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LETTER TO THE EDITOR

Alternative approach to non-relativistic perturbation theory

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Abstract. We develop a simple alternative approach to perturbation theory in one-dimensional non-relativistic quantum mechanics. The formulae for the energy shifts and wavefunctions do not involve cumbersome sums over intermediate states which appear in the usual Rayleigh-Schrödinger expansion. Unlike standard logarithmic perturbation theory, our approach does not utilize taking the logarithm of the wavefunction, and is therefore applicable in the same form to both the ground state and excited bound states.

Performing explicit calculations in non-relativistic quantum mechanics using the familiar Rayleigh-Schrödinger perturbation expansion is rendered difficult by the presence of summations over all intermediate unperturbed eigenstates. Alternative perturbation procedures have been proposed to avoid this difficulty, notably the logarithmic perturbation theory (LPT) [1-4] and the Dalgarno-Lewis technique [5-8]. Indeed, in applying these methods to the nth excited state, one requires knowledge of the unperturbed eigenfunction $\psi_n^0(x)$ but no knowledge of the other eigenvalues or eigenfunctions is necessary. LPT results are particularly simple for the ground state ($n=0$); however, the two presently known procedures for applying LPT to excited states ($n>0$) involve either tedious explicit factoring out of the zeros of $\psi_n^{(0)}(x)$ [1, 2], or introduction of ghost states [4]. In this letter, starting from first principles, we develop a more economical scheme which yields simple perturbation theory formulae for both energy level shifts and corrections to the wavefunction for all states. Since our approach does not involve the logarithm of the wavefunction, no factoring out of the zeros of $\psi_n^{(0)}(x)$ is needed. In fact, the formulae, worked out below for one-dimensional situations, are equally applicable to the excited states as well as to the ground state. Our results can be thought of as a generalization of LPT.

Derivation. The Schrödinger equation with an unperturbed potential $V(x)$ and a perturbing potential $\lambda h(x)$ is ($\hbar = 2m = 1$)

$$-\psi_n'' + (V + \lambda h)\psi_n = E_n \psi_n \tag{1}$$

where λ serves as the coupling constant and the primes denote differentiation with respect to x. Let us write the wavefunction $\psi_n(x)$ as

$$\psi_n(x) = f_n(x)\psi_n^{(0)}(x) \tag{2}$$

in which $\psi_n^{(0)}(x)$ is the known normalized eigenfunction of the unperturbed Schrödinger equation. Substituting (2) into (1) yields

$$\psi_n^{(0)} f_n'' + 2\psi_n^{(0)\prime} f_n' - \lambda h \psi_n^{(0)} f_n = (E_n^{(0)} - E_n)\psi_n^{(0)} f_n. \tag{3}$$

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Now expand E_n and $f_n(x)$ in powers of λ:

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \tag{4}$$

$$f_n(x) = f_n^{(0)}(x) + \lambda f_n^{(1)}(x) + \lambda^2 f_n^{(2)}(x) + \dots \qquad f_n^{(0)}(x) = 1. \tag{5}$$

Upon substituting (4) and (5) into (3) and equating powers of λ, we obtain the following hierarchy of differential equations:

$$\psi_n^{(0)} f_n^{(1)\prime\prime} + 2\psi_n^{(0)\prime} f_n^{(1)\prime} = (h - E_n^{(1)})\psi_n^{(0)} \tag{6}$$

$$\psi_n^{(0)} f_n^{(2)\prime\prime} + 2\psi_n^{(0)\prime} f_n^{(2)\prime} = (h - E_n^{(1)})\psi_n^{(0)} f_n^{(1)} - E_n^{(2)}\psi_n^{(0)} \tag{7}$$

$$\psi_n^{(0)} f_n^{(3)\prime\prime} + 2\psi_n^{(0)\prime} f_n^{(3)\prime} = (h - E_n^{(1)})\psi_n^{(0)} f_n^{(2)} - E_n^{(2)}\psi_n^{(0)} f_n^{(1)} - E_n^{(3)}\psi_n^{(0)} \tag{8}$$

$$\psi_n^{(0)} f_n^{(k)\prime\prime} + 2\psi_n^{(0)\prime} f_n^{(k)\prime} = (h - E_n^{(1)})\psi_n^{(0)} f_n^{(k-1)} - \psi_n^{(0)} \sum_{i=2}^{k} E_n^{(i)} f_n^{(k-i)}. \tag{9}$$

Each of the above linear differential equations is trivially solved by using an integrating factor $\psi_n^{(0)}(x)$.

Multiplying (6) by $\psi_n^{(0)}(x)$ gives

$$(\psi_n^{(0)2} f_n^{(1)\prime})' - (h - E_n^{(1)})\psi_n^{(0)2}. \tag{10}$$

Since $\psi_n^{(0)}(x) \to 0$ as $x \to \pm\infty$, we obtain

$$\psi_n^{(0)2} f_n^{(1)\prime}(x) = \int_{-\infty}^{x} (h - E_n^{(1)})\psi_n^{(0)2}\, \mathrm{d}x'. \tag{11}$$

For $x \to +\infty$, we obtain the familiar first-order result

$$E_n^{(1)} = \int_{-\infty}^{\infty} h(x)\psi_n^{(0)2}(x)\, \mathrm{d}x. \tag{12}$$

Also, the first-order correction to the wavefunction is

$$f_n^{(1)}(x) = \int^{x} \frac{\mathrm{d}x'}{\psi_n^{(0)2}(x')} \int_{-\infty}^{x'} [h(x'') - E_n^{(1)}]\psi_n^{(0)2}(x'')\, \mathrm{d}x''. \tag{13}$$

Proceeding in the same manner, one obtains the following higher-order results

$$E_n^{(2)} = \int_{-\infty}^{\infty} [h(x) - E_n^{(1)}] f_n^{(1)}(x)\psi_n^{(0)2}(x)\, \mathrm{d}x \tag{14}$$

$$f_n^{(2)}(x) = \int^{x} \frac{\mathrm{d}x'}{\psi_n^{(0)2}(x')} \int_{-\infty}^{x'} \{[h(x'') - E_n^{(1)}] f_n^{(1)}(x'') - E_n^{(2)}\}\psi_n^{(0)2}(x'')\, \mathrm{d}x'' \tag{15}$$

$$E_n^{(k)} = \int_{-\infty}^{\infty} \left\{[h(x) - E_n^{(1)}] f_n^{(k-1)}(x) - \sum_{i=2}^{k-1} E_n^{(i)} f_n^{(k-i)}(x)\right\}\psi_n^{(0)2}(x)\, \mathrm{d}x \tag{16}$$

$$f_n^{(k)}(x) = \int^{x} \frac{\mathrm{d}x'}{\psi_n^{(0)2}(x')} \int_{-\infty}^{x'} \left\{[h(x'') - E_n^{(1)}] f_n^{(k-1)}(x'') - \sum_{i=2}^{k} E_n^{(i)} f_n^{(k-i)}(x'')\right\} \times \psi_n^{(0)2}(x'')\, \mathrm{d}x''. \tag{17}$$

Equations (12)-(17) are the main results of this letter.

One can see that, in general, $f_n^{(k)}(x)$ is singular at the zeros of $\psi_n^{(0)}(x)$ while $\psi_n^{(0)}(x) f_n^{(k)}(x)$ remains finite at these points. This amounts to a shift in the position of zeros of the unperturbed wavefunction under the influence of a perturbing potential.

Also, the indefiniteness of integrals in the expression for $f_n^{(k)}$ is justified when one requires $\psi_n^{(0)}$ to be orthogonal to $\psi_n^{(0)} f_n^{(k)}$. Finally, the above results, being an expansion in powers of λ, necessarily agree with the Rayleigh–Schrödinger results. For completeness it is proper to mention that there are several published treatments of Rayleigh–Schrödinger perturbation theory using wave and reaction operators, which do not involve summations over all intermediate unperturbed eigenstates [9–11]. However, our derivation is simpler and more direct, and hence provides a useful alternative.

For a ground state, one can easily show that the new formulae reduce to LPT results. For instance, take (14) for $n=0$ and perform integration by parts

$$E_0^{(2)} = \int_{-\infty}^{\infty} f_0^{(1)}(x) \left[\frac{\mathrm{d}}{\mathrm{d}x} \int_{-\infty}^{x} (h - E_0^{(1)}) \psi_0^{(0)2}(x')\, \mathrm{d}x' \right] \mathrm{d}x$$

$$= -\int_{-\infty}^{\infty} \left[\frac{1}{\psi_0^{(0)2}(x)} \int_{-\infty}^{x} (h - E_0^{(1)}) \psi_0^{(0)2}(x')\, \mathrm{d}x' \right] \mathrm{d}x. \tag{18}$$

This is identical to the usual LPT ground state result, and the proof can be extended to higher orders.

Example (a). Harmonic oscillator with linear perturbation ($n=1$ state). Consider a one-dimensional harmonic oscillator potential $V(x) = \frac{1}{4}\omega^2 x^2$ with a linear perturbation of the form

$$h(x) = Ax + B. \tag{19}$$

Let us calculate the energy level shifts and corrections to the wavefunction for the first excited state. The normalized unperturbed eigenfunction is

$$\psi_1^{(0)}(x) = N_1 x\, \mathrm{e}^{-\omega x^2/4} \qquad N_1 = \left[\frac{\omega^3}{2\pi} \right]^{1/4}. \tag{20}$$

The first-order energy shift is easily obtained to be $E_1^{(1)} = B$. Knowing $E_1^{(1)}$, we go on to calculate $f_1^{(1)}(x)$ using (13).

$$f_1^{(1)}(x) = -\frac{A}{\omega}\left(x - \frac{2}{\omega x} \right). \tag{21}$$

Note that $f_1^{(1)}$ has a pole at $x=0$, where $\psi_1^{(0)}$ vanishes.

The first-order correction to the wavefunction is given by

$$\psi_1^{(0)}(x) f_1^{(1)} = -\frac{A}{\omega} N_1 x\, \mathrm{e}^{-\omega x^2/4} \left(x - \frac{2}{\omega x} \right). \tag{22}$$

Now the second-order calculations can be performed. First, we compute $E_1^{(2)}$ from (14).

$$E_1^{(2)} = -\frac{A^2}{\omega^2}. \tag{23}$$

With $E_1^{(2)}$ available, we calculate the second-order correction to the wavefunction

$$f_1^{(2)}(x) = \frac{A^2 x^2}{2\omega^2}. \tag{24}$$

The un-normalized wavefunction, up to second order in A, is

$$\psi_1^{(0)}[1 + f_1^{(1)}(x) + f_1^{(2)}(x)] = N_1 x\, \mathrm{e}^{-\omega x^2/4} \left[1 - \frac{A}{\omega}\left(x - \frac{2}{\omega x} \right) + \frac{A^2 x^2}{2\omega^2} \right]. \tag{25}$$

The energy level shifts due to higher orders in A can be seen to vanish since all of the integrands are odd functions.

Example (b). Infinite square well with linear perturbation ($n=2$ state). Consider the infinite square well potential

$$V(x)=\begin{cases}0 & -\pi/2<x<\pi/2\\ \infty & \text{otherwise.}\end{cases} \tag{26}$$

Take a perturbation of the form

$$h(x)=Ax+B. \tag{27}$$

Again, calculate the energy level shifts and corrections to the wavefunction:

$$\psi_2^{(0)}(x)=\sqrt{\frac{2}{\pi}}\cos 3x. \tag{28}$$

We first calculate $E_2^{(1)}=B$, and

$$f_2^{(1)}=\frac{A}{4}\left[\frac{1}{3}\left(x^2-\frac{\pi^2}{4}\right)\tan 3x+\frac{1}{9}x\right]. \tag{29}$$

The second-order energy level correction is

$$E_2^{(2)}=\frac{A^2}{36}\left(\frac{\pi^2}{12}-\frac{5}{36}\right). \tag{30}$$

The higher-order calculations are just exercises in elementary integrals.

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