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Higher-order corrections to the excited states using the logarithmic perturbation method

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Based on the logarithmic perturbation method proposed by Aharonov and Au [Phys. Rev. Lett. **42**, 1582 (1979)], we calculate explicitly up to fourth order and arrive at different results for the energy corrections and nodal point shifts of the first excited state. [S1050-2947(98)04707-6]

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I. INTRODUCTION

Aharonov and Au proposed an approach to the nonrelativistic stationary-state perturbation theory [1]. In the commonly known logarithmic perturbation method (LPM), they show that in problems reducible to one dimension, the corrections of eigenenergies, wave functions, as well as the positions of the nodes, to any order, can be expressed in quadrature in a hierarchy scheme. This method was later extended to three-dimensional problems [2] and applied to different cases [3,4]. All these studies [2–4] primarily concentrated on calculating the energy corrections of the ground state in which the wave function is nodeless. In order to avoid cumbersome sums over intermediate states, alternative approaches [5,6] with a similar spirit were developed to treat the excited states.

In this work we would like to point out that the formulas we derived are different from those in Ref. [1] regarding the energy corrections and nodal shifts of the higher excited states. Thus our purposes of presenting this work are first to investigate the perturbative approach of nodal point shifts, which is, after all, the LPM is designed to undertake, and second for practical reasons, since this method is widely applied in atomic, molecular, and condensed-matter physics [2–4]. Recently, it has been extended further to calculate the quasinormal mode frequencies [7] of black holes and the Dirac equation in one dimension [8]. Hence it is our belief that the present results will be helpful to researchers in many areas.

II. DERIVATIONS

We use the same notation as in Ref. [1], but we set $2\mu=1$ and $\hbar=1$. (In Ref. [1], $\mu=1$.) Nevertheless, this will change the results only slightly. For definiteness, we consider the first excited state, which can be expressed as

$$\psi(x)=(x-\alpha)\exp[-G(x)], \tag{1}$$

where α is the nodal position and $G(x)$ is regular and expandable in powers of the coupling constant λ and so is its derivative $g(x)$, i.e., $g(x)=dG(x)/dx$. Thus we write

$$\begin{aligned}\alpha&=\alpha_0+\lambda\alpha_1+\lambda^2\alpha_2+\lambda^2\alpha_3+\cdots,\\ g&=g_0+\lambda g_1+\lambda^2 g_2+\lambda^3 g_3+\cdots,\\ E&=E_0+\lambda E_1+\lambda^2 E_2+\lambda^3 E_3+\cdots.\end{aligned} \tag{2}$$

After substituting the wave function (1), the Schrödinger equation becomes

$$(g^2-g')(x-\alpha)-2g=-(E-V_0-\lambda V_1)(x-\alpha), \tag{3}$$

where $g'=dg/dx$. Gathering all the terms zeroth order in λ after substituting Eq. (2) into Eq. (3), we get the unperturbed Schrödinger equation

$$(g_0^2-g_0')(x-\alpha_0)-2g_0=-(E_0-V_0)(x-\alpha_0), \tag{4}$$

where α_0 is the node of the unperturbed wave function. Then we collect terms first order in λ,

$$\begin{aligned}&(2g_0g_1-g_1')(x-\alpha_0)-2g_1-\alpha_1(g_0^2-g_0')\\ &\quad=-(E_1-V_1)(x-\alpha_0)+\alpha_1(E_0-V_0).\end{aligned} \tag{5}$$

Multiplying both sides of Eq. (5) by $(x-\alpha_0)\exp(-2G_0)$ and using Eq. (4), we have

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$$-[g_1(x-\alpha_0)^2\exp(-2G_0)]' = -(E_1-V_1)(x-\alpha_0)^2\exp(-2G_0)-\alpha_1[\exp(-2G_0)]. \tag{6}$$

Notice that the negative sign in front of the last term on the right-hand side is different from that in Eq. (34) of Ref. [1]. This will not change the first-order correction energy connection but the sign of the first-order correction to the nodal position of the wave function. As we integrate from $-\infty$ to ∞, we get the first-order energy correction E_1,

$$E_1=\int_{-\infty}^{\infty}V_1(x-\alpha_0)^2\exp(-2G_0)dx=\int_{-\infty}^{\infty}V_1\Psi_0^2(x)dx \tag{7}$$

and from $-\infty$ to α_0 we get the first-order correction of the nodal point shift

$$\alpha_1=-\exp[2G_0(\alpha_0)]\int_{-\infty}^{\alpha_0}(E_1-V_1)\rho_0(x)dx,$$

where

$$\rho_0(x)=(x-\alpha_0)^2\exp[-2G_0(x)]. \tag{8}$$

We notice that the sign of α_1 is different from Eq. (37) of Ref. [1]. Accordingly, $g_1(x)$ is also different,

$$g_1(x)=\frac{1}{\rho_0(x)}\int_{-\infty}^{x}(E_1-V_1)\rho_0(x')dx'+\frac{\alpha_1}{(x-\alpha_0)^2}. \tag{9}$$

As x approaches α_0, the limit of g_1 can be obtained by using Eq. (7),

$$g_1(\alpha_0)=\alpha_1 g_0(\alpha_0)-\alpha_1 g_0'(\alpha_0). \tag{10}$$

Thus g_1 is proved to be singularity free.

In the second-order calculation, we accumulate all the terms proportional to λ^2. Then

$$(x-\alpha_0)(g_1^2+2g_0g_2-g_2') -\alpha_1(2g_0g_1-g_1')-\alpha_2(g_0^2-g_0')-2g_2 = -E_2(x-\alpha_0)+\alpha_1(E_1-V_1)+\alpha_2(E_0-V_0). \tag{11}$$

We multiply both sides of Eq. (11) by $\exp(-2G_0)$ and making use of the zeroth- and first-order corrections we get

$$-[g_2(x-\alpha_0)^2\exp(-2G_0)]' = -\alpha_2[\exp(-2G_0)]'-E_2\rho_0+F_2,$$

where

$$F_2(x)=\left\{2\alpha_1\left[g_1+\frac{\alpha_1 g_0}{x-\alpha_0}\right]-g_1^2(x-\alpha_0)^2\right\}\exp(-2G_0). \tag{12}$$

We can easily show that $F_2(x)$ is the same as Eq. (40) of Ref. [1]; however, α_1 has to be the one described in Eq. (8). Based on the fact that g_1 and $g_0/(x-\alpha_0)$ are singularity free, it is not difficult to show that F_2 is a well-behaved function. Using the same procedures, that is, integrating from $-\infty$ to ∞, we have the second-order correction to the energy

$$E_2=\int_{-\infty}^{\infty}F_2(x)dx'. \tag{13}$$

Integrating from $-\infty$ to α_0, we get the correction to the nodal point shift

$$\alpha_2=\exp[2G_0(\alpha_0)]\int_{-\infty}^{\alpha_0}[F_2(x')-E_2\rho_0(x')]dx'. \tag{14}$$

Thus $g_2(x)$ can be obtained by integrating from $-\infty$ to x,

$$g_2(x)=-\frac{1}{\rho_0(x)}\int_{-\infty}^{x}[F_2(x')-E_2\rho_0(x')]dx'+\frac{\alpha_2}{(x-\alpha_0)^2}. \tag{15}$$

We collect the terms proportional to λ^3 and proceed to calculate the third-order correction

$$(2g_0g_3+2g_1g_2-g_3')(x-\alpha_0)-(g_1^2+2g_0g_2-g_2')\alpha_1 -(2g_0g_1-g_1')\alpha_2-(g_0^2-g_0')\alpha_3-2g_3 = -E_3(x-\alpha_0)+\alpha_1E_2+\alpha_2(E_1-V_1)+\alpha_3(E_0-V_0). \tag{16}$$

Repeating the previous procedures, we substitute all the lower corrections into Eq. (16) and multiply both sides of it by $(x-\alpha_0)\exp(-2G_0)$,

$$-[g_3(x-\alpha_0)^2\exp(-2G_0)]' = -\alpha_3[\exp(-2G_0)]'-E_3\rho_0+F_3, \tag{17}$$

where

$$F_3(x)=((x-\alpha_0)\{\alpha_1[(g_1^2+2g_0g_2-g_2')+E_2] +\alpha_2[(2g_0g_1-g_1')+(E_1-V_1)]\} -2g_1g_2(x-\alpha_0)^2)\exp(-2G_0). \tag{18}$$

Together with

$$(g_0^2-g_0')+(E_0-V_0)=\frac{2g_0}{(x-\alpha_0)}, \tag{19}$$

we can see that the above expression (18) is quite different from Eq. (40) of Ref. [1]. Again, we carry out the previous procedures, i.e., when we integrate from $-\infty$ to ∞, we obtain the third-order energy correction

$$E_3=\int_{-\infty}^{\infty}F_3(x)dx. \tag{20}$$

After that, integrating from $-\infty$ to α_0, we have the third-order nodal point shift

$$\alpha_3=\exp[2G_0(\alpha_0)]\int_{-\infty}^{\alpha_0}[F_3(x')-E_3\rho_0(x')]dx'. \tag{21}$$

Finally, we integrate from $-\infty$ to x and obtain

$$g_3(x)=\frac{1}{\rho_0(x)}\int_{-\infty}^{x}[E_3\rho_0(x')-F_3(x')]dx'+\frac{\alpha_3}{(x-\alpha_0)^2}. \tag{22}$$

Based on the behaviors of the $g_i(x)$'s $(i=1,2)$, it is not difficult to deduce that $g_3(x)$ is also singularity free, except it does not agree with the one derived from Ref. [1].

Before reaching the general formula, we work out the fourth-order correction, which is calculated by collecting all the terms proportional to λ^4,

$$\begin{aligned}&[(x-\alpha_0)^2(2g_0g_4-g_4')-2g_4(x-\alpha_0)]\\&\quad-\alpha_1(x-\alpha_0)[(2g_0g_3+2g_1g_2-g_3')+E_3]\\&\quad-\alpha_2(x-\alpha_0)[(2g_0g_2+g_1^2-g_2')+E_2]\\&\quad-\alpha_3(x-\alpha_0)[(2g_0g_1-g_1')+(E_1+V_1)]\\&\quad-\alpha_4(x-\alpha_0)[(g_0^2-g_0')+(E_0-V_0)]\\&=-E_4(x-\alpha_0)^2-(2g_1g_3+g_2^2)(x-\alpha_0)^2.\end{aligned} \tag{23}$$

Multiplying both sides by $\exp(-2G_0)$, we get

$$\begin{aligned}&-[g_4(x-\alpha_0)^2\exp(-2G_0)]'\\&\quad=-\alpha_4[\exp(-2G_0)]'-E_4\rho_0+F_4,\end{aligned} \tag{24}$$

where

$$\begin{aligned}F_4(x)=&((x-\alpha_0)\{\alpha_1[(2g_0g_3+2g_1g_2-g_3')+E_3]\\&+\alpha_2[(2g_0g_2+g_1^2-g_2')+E_2]\\&+\alpha_3[(2g_0g_1-g_1')+(E_1-V_1)]\}\\&-(2g_1g_3+g_2^2)(x-\alpha_0)^2)\exp(-2G_0).\end{aligned} \tag{25}$$

We obtain the fourth-order correction in energy E_4, nodal point shift α_4, and $g_4(x)$ by repeating the previous procedures. We also show that $F_4(x)$ is singularity free by making use of the $g_i(x)$'s $(i=1,$ 2, and 3). Nevertheless, $F_4(x)$ is different from that shown in Ref. [1].

Now we deduce the hierarchy equation that is of the same form as Eq. (39) of Ref. [1] [the expression for $F_i(x)$ appears to be different from Eq. (40) of Ref. [1]]

$$\begin{aligned}&-[g_i(x-\alpha_0)^2\exp(-2G_0)]'\\&\quad=-\alpha_i[\exp(-2G_0)]'-2E_i\rho_0+F_i,\end{aligned} \tag{26}$$

where

$$\begin{aligned}F_i(x)=&\left\{2\alpha_{i-1}\left[g_1+\frac{g_0\alpha_1}{x-\alpha_0}\right]\right.\\&+\sum_{m=2}^{i-1}\alpha_{i-m}\left[\sum_{j=0}^{m}g_jg_{m-j}-g_m'+E_m\right](x-\alpha_0)\\&\left.-\sum_{j=1}^{i-1}g_jg_{i-j}(x-\alpha_0)^2\right\}\exp(-2G_0).\end{aligned} \tag{27}$$

The second term in $F_i(x)$ contributes when $i\geqslant 3$. After careful examination, it is not difficult to notice that our Eq. (27) is different from Eqs. (37), (38), and (40) in Ref. [1]. The disagreements occur not only at the negative sign in front of α_i, but also in the expression of $F_i(x)$, we notice that in the second term there is an additional term E_m in the second set of large square brackets and an extra prefactor α_{i-m} in front of it. Equation (27) can be integrated to yield the corrections of the eigenenergies, the wave functions, and the positions of the nodal points.

We now illustrate the corrected formulas by calculating explicitly the energy corrections and nodal point shifts caused by cubic and quartic perturbations to the simple harmonic oscillator up to fourth order.

Case I. The cubic perturbation potential

$$V'(x)=\beta x^3. \tag{28}$$

Using the above-derived formulas, we calculate the three lowest-order corrections in energy and nodal point position. Here the zeroth-order first excited state of the harmonic-oscillator wave function is

$$\Psi_1(x)=\sqrt{(2\alpha/\sqrt{\pi})}\;\alpha x\;\exp\left(-\frac{\alpha^2x^2}{2}\right), \tag{29}$$

where $\alpha=\sqrt{\omega/2}$ and ω is the frequency (recall that $2\mu=1$ and $\hbar=1$). It is very easy to see that the zeroth nodal point α_0 for $\Psi_1(x)$ [Eq. (29)] is at the origin and $g_0(x)=\alpha^2x$.

In first order, we have

$$E_1=0,\quad \alpha_1=-\frac{\beta}{\alpha^6},\quad g_1(x)=\frac{\beta}{\alpha^4}\left(\frac{1}{2}\alpha^2x^2+1\right). \tag{30}$$

The vanishing first-order correction in energy is expected because of the asymmetry of $V'(x)$ and the same reason explains why the wave function is shifted to the left.

Now in second order we have

$$\begin{aligned}&E_2=-\frac{71}{16}\frac{\beta^2}{\alpha^8},\quad \alpha_2=0,\\&g_2(x)=-\frac{\beta^2}{\alpha^9}\left(\frac{1}{8}\alpha^3x^3+\frac{13}{16}\alpha x\right).\end{aligned} \tag{31}$$

The correction in energy agrees with that of the conventional method, but the nodal point is not shifted in this order.

Then the third-order corrections are

$$\begin{aligned}&E_3=0,\\&\alpha_3=-\frac{59}{16}\frac{\beta^3}{\alpha^{16}},\\&g_3(x)=\frac{\beta^3}{\alpha^{14}}\left(\frac{1}{32}\alpha^4x^4+\frac{23}{64}\alpha^2x^2+\frac{11}{16}\right).\end{aligned} \tag{32}$$

Again, we see similar behavior to that of first order. The energy correction vanishes and the wave function shifts to the left.

Finally, in fourth order we have

$$E_4=-\frac{13\,905}{512}\frac{\beta^4}{\alpha^{18}},\quad \alpha_4=0. \tag{33}$$

This result is the same as the second-order results. We attribute all these to the odd parity of $V'(x)$. Thus, in the next example, we adopt a perturbation potential of even parity.

Case II. The quartic oscillator

$$V'(x)=\gamma x^4. \tag{34}$$

Similarly, we carry out the same procedures. The results of the perturbation calculation are, in first order,

$$E_1=\frac{15}{4}\frac{\gamma}{\alpha^4},\quad \alpha_1=0,\quad g_1(x)=\frac{\gamma}{\alpha^5}\left(\frac{1}{2}\alpha^3x^3+\frac{5}{4}\alpha x\right) \tag{35}$$

and, in second order,

$$E_2=-\frac{165}{16}\frac{\gamma^2}{\alpha^{10}},$$

$$\alpha_2=0, \tag{36}$$

$$g_2(x)=\frac{\gamma}{\alpha^{11}}\left(\frac{1}{8}\alpha^5x^5+\frac{17}{16}\alpha^3x^3+\frac{55}{16}\alpha x\right).$$

In third order we have $E_3=\frac{3915}{64}(\gamma^3/\alpha^{16})$, $\alpha_3=0$, and

$$g_3(x)=\frac{\gamma^3}{\alpha^{17}}\left(\frac{1}{16}\alpha^7x^7+\frac{31}{32}\alpha^5x^5+\frac{103}{16}\alpha^3x^3+\frac{1305}{64}\alpha x\right). \tag{37}$$

Finally, the fourth-order corrections are

$$E_4=-\frac{520\,485}{1024}\frac{\gamma^4}{\alpha^{22}},\quad \alpha_4=0. \tag{38}$$

All the above energy corrections are checked with the conventional method and clearly all the $g_i(x)$'s ($i=1,2,3$) are singularity free. Even though the examples we showed are very standard, there is one interesting phenomenon that is not revealed by other methods, that is, the first excited-state wave function is either, up to the four lower orders, only pushed to the left (case I) or not shifted at all (case II). We attribute these behaviors to the odd or even parity of the perturbation potentials.

III. CONCLUSION

In this work, after rederiving the hierarchy equations, we presented general formulas for the energy corrections and nodal point shifts of the first excited state based on the logarithmic perturbation expansion proposed by Aharonov and Au [1]. In order to demonstrate them explicitly, we calculated the energy corrections and nodal shifts of the first excited-state wave function up to fourth order and applied them to two specific examples.

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