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Zel'dovich's method of perturbation theory in quantum mechanics

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Abstract. Many years ago Zel'dovich showed how the Lagrange condition in the theory of differential equations can be utilized in the perturbation theory of quantum mechanics. Zel'dovich's method enables us to circumvent the summation over intermediate states. As compared with other similar methods, in particular the logarithmic perturbation expansion method, we emphasize that this relatively unknown method of Zel'dovich has a remarkable advantage in dealing with excited states. That is, the ground and excited states can all be treated in the same way. The nodes of the unperturbed wavefunction do not give rise to any complication.

1. Introduction

The Rayleigh–Schrödinger perturbation theory in quantum mechanics involves summations over intermediate states. This usually requires evaluating a large number of matrix elements of the perturbative interaction. There are alternative forms of perturbation theory in which the summations can be circumvented. They are Sternheimer's method [1], Dalgarno and Lewis' (DL) method [2–4] and the logarithmic perturbation expansion (LPE) method developed by Aharonov and Au [5–8]. In both the Sternheimer's and DL methods one has to solve an inhomogeneous differential equation. The LPE method is more straightforward in the sense that it does not require solving any equation. The entire perturbation calculation is reduced to that of quadrature. If the unperturbed wavefunction has a node or nodes, however, the LPE method becomes quite involved. This is the case for excited states.

The purpose of this paper is to examine yet another form of perturbation theory that was developed by Zel'dovich in 1956 [9, 10]. In solving the Schrödinger equation in the presence of perturbation, Zel'dovich made ingenious use of the Lagrange condition of the theory of differential equations and reformulated the perturbation theory in such a way so that the summation over the intermediate states is avoided. In Zel'dovich's method the entire perturbation calculation is again reduced to that of quadrature. In this respect, Zel'dovich's method is similar to the LPE method which was developed much later. In dealing with excited states, however, this seldom quoted method of Zel'dovich has a remarkable advantage over the LPE method. Unlike in the LPE method, the nodes of the unperturbed wavefunction do not give rise to any complication. Zel'dovich's method can handle excited states and the ground state exactly in the same manner.

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We summarize Zel'dovich's method in section 2 and examine its relation to the DL and LPE methods in section 3. In section 4 we illustrate Zel'dovich's method by applying it to examples. A summary is given in section 5.

2. Zel'dovich's method

We consider a particle in a stationary bound state in one dimension, which can be the ground state or any of the excited states. This can be extended to the three-dimensional case with a central potential in a straightforward manner. Let us start with the unperturbed system that is described by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\psi_0''(x) + V_0(x)\psi_0(x) = E_0\psi_0(x) \tag{1}$$

where the notation is standard. For example, m is the mass of the particle and $\psi_0''(x) = \mathrm{d}^2\psi_0(x)/\mathrm{d}x^2$. It is understood that equation (1) can be solved exactly. We are interested in finding approximate solutions of

$$-\frac{\hbar^2}{2m}\psi''(x) + [V_0(x) + V_1(x)]\psi(x) = E\psi(x) \tag{2}$$

where $V_1(x)$ is the perturbation potential.

Let $R(x)$ and $I(x)$ be a regular and an irregular solution, respectively, of the unperturbed Schrödinger equation (1) with eigenvalue E_0. $R(x)$ satisfies the physically required boundary condition for a bound state but $I(x)$ does not. $R(x)$ can be taken as the unperturbed, normalized wavefunction as follows:

$$\psi_0(x) = R(x) \qquad \int_{-\infty}^{\infty} \mathrm{d}x\, R^2(x) = 1. \tag{3}$$

$I(x)$ may or may not be normalizable.

Let us now briefly digress into the three-dimensional case. By separating the angular part we obtain an equation for the radial part of the wavefunction with variable r with its range $(0, \infty)$. The unperturbed potential is of the form

$$\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V_0(r). \tag{4}$$

If $V_0(0)$ is finite, $R(r)$ and $I(r)$ behave as r^{l+1} and r^{-l}, respectively, as $r \to 0$. If $V(r) \to 0$ as $r \to \infty$, then $R(r) \to 0$ while $I(r)$ diverges. Such an $I(r)$ is not normalizable.

Returning to the one-dimensional case with variable x in $(-\infty, \infty)$, we now write the unknown $\psi(x)$ of (2) as

$$\psi(x) = \alpha(x)R(x) + \beta(x)I(x) \tag{5}$$

where $\alpha(x)$ and $\beta(x)$ are unknown functions. In order for the irregular solution $I(x)$ not to disturb the boundary condition for $\psi(x)$, we require that

$$\beta(-\infty) = \beta(\infty) = 0. \tag{6}$$

Furthermore, we require that $\alpha(x)$ and $\beta(x)$ satisfy the 'Lagrange condition'

$$\alpha'(x)R(x) + \beta'(x)I(x) = 0 \tag{7}$$

where $\alpha'(x) = \mathrm{d}\alpha(x)/\mathrm{d}x$. By substituting (5) into (2) and remembering (7), we obtain

$$\frac{\hbar^2}{2m}[\alpha'(x)R'(x) + \beta'(x)I'(x)] + [\Delta E - V_1(x)][\alpha(x)R(x) + \beta(x)I(x)] = 0 \tag{8}$$

where ΔE is the energy shift caused by $V_1(x)$,

$$E = E_0 + \Delta E. \tag{9}$$

Equations (7) and (8) lead to

$$\frac{\alpha'(x)}{I(x)} = -\frac{\beta'(x)}{R(x)} = -\frac{2m}{\hbar^2 W}[\Delta E - V_1(x)][\alpha(x)R(x) + \beta(x)I(x)]. \tag{10}$$

Here W is the Wronskian

$$W = R'(x)I(x) - R(x)I'(x) \tag{11}$$

which is a constant. We have not made any approximations so far.

We now expand ΔE, $\psi(x)$, $\alpha(x)$ and $\beta(x)$ as

$$\Delta E = E_1 + E_2 + \cdots \tag{12}$$

$$\psi(x) = \psi_0(x) + \psi_1(x) + \psi_2(x) + \cdots \tag{13}$$

$$\alpha(x) = \alpha_0 + \alpha_1(x) + \alpha_2(x) + \cdots \qquad \alpha_0 = 1 \tag{14}$$

$$\beta(x) = \beta_0 + \beta_1(x) + \beta_2(x) + \cdots \qquad \beta_0 = 0 \tag{15}$$

where the suffix refers to the order of perturbation,

$$\psi_n(x) = \alpha_n(x)R(x) + \beta_n(x)I(x). \tag{16}$$

Each $\beta_1, \beta_2, \ldots$ has to conform to (6). By putting the above expansions into (8) and collecting the first-order terms, we obtain

$$\frac{\alpha_1'(x)}{I(x)} = -\frac{\beta_1'(x)}{R(x)} = -\frac{2m}{\hbar^2 W}[E_1 - V_1(x)]R(x) \tag{17}$$

which leads to

$$\alpha_1(x) = -\frac{2m}{\hbar^2 W}\int_{-\infty}^{x} \mathrm{d}y\,[E_1 - V_1(y)]R(y)I(y) \tag{18}$$

$$\beta_1(x) = \frac{2m}{\hbar^2 W}\int_{-\infty}^{x} \mathrm{d}y\,[E_1 - V_1(y)]R^2(y). \tag{19}$$

There is an arbitrariness regarding the lower end of the integral of (18). We have taken it to be $-\infty$ since we usually find this most convenient. We discuss this choice in section 3. If we choose a different lower end, this effectively changes α_0. This change can be suppressed by renormalizing $R(x)$. Condition (6) together with (19) leads to

$$E_1 = \int_{-\infty}^{\infty} \mathrm{d}x\, V_1(x)R^2(x) \tag{20}$$

which is the well known first-order energy shift.

In the second order we obtain

$$\frac{\alpha_2'(x)}{I(x)} = -\frac{\beta_2'(x)}{R(x)} = -\frac{2m}{\hbar^2 W}\{E_2 R(x) + [E_1 - V_1(x)][\alpha_1(x)R(x) + \beta_1(x)I(x)]\}. \tag{21}$$

Recalling (6) that implies $\beta_2(\infty) = 0$ we obtain from (21)

$$\begin{aligned} E_2 &= -\int_{-\infty}^{\infty} \mathrm{d}x\,[E_1 - V_1(x)][\alpha_1(x)R(x) + \beta_1(x)I(x)]R(x) \\ &= \frac{2m}{\hbar^2 W}\int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{x} \mathrm{d}y\,[E_1 - V_1(x)][E_1 - V_1(y)] \\ &\quad \times R(x)R(y)[R(x)I(y) - I(x)R(y)]. \end{aligned} \tag{22}$$

Let us examine the integral that contains the term $R(x)I(y)$ of the last square brackets. It can be manipulated as

$$\begin{aligned}\int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{x} \mathrm{d}y\,[E_1 - V_1(x)][E_1 - V_1(y)]R^2(x)R(y)I(y) \\ &= \int_{-\infty}^{\infty} \mathrm{d}x \int_{x}^{\infty} \mathrm{d}y\,[E_1 - V_1(x)][E_1 - V_1(y)]R(x)R^2(y)I(x) \\ &= -\int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{x} \mathrm{d}y\,[E_1 - V_1(x)][E_1 - V_1(y)]R(x)I(x)R^2(y). \qquad (23)\end{aligned}$$

From the first to the second line, we have changed the order of integrations and interchanged the variables x and y. From the second to the third line, we have used (20). By using the above results, E_2 can be reduced to

$$E_2 = -\frac{4m}{\hbar^2 W}\int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{x} \mathrm{d}y\,[E_1 - V_1(x)][E_1 - V_1(y)]R(x)I(x)R^2(y). \qquad (24)$$

If $I(x)$ is known as well as $R(x)$, E_2 can immediately be evaluated. If $I(x)$ is not known, we can determine $I(x)$ in terms of $R(x)$. This can be done by using

$$R^2(x)\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{I(x)}{R(x)}\right] = -W \qquad (25)$$

$$I(x) = -WR(x)\int^{x} \frac{\mathrm{d}z}{R^2(z)}. \qquad (26)$$

This concludes our review of Zel'dovich's method [9, 10]. What we present below is new.

In (26) we have not specified the lower limit of the integral. This is because the lower limit does not affect E_2, as can be seen from (22). This practically means that the integral of (26) can be taken as an indefinite integral. One may well wonder about the following question. Suppose $R(x)$ has a node, say at $x = 0$, then how does $I(x)$ behave around $x = 0$? When $R(0) = 0$ we can safely assume that $R'(0) \neq 0$. Then (11) leads to

$$I(0) = \frac{W}{R'(0)}. \qquad (27)$$

Hence $I(x)$ should have no singularity at $x = 0$. Although the integral of (26) as such is questionable, we can interpret the product of the integral and $R(x)$ such that the product conforms to (27). Let us assume that $R(x)$ has only one node at $x = 0$ and write it as

$$R(x) = xf(x) \qquad f(0) = R'(0) \neq 0. \qquad (28)$$

Then we proceed as

$$\begin{aligned} I(x) &= -Wxf(x)\int^{x} \frac{\mathrm{d}z}{z^2 f^2(z)} \\ &= -Wxf(x)\left[-\frac{1}{xf^2(x)} + \int^{x} \frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{f^2(z)}\right]. \qquad (29)\end{aligned}$$

In the last z integration with the factor $1/z$, we take the principal part. One can confirm that this $I(x)$ does satisfy the Schrödinger equation (1) by directly substituting it into the equation. In the above we assumed that the node is at $x = 0$ but it can be shifted to an arbitrary position. The case with more than one node can be done in a similar fashion. In (24) we have the combination of $R(x)I(x)$. The additional factor of $R(x)$ that appears in E_2 doubly ensures that the node of $R(x)$ does not do any harm.

In the case where we deal with (26) numerically, one can proceed in the following way. Let us assume that $R(x)$ has only one node at $x = 0$. In numerical work we have to specify the

lower end of the integral. Let us start with the case of $x < 0$. We choose the lower end to be an arbitrary negative number. Then (26) is well defined. We can evaluate it with no difficulty. It is understood that one takes exactly the same mesh points for x and z. Next, if $x > 0$ we take the lower end to be a positive number so that (26) is again well defined. The $I(x)$ calculated in this way is discontinuous at $x = 0$. We simply make it continuous at $x = 0$ by adding a constant to the positive (or negative) x part of $I(x)$. The $I(0)$ so determined is related to W through (27). Recall that W can be chosen arbitrarily. If there is more than one node, this procedure can be repeated. If the two nodes are at $x = 0$ and $x = 1$, for example, we calculate $I(x)$ piecewise in the regions of $(-\infty, 0)$, $(0, 1)$ and $(1, \infty)$. In each of the regions we choose the lower end of the integral such that the integral is well defined. Then we join the obtained integrals smoothly at $x = 0$ and $x = 1$.

One can go on to higher orders in a successive manner. For example, in the third order we obtain

$$\frac{\alpha_3'(x)}{I(x)} = -\frac{\beta_3'(x)}{R(x)} = -\frac{2m}{\hbar^2 W}\{E_3 R(x) + E_2[\alpha_1(x)R(x) + \beta_1(x)I(x)] + [E_1 - V_1(x)][\alpha_2(x)R(x) + \beta_2(x)I(x)]\}. \tag{30}$$

This leads to

$$E_3 = -\int_{-\infty}^{\infty} \mathrm{d}x\, R(x)\{E_2[\alpha_1(x)R(x) + \beta_1(x)I(x)] + [E_1 - V_1(x)][\alpha_2(x)R(x) + \beta_2(x)I(x)]\}. \tag{31}$$

All the formulae presented in this section can be applied to any of the excited states as well as to the ground state. This is an important advantage of Zel'dovich's method over the LPE method.

3. Relation to the DL and LPE methods

Let us first examine the relation between Zel'dovich's method and the DL method. From their construction, it is clear that $\psi_0(x)$ and $\psi_1(x)$ satisfy the DL equation

$$-\frac{\hbar^2}{2m}\psi_1''(x) + V_0(x)\psi_1(x) = [E_1 - V_1(x)]\psi_0(x). \tag{32}$$

The first line of (22) is nothing but

$$E_2 = -\int_{-\infty}^{\infty} \mathrm{d}x\, [E_1 - V_1(x)]\psi_0(x)\psi_1(x). \tag{33}$$

Therefore, the two methods are equivalent.

Below (19) we mentioned the arbitrariness regarding the lower limit of the integral of $\alpha_1(x)$ of (18). Essentially the same arbitrariness appears in solving the DL equation. This was discussed by Mavromatis in some detail [4]. The choice of $-\infty$ in (18) (and $-a$ in examples 1 and 2 of section 4) is a matter of convenience.

Next let us examine the relation to the LPE method. Equation (24) can be rewritten as

$$E_2 = -\frac{2m}{\hbar^2 W}\int_{-\infty}^{\infty} \mathrm{d}x\, \frac{I(x)}{R(x)}\frac{\mathrm{d}}{\mathrm{d}x}\left\{\int_{-\infty}^{x} \mathrm{d}y\, [E_1 - V_1(y)]R^2(y)\right\}^2. \tag{34}$$

By integrating the right-hand side by parts and using (26) we obtain

$$E_2 = -\frac{2m}{\hbar^2}\int_{-\infty}^{\infty} \frac{\mathrm{d}x}{R^2(x)}\left\{\int_{-\infty}^{x} \mathrm{d}y\, [E_1 - V_1(y)]R^2(y)\right\}^2. \tag{35}$$

This expression for E_2 is the same as (23) of Aharonov and Au [5] which they derived for the ground state. See also (19) of [7]. For the ground state Zel'dovich's method is therefore equivalent to the LPE method .

There is a problem, however, on the part of the LPE method in dealing with excited states. The $R(x)$ of an excited state has a node or nodes. Suppose $R(x)$ has a node, then the x-integral $\int_{-\infty}^{\infty}(\mathrm{d}x/R^2)\ldots$ of (35) is simply divergent. This is so unless the $\{\cdots\}$ of (35) vanishes exactly at the position of the node (which does not usually happen). In the presence of the node, then, the transformation from (34) to (35), as such, by means of integration by parts is not valid. In the LPE method the singularity due to the node of $R(x)$ has to be dealt with carefully as was done in [5,6,8]. Every time another node appears in $R(x)$ almost the entire set of formulae will change. The LPE method in such a case is quite cumbersome. In contrast to this, Zel'dovich's method has no such complication as we stated at the end of section 2. We will illustrate it in the next section. In Zel'dovich's method, we use (24) for E_2, but not (35). The latter, of course, can be used if $R(x)$ has no node.

Suppose $R(x)$ has a node at $x = c_0$, then $\psi(x)$ will have a node at, say, $x = c$ that is shifted from but in the vicinity of $x = c_0$:

$$R(c_0) = \psi_0(c_0) = 0 \qquad \psi(c) = 0. \tag{36}$$

Aharonov and Au developed a method for determining the shift of the node position [5]. In Zel'dovich's method this can be done as follows. Let us expand c as

$$c = c_0 + c_1 + c_2 + \cdots. \tag{37}$$

By expanding $\psi(c) = 0$, we obtain

$$c_1\psi_0'(c_0) + \psi_1(c_0) = 0 \tag{38}$$

$$c_2\psi_0'(c_0) + c_1\psi_1'(c_0) + \psi_2(c_0) = 0 \tag{39}$$

and so on. Equation (38) leads to

$$c_1 = -\frac{\psi_1(c_0)}{\psi_0'(c_0)} = -\frac{\beta_1(c_0)I(c_0)}{R'(c_0)}. \tag{40}$$

By using (28) with a node at $x = c_0$, we find that $I(c_0) = W/R'(c_0)$. Thus we obtain

$$c_1 = -\frac{W\beta_1(c_0)}{R'^2(c_0)}. \tag{41}$$

This is how the node of the perturbed wavefunction can be determined. Equation (40) is the same as (37) of [5], but it seems to us that the derivation given above is simpler than that given in [5].

In the LPE method, in order to be able to calculate E_2, one has to know c_1. In Zel'dovich's method, E_2 can be calculated without knowing c_1. If one wants to know c_1 within Zel'dovich's method, one can use (40) or one can directly determine it from $\psi_0(x) + \psi_1(x) = 0$, where $\psi_1(x) = \alpha_1(x)R(x) + \beta_1(x)I(x)$.

4. Examples

We examine two examples, an infinite square-well potential and a harmonic oscillator. We examine excited states as well as the ground state. We assume the same perturbation potential in both examples:

$$V_1(x) = \lambda x \tag{42}$$

where λ is a constant.

Example 1. Infinite square-well potential. The unperturbed potential is

$$V_0(x) = \begin{cases} 0 & \text{if} \quad |x| < a \\ \infty & \text{if} \quad |x| > a. \end{cases} \tag{43}$$

This reduces the space from $(-\infty, \infty)$ to $(-a, a)$. The unperturbed wavefunction can be taken as

$$\psi_0(x) = R(x) = \frac{1}{\sqrt{a}} \cos\left(kx - \frac{\nu\pi}{2}\right) \qquad k = \frac{\pi}{2a}(\nu + 1) \tag{44}$$

where $\nu = 0$ for the ground state and $\nu = 1, 2, \ldots$ for excited states. The unperturbed energy is $E_0 = (\hbar k)^2/(2m)$. For the irregular solution we take

$$I(x) = \frac{1}{\sqrt{a}} \sin\left(kx - \frac{\nu\pi}{2}\right). \tag{45}$$

This can be obtained from (26) by choosing the Wronskian as

$$W = -\frac{k}{a}. \tag{46}$$

Note that $\int^x \mathrm{d}z/R^2(z) = (a/k)\tan(kx - \nu\pi/2)$ is singular at the nodes of $R(x)$. This singularity is cancelled when the integral is multiplied with $R(x)$.

It is clear that $E_1 = 0$. For $\alpha_1(x)$ and $\beta_1(x)$ we obtain

$$\alpha_1(x) = -\frac{2m}{\hbar^2}\frac{\lambda}{8k^3}[2ka + (-1)^\nu(\sin 2kx - 2kx\cos 2kx)] \tag{47}$$

$$\beta_1(x) = \frac{2m}{\hbar^2}\frac{\lambda}{8k^3}[2k^2(x^2 - a^2) + 1 + (-1)^\nu(\cos 2kx + 2kx\sin 2kx)]. \tag{48}$$

Note that $\beta_1(a) = \beta_1(-a) = 0$. Putting the above $R(x)$ and $I(x)$ into (24), we obtain

$$E_2 = \frac{2m}{\hbar^2}\frac{\lambda^2}{48k^4}[4(ka)^2 - 15]. \tag{49}$$

If we put $a = \pi/2$, the above E_2 for the ground state ($\nu = 0$) agrees with that of example A of [4]. Equation (49) is also valid for all excited states.

Let us examine the nodes of the wavefunction. We can determine the positions of all the nodes but let us focus on the cases where the unperturbed wavefunction has odd parity and see how the node at the origin is shifted by perturbation. We start with $c_0 = 0$ and determine c_1. Equation (39) gives

$$c_1 = \frac{2m}{\hbar^2}\frac{\lambda}{k^4}[-2(ka)^2 + 1 + (-1)^\nu] \tag{50}$$

which is negative. The node is shifted to the negative side of the origin. This is because the perturbation force acts in that direction.

Example 2. Harmonic oscillator. The unperturbed potential is

$$V_0(x) = \tfrac{1}{2}m\omega^2x^2 \tag{51}$$

where $\omega > 0$ is a constant. We assume the same $V_1(x)$ of (42). The unperturbed wavefunction can be taken as [11]

$$\psi_0(x) = R(x) = N_\nu H_\nu(\gamma x)\mathrm{e}^{-\frac{1}{2}(\gamma x)^2} \qquad \gamma^2 = \frac{m\omega}{\hbar} \qquad N_\nu{}^2 = \frac{\gamma}{2^\nu\sqrt{\pi}\,\nu!} \tag{52}$$

where $\nu = 0, 1, 2, \ldots$. H_ν is the Hermite polynomial of order ν; $H_0(\xi) = 1$, $H_1(\xi) = 2\xi$, $H_2(\xi) = 4\xi^2 - 2$, etc. Note that suffix ν refers to the unperturbed state that is being considered.

It should not be confused with suffix n of ψ_n, E_n, etc, that refers to the order of perturbation. The unperturbed energy is $E_0 = (\nu + \frac{1}{2})\hbar\omega$. It is clear that $E_1 = 0$.

The unperturbed Schrödinger equation (1) with $E_0 = (\nu + \frac{1}{2})\hbar\omega$ has the following two independent solutions:

$$\boldsymbol{E}_\nu^{(0)}(\gamma x) = \sqrt{2}\mathrm{e}^{-\frac{1}{4}(\gamma x)^2}{}_1F_1\left(-\frac{\nu}{2}; \frac{1}{2}; \frac{(\gamma x)^2}{2}\right) \tag{53}$$

$$\boldsymbol{E}_\nu^{(1)}(\gamma x) = 2\gamma x\mathrm{e}^{-\frac{1}{4}(\gamma x)^2}{}_1F_1\left(\frac{1-\nu}{2}; \frac{3}{2}; \frac{(\gamma x)^2}{2}\right) \tag{54}$$

where $\boldsymbol{E}_\nu^{(0)}$ and $\boldsymbol{E}_\nu^{(1)}$ are the Weber functions and the ${}_1F_1$ are the confluent hypergeometric (or Kummer) functions [11]. They have no singularity except that they diverge as $x \to \infty$ or $-\infty$. The $R(x)$ of (52) is a special linear combination of the two solutions such that it vanishes as $|x| \to \infty$ [12]. Any one of the two solutions or their linear combination, other than that of $R(x)$, can be taken as $I(x)$. It would be more interesting, however, to determine $I(x)$ by means of (26), which we will do below.

Let us focus on the three states ($\nu = 0, 1, 2$) of the lowest energies. For the ground state with $\nu = 0$, the irregular solution is given by

$$I(x) = -\frac{W}{N_0}\mathrm{e}^{-\frac{1}{2}(\gamma x)^2}\int^x \mathrm{e}^{(\gamma z)^2}\,\mathrm{d}z. \tag{55}$$

It is straightforward to work out (24) to find

$$\begin{aligned} E_2 &= \frac{4m(N_0\lambda)^2}{\hbar^2}\int_{-\infty}^{\infty} x\mathrm{e}^{-(\gamma x)^2}\,\mathrm{d}x\int^x \mathrm{e}^{(\gamma z)^2}\,\mathrm{d}z\int_{-\infty}^x y\mathrm{e}^{-(\gamma y)^2}\,\mathrm{d}y \\ &= -\frac{2m(N_0\lambda)^2}{(\hbar\gamma)^2}\int_{-\infty}^{\infty} x\mathrm{e}^{-2(\gamma x)^2}\,\mathrm{d}x\int^x \mathrm{e}^{(\gamma z)^2}\,\mathrm{d}z = -\frac{\lambda^2}{2m\omega^2}. \end{aligned} \tag{56}$$

As we stated earlier, E_2 does not depend on the choice of the lower limits of the z integrations of (55) and (56).

For the first excited state with $\nu = 1$ we obtain

$$\begin{aligned} I(x) &= -\frac{W}{N_1}\gamma x\mathrm{e}^{-\frac{1}{2}(\gamma x)^2}\int^x \frac{\mathrm{e}^{(\gamma z)^2}}{(\gamma z)^2}\,\mathrm{d}z \\ &= \frac{W}{N_1\gamma}\mathrm{e}^{\frac{1}{2}(\gamma x)^2}\left[1 - 2\gamma^2 x\mathrm{e}^{-(\gamma x)^2}\int^x \mathrm{e}^{(\gamma z)^2}\,\mathrm{d}z\right]. \end{aligned} \tag{57}$$

The $R(x)$ has a node at $x = 0$. We have to interpret the z integration of (57) as we explained towards the end of section 2. This $I(x)$ satisfies (1).

The energy shift E_2 can be worked out as follows:

$$\begin{aligned} E_2 &= \frac{4m(N_1\lambda)^2}{\hbar^2}\int_{-\infty}^{\infty} x(\gamma x)^2\mathrm{e}^{-(\gamma x)^2}\,\mathrm{d}x\int^x \frac{\mathrm{e}^{(\gamma z)^2}}{(\gamma z)^2}\,\mathrm{d}z\int_{-\infty}^x y(\gamma y)^2\mathrm{e}^{-(\gamma y)^2}\,\mathrm{d}y \\ &= -\frac{2m(N_1\lambda)^2}{\hbar^2}\int_{-\infty}^{\infty} x^3[(\gamma x)^2 + 1]\mathrm{e}^{-2(\gamma x)^2}\,\mathrm{d}x\int^x \frac{\mathrm{e}^{(\gamma z)^2}}{(\gamma z)^2}\,\mathrm{d}z = -\frac{\lambda^2}{2m\omega^2}. \end{aligned} \tag{58}$$

From the second line to the last we performed integration by parts but there is no danger in that.

If we apply (35) of the LPE method to the first excited state, we meet difficulty in the x integration. It is clear that the y integral of (35) does not vanish for $x = 0$ where $R(x)$ has a node. Hence the x integral diverges. Aharonov and Au developed different formulae for excited states but we do not pursue those here [5, 6, 8].

Let us examine the node of the perturbed wavefunction of $\nu = 1$. We know that $c_0 = 0$ and we want to determine c_1. $\beta_1(x)$ is given by

$$\beta_1(x) = \frac{2m\lambda}{\sqrt{\pi}\hbar^2 W\gamma}[(\gamma x)^2 + 1]\mathrm{e}^{-(\gamma x)^2}. \tag{59}$$

Then we obtain from (40)

$$c_1 = -\frac{\lambda}{m\omega^2}. \tag{60}$$

As the last exercise let us briefly examine the second excited state, $\nu = 2$. $R(x)$ of this state has two nodes. Again, by using (26) we obtain the irregular solution as

$$\begin{aligned} I(x) &= -\frac{W}{2N_2}[2(\gamma x)^2 - 1]\mathrm{e}^{-\frac{1}{2}(\gamma x)^2}\int^x \frac{\mathrm{e}^{(\gamma z)^2}}{[2(\gamma z)^2 - 1]^2}\,\mathrm{d}z \\ &= \frac{W}{4N_2\gamma}\mathrm{e}^{\frac{1}{2}(\gamma x)^2}\left\{1 - [2(\gamma x)^2 - 1]\mathrm{e}^{-(\gamma x)^2}\int^x \mathrm{e}^{(\gamma z)^2}\,\mathrm{d}z\right\}. \end{aligned} \tag{61}$$

This $I(x)$ has no singularity. The energy shift E_2 can be calculated by using (24) in the same manner as in the $\nu = 1$ case. The calculation involved is somewhat complicated but straightforward. We again find $E_2 = -\lambda^2/(2m\omega^2)$. This exercise clearly illustrates the superiority of Zel'dovich's method over the LPE method. The state with a wavefunction with two nodes is almost prohibitive in the LPE method. In fact, the LPE method has not been developed for states with more than one node.

5. Summary

We reviewed Zel'dovich's method of perturbation theory and compared it with the DL and LPE methods. Zel'dovich's method enables us to circumvent summations over the intermediate states. In this respect Zel'dovich's method is similar to the DL and LPE methods. Unlike the DL method, Zel'dovich's method does not involve solving any equations. The entire calculation is reduced to that of quadrature. This feature of Zel'dovich's method is very similar to that of the LPE method of Aharonov and Au [4–6]. Zel'dovich's method, however, has a remarkable advantage over the LPE method. It can be applied to excited states exactly in the same manner as to the ground state. The nodes of the wavefunction that are found for an excited state do not require any modifications of the method. We have illustrated Zel'dovich's method in two examples, and shown how the ground and excited states can be handled exactly in the same straightforward manner.

One appreciates the advantage of Zel'dovich's method over the LPE method if one sees the modifications that are required in the latter in handling excited states [5, 6, 8]. The LPE method has been developed only for the cases of no node and one node of the unperturbed wavefunction. If there are two or more nodes, the LPE is almost prohibitive. We believe that Zel'dovich's method deserves much more attention than it has received so far.

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