cot\delta. \tag{36}$$

For very large λ, p is very close to π, so

$$\delta \ll 1. \tag{37}$$

The exact lowest excited state is, for $|x| < 1$,

$$\mathrm{e}^{-S}\chi = \sin\pi x \tag{38}$$

with the excitation energy

$$\epsilon = \frac{1}{2}(\pi^2 - p^2) = \pi\delta - \frac{1}{2}\delta^2 \ll 1, \tag{39}$$

and for $x \geq 0$, χ is given by

$$\chi(x) = \frac{\sin\pi x}{\sin p(1-x)}. \tag{40}$$

In order to test the effectiveness of the iterative solution (33) and the supplementary condition (27), we shall start from the groundstate solution (35) and a trial function

$$\chi_0 = x. \tag{41}$$

Since Eq.(33) yields only the ratio $\chi_n(x)/\epsilon_n$, we follow Eq.(27) by choosing

$$x^0 = 1 \tag{42}$$

and therefore

$$\chi_n(1) = \chi_0(1) = 1. \tag{43}$$

It is clear that the trial function

$$\mathrm{e}^{-S}\chi_0 = x\sin p(1-x) \tag{44}$$

is *not* a very good guess of the first excited state (38), nor does (41) resembles (40), except that at $x = 0$, $\chi_0(0) = \chi(0) = 0$. Nevertheless, we shall show that the iterative solution (33) with the supplementary condition (43) does lead to a rapidly convergent sequence.

Substituting Eqs.(35) and (41) into Eq.(33), we find, for $x \geq 0$,

$$\left[\frac{4p}{2\epsilon_1}\sin p\right]\chi_1\mathrm{e}^{-S}$$
$$= \sin px - (\sin p)\left[\frac{x}{p}\sin p(1-x) + x^2\cos p(1-x)\right]. \tag{45}$$

The supplementary condition (43) leads to

$$\epsilon_1 = \frac{2p^2}{1 - p\cot p}. \tag{46}$$

For $\delta = \pi - p$ small, Eq.(46) gives

$$\epsilon_1 = 2\pi\delta - 4\delta^2 + 2\left(\frac{1}{\pi} + \frac{\pi}{3}\right)\delta^3 - 2\delta^4 + O(\delta^5), \tag{47}$$

whereas the exact ϵ is given by Eq.(39) with $\epsilon_1 \cong 2\epsilon$. However, on second and third iterations, we find

$$\epsilon_2 = \pi\delta + \left(\frac{1}{\pi} - \frac{\pi}{3}\right)\delta^3 + \left(\frac{1}{3} - \frac{2}{\pi^2}\right)\delta^4 + O(\delta^5), \quad (48)$$

$$\epsilon_3 = \pi\delta - \frac{1}{2}\,\delta^2 + \frac{-6+\pi^2}{12\pi}\,\delta^3 - \frac{15}{8\pi^2}\,\delta^4 + O(\delta^5). \quad (49)$$

Comparing to the exact value, the second order solution ϵ_2 gives the correct $\pi\delta$ and the third order ϵ_3 gives the correct first two terms: $\pi\delta - \frac{1}{2}\,\delta^2$.

For $\delta = 0.1$, Eqs.(47)–(49) yield

$$\epsilon_1 = 0.59086, \quad \epsilon_2 = 0.31348, \quad \epsilon_3 = 0.30924, \quad (50)$$

which can be compared with the exact solution

$$\epsilon = 0.30916.$$

The $\chi_n(x)$ for $n = 0,\ 1,\ 2,\ 3$ are plotted in Fig.1, together with the exact solution $\chi(x)$. In fact, χ_2, χ_3 and χ are on the same curve. This shows the rapid convergence of the iterative process.

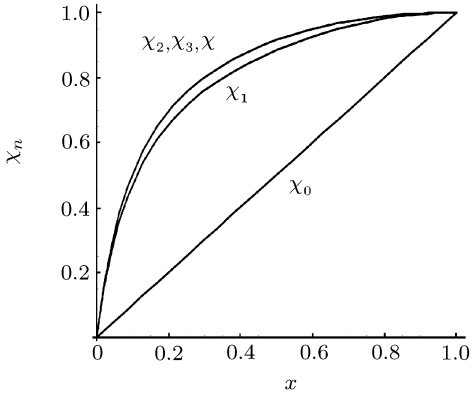


Fig.1. χ and χ_n for $n = 0,\ 1,\ 2,\ 3$ for the soluble problem (Section 3).

4. One-dimensional quartic potential

Consider the one-dimensional quartic potential

$$V = \frac{g^2}{2}(x^2 - 1)^2. \quad (51)$$

Assume that the groundstate wavefunction e^{-S} has been obtained by using the method described in our recent paper.[5] The first excited state $e^{-S}\chi$ satisfies Eq.(25) and the corresponding nth order iterative solution is $e^{-S}\chi_n$, with χ_n given by Eq.(33). When $n = 0$, we choose the trial function χ_0 to be an odd function, with

$$\chi_0(-x) = -\chi_0(x)$$

and for x positive

$$\chi_0(x) = \begin{cases} x(2-x), & \text{for} \quad 0 < x < 1, \\ 1, & \text{for} \quad x > 1. \end{cases} \quad (52)$$

As in Eqs.(27) and (42)–(43), we choose $x^0 = 1$ and set

$$\chi_n(1) = \chi_0(1) = 1. \quad (53)$$

In the following, we also set

$$g = 3. \quad (54)$$

Using the iteration method of Refs.[1, 5], we find the groundstate energy to be

$$E_{\rm gd} = 2.48291. \quad (55)$$

The lowest excitation energy ϵ_n for the first four iterations ($n = 1,\ 2,\ 3,\ 4$) based on Eqs.(33) and (53) are

$$\epsilon_1 = 0.41776, \ \epsilon_2 = 0.41367,$$

$$\epsilon_3 = 0.413568, \ \epsilon_4 = 0.413568. \quad (56)$$

Thus, with three iterations, ϵ_3 is already accurate to seven significant figures. The corresponding wavefunctions χ_n are plotted in Fig.2. The groundstate e^{-S} and the first excited state $e^{-S}\chi$ are given in Fig.3. To the same seven significant figures the eigenvalue for the first excited state can be expressed as $E_{\rm odd} = E_{\rm gd} + \epsilon_4$.

To test the sensitivity to the choice x^0 we set, instead of Eq.(53), $x^0 = 1/2$ and require

$$\chi_n\left(\frac{1}{2}\right) = \chi_0\left(\frac{1}{2}\right). \quad (57)$$

The corresponding excitation energies ϵ_n of the lowest excited state for the first 4 iterations are, in place of Eq.(56),

$$\epsilon_1 = 0.41363, \ \epsilon_2 = 0.41358,$$

$$\epsilon_3 = 0.413569, \ \epsilon_4 = 0.413568. \quad (58)$$

Although the value of ϵ_1 in Eq.(58) differs from the corresponding one in Eq.(56), after the fourth iteration ϵ_4 becomes essentially the same for both cases. This means that the iteration result is not too sensitive to the choice of x^0.

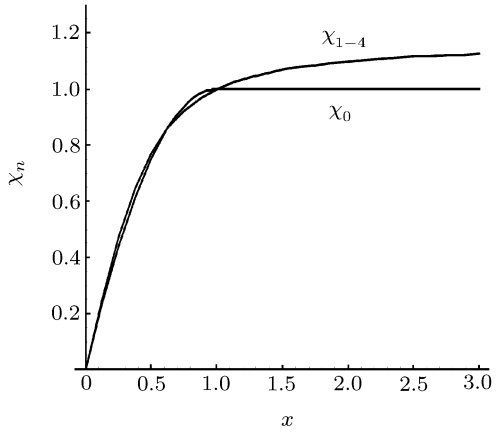


Fig.2. χ_n for $n = 0,\ 1,\ 2,\ 3,\ 4$ for the quartic potential (51) with $g = 3$.

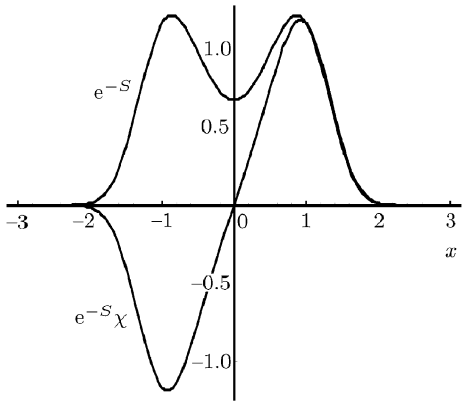


Fig.3. The groundstate wavefunction e^{-S} and the first excited state wavefunction $e^{-S}\chi$ for the quartic potential (51) with $g = 3$.

Appendix A

In our earlier work[6] an asymptotic expansion of the average $E = \frac{1}{2}(E_{\rm gd} + E_{\rm odd})$ and that of the difference $\Delta = 1/2\ \epsilon$ were obtained. To compare our present results with these asymptotic expansions, we take a larger coupling $g = 8$. This enables us to use the asymptotic expansion up to order $1/g^3$ for the wavefunction $\phi_\pm$ of Ref.[6]. We find

$$E_{\rm asymp} = 7.728854\ . \tag{A1}$$

Using the expressions

$$\Delta = \frac{\lambda}{2}\ \frac{1}{\int\limits_0^\infty \phi_+^2(x){\rm d}x} \tag{A2}$$

and

$$\lambda = \phi'_+\phi_- - \phi_+\phi'_- \tag{A3}$$

of Ref.[6], we obtain

$$\epsilon_{\rm asymp} = 2\Delta_{\rm asymp} = 0.003027. \tag{A4}$$

For $g = 8$, the iterative method of Ref.[5] gives

$$E_{\rm gd} = 7.727340. \tag{A5}$$

The corresponding nth order iterative excitation energy ϵ_n of Section 4 for $n = 1 - 4$ are

$$\epsilon_1 = 0.00310125,\ \epsilon_2 = 0.00301796,$$
$$\epsilon_3 = 0.003017947,\ \epsilon_4 = 0.003017947. \tag{A6}$$

Keeping the accuracy to seven significant figures, we find

$$E = E_{\rm gd} + \frac{1}{2}\ \epsilon = 7.728849 \tag{A7}$$

and

$$\epsilon = 0.003018. \tag{A8}$$

Thus, the asymptotic values $E_{\rm asymp}$ and $\epsilon_{\rm asymp}$ of Eqs.(A1) and (A4) compare well with E and ϵ of Eqs.(A7) and (A8). However, inclusions of still higher and higher order terms in the asymptotic expansion would lead to divergent results for $E_{\rm asymp}$ and $\epsilon_{\rm asymp}$.

The wavefunctions $\chi_n(x)$ for $g = 8$ are plotted in Fig.4. As we can see, the deviation of the $\chi_n(x)$ from 1 happens only at small x.

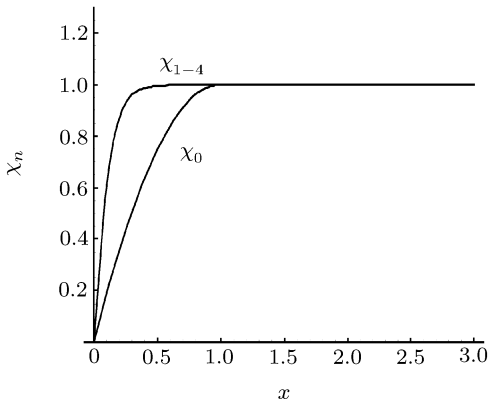


Fig.4. χ_n for $n = 0,\ 1,\ 2,\ 3,\ 4$ for the quartic potential (51) with $g = 8$.

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