New Approach to Perturbation Theory

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We present here a new approach to nonrelativistic perturbation theory. We show that in problems reducible to one dimension, the energy shifts and wave-function corrections, including corrections to the position of the nodes, to any order, can be expressed in quadrature in a hierarchy scheme. The second-order energy shift calculated is explicitly shown to be equivalent to that in the ordinary Rayleigh-Schrödinger theory.

The subject of stationary-state perturbation theory is well discussed in most quantum mechanics textbooks.[1] In the usual treatment, the energy shifts and corrections to the wave functions are expressed in terms of sums over intermediate states or integrals involving the Green's functions. In this Letter, we shall describe a new technique that, in one-dimensional problems, and hence in any problem reducible to one dimension, yields, in a hierarchical scheme, quadrature forms for the energy shifts and corrections to wave functions to any given order in perturbation theory. We obtain an extra bonus in that the shift in the nodal positions of the wave function, to any order, is also expressible in quadrature. The possible application of this new technique and extension to three-dimensional problems will be discussed in detail in a later publication.

Consider a perturbation $\lambda V_1(x)$ being introduced to a nonrelativistic system with a Hamiltonian $H_0 = p^2/2m + V_0(x)$ whose unperturbed solutions are known. The Schrödinger equation then becomes

$$H|\psi\rangle = (H_0 + \lambda V_1)|\psi\rangle = E|\psi\rangle. \tag{1}$$

The state $|\psi\rangle$ and its eigenvalue E can be expressed as series in λ:

$$|\psi\rangle = |\psi_0\rangle + \lambda|\psi_1\rangle + \lambda^2|\psi_2\rangle + \cdots \tag{2}$$

and

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots, \tag{3}$$

where

$$H_0|\psi_0\rangle = E_0|\psi_0\rangle \tag{4}$$

is the unperturbed Schrödinger equation and its eigenvector $|\psi_0\rangle$ and eigenvalue E_0 are presumed known. In the x representation, the wave functions $\psi(x) = \langle x|\psi\rangle$ and $\psi_0(x) = \langle x|\psi_0\rangle$ are nodeless in the ground state and have N nodes in the Nth excited state, and we can ordinarily write, for systems in well-behaved potentials,

$$\psi^N(x) = \left[\prod_{i=1}^{N}(x - \alpha^i)\right]\exp[-G^N(x)] \tag{5}$$

and

$$\psi_0^N(x) = \left[\prod_{i=1}^{N}(x - \alpha_0^i)\right]\exp[-G_0^N(x)], \tag{6}$$

where the perturbed and unperturbed nodal positions are denoted by α^i and α_0^i, respectively, and the functions $G^N(x)$ and $G_0^N(x)$ are regular. The perturbed ith nodal position can likewise be written as a series in λ:

$$\alpha^i = \alpha_0^i + \lambda\alpha_1^i + \lambda^2\alpha_2^i + \cdots. \tag{7}$$

In this Letter, we present our new approach to perturbation theory for the cases $N=0$ (ground state) and $N=1$ (first excited state). The generalization to higher excited states is straightforward.

The ground state.—The ground-state wave function of a system is nodeless. Thus the perburbed and unperturbed wave functions can be written, in accordance with Eqs. (5) and (6), as

$$\psi(x) = \exp[-G(x)] \tag{8}$$

and

$$\psi_0(x) = \exp[-G_0(x)]. \tag{9}$$

The function G and its derivative $g(x) \equiv G'(x)$ can be expanded as power series in λ:

$$G(x) = G_0(x) + \lambda G_1(x) + \lambda^2 G_2(x) + \cdots = \sum_{i=0}^{\infty}\lambda^i G_i(x) \tag{10}$$

and

$$g(x) = \sum_{i=0}^{\infty}\lambda^i g_i(x), \tag{11}$$

where $g_0(x) \equiv G_0'(x)$. Substituting Eqs. (8)–(11) into the Schrödinger equation (1), we obtain

$$-\tfrac{1}{2}(g^2 - g')e^{-G} - (E - V_0 - \lambda V_1)e^{-G}. \tag{12}$$

On comparing coefficients for various powers of λ, we have

$$-(g_0^2 - g_0') = 2(E_0 - V_0), \tag{13}$$

$$-(2g_0g_1 - g_1') = 2(E_1 - V_1), \tag{14}$$

and

$$-(2g_0g_i - g_i') = 2\left(E_i + \tfrac{1}{2}\sum_{j=1}^{i-1} g_j g_{i-j}\right), \quad i \geq 2. \quad (15)$$

Equation (13) is the Schrödinger equation for the unperturbed system. On multiplication of Eq. (14) with the integrating factor $\exp(-2G_0)$, it becomes

$$-[g_1 \exp(-2G_0)]' = 2(V_1 - E_1)\exp(-2G_0). \quad (16)$$

On integrating both sides from $-\infty$ to $+\infty$, and using the fact that ψ_0 is normalized and vanishes at both limits, we obtain

$$E_1 = \int V_1 \psi_0^2(x)\,dx \equiv \int V_1 \rho(x)\,dx \quad (17)$$

in agreement with conventional perturbation theory. With E_1 thus known, we can perform an indefinite integral on Eq. (16) to obtain

$$g_1(x) = -[2/\rho(x)]\int_{-\infty}^{x}(V_1 - E_1)\rho(x')\,dx', \quad (18)$$

and hence

$$G_1(x) = \int_{x_0}^{x} g_1(x')\,dx', \quad (19)$$

and the lower limit is determined by requiring that the first-order perturbed wave function is normalized to unity. The same integrating factor can be applied to Eq. (15), and it leads to

$$G_i(x) = \int_{x_0}^{+\infty} \tfrac{1}{2}\left(\sum_{j=1}^{i-1} g_j g_{i-j}\right)\rho(x)\,dx, \quad (20)$$

and

$$g_i(x) = [2/\rho(x)]\int_{-\infty}^{x}\left(E_i + \tfrac{1}{2}\sum_{j=1}^{i-1} g_j g_{i-j}\right)\rho(x')\,dx'. \quad (21)$$

Equations (20) and (21) form a hierarchical scheme by which the corrections to the wave function and energy of the ground state can be calculated to any order in the coupling constant λ. These are in quadrature forms and do not involve the Green's function of the problem.[2]

It is interesting to show explicitly that the second-order energy shift, as given by Eq. (20), agrees with the usual expression from the Rayleigh-Schrödinger theory. For simplicity, we take the first-order energy correction to be zero, since one always has the freedom to redefine the perturbation as $V_1 - \langle 0|V_1|0\rangle$. Under this assumption, we have

$$g_1(x) = -[2/\rho(x)]\int_{-\infty}^{x} V_1\rho(x')\,dx' \quad (22)$$

and

$$E_2 = -\int_{-\infty}^{+\infty} \tfrac{1}{2} g_1^2(x)\rho(x)\,dx\,; \quad (23)$$

whereas according to the Rayleigh-Schrödinger theory,

$$E_2^{RS} = \sum_{n\neq 0}\frac{\langle 0|V_1|n\rangle\langle n|V_1|0\rangle}{E_0 - E_n} = \int \psi_1 V_1 \psi_0. \quad (24)$$

$$= \int \psi_1 V_1 \psi_0.$$

We now demonstrate the equivalence between Eq. (23) and (24). On comparing Eqs. (2), (8), and (10), we have

$$\psi_1 = -G_1\psi_0, \quad (25)$$

and so

$$E_2^{RS} = -\int_{-\infty}^{+\infty} G_1 V_1 \rho. \quad (26)$$

On the other hand, from Eq. (16), we have

$$(g_1\rho)' = -2V_1\rho. \quad (27)$$

Hence

$$E_2^{RS} = \int_{-\infty}^{\infty} \tfrac{1}{2} G_1 (g_1\rho)'. \quad (28)$$

On integration by parts and using the fact that ρ vanishes at both limits, we obtain

$$E_2^{RS} = -\int_{-\infty}^{\infty} \tfrac{1}{2} g_1^2 \rho, \quad (29)$$

which is Eq. (23) in our present approach.

The excited states.—We now extend our technique to excited states. We shall see that in the present approach, the corrections to the nodal positions of the wave function of the excited states are expressible as quadratures.

For definiteness, we consider the first excited state which has one node. Its wave function, according to Eq. (5), can be written as

$$\psi(x) = (x - \alpha)\exp[-G(x)], \quad (30)$$

where $G(x)$ is regular and is expandable in powers of λ as before, and so is its derivative g. The Schrödinger equation then becomes

$$-\tfrac{1}{2}[g^2 - g' - 2g/(x-\alpha)] = E - V_0 - \lambda V_1. \quad (31)$$

On expanding both sides in powers of λ, we have

$$(x-\alpha_0)(g_0^2 - g_0') - 2g_0$$

$$= -2(E_0 - V_0)(x - \alpha_0), \quad (32)$$

which is the unperturbed Schrödinger equation, and α_0 is the node of the unperturbed wave func-

tion. To first order in λ we have

$$(x-\alpha_0)(2g_0g_1-g_1')-2g_1-\alpha_1(g_0^2-g_0')=-2(E_1-V_1)(x-\alpha_0)+2\alpha_1(E_0-V_0). \tag{33}$$

On multiplying this throughout by $(x-\alpha_0)\exp(-2G_0)$ and making use of Eq. (32) we find

$$-[g_1(x-\alpha_0)^2\exp(-2G_0)]'=-2(E_1-V_1)(x-\alpha_0)^2\exp(-2G_0)+\alpha_1[\exp(-2G_0)]'. \tag{34}$$

On integrating from $-\infty$ to $+\infty$ on both sides, we get

$$E_1=\int_{-\infty}^{+\infty}V_1(x-\alpha_0)^2\exp(-2G_0)\,dx \tag{35}$$

$$=\int_{-\infty}^{+\infty}V_1\psi_0^2(x)\,dx=\int_{-\infty}^{+\infty}V_1\rho(x)\,dx, \tag{36}$$

in agreement with the conventional Rayleigh-Schrödinger theory. On integrating both sides from $-\infty$ to α_0, we obtain the first-order corrections to the nodal position of the wave function,

$$\alpha_1=\exp[2G_0(\alpha_0)]\int_{-\infty}^{\alpha_0}2(E_1-V_1)\rho(x)\,dx. \tag{37}$$

On integrating from $-\infty$ to x on both sides, we obtain a solution to g_1:

$$g_1(x)=[1/\rho(x)]\{\int_{-\infty}^{x}2(E_1-V_1)\rho(x')dx'-\alpha_1\exp[-2G_0(x)]\}. \tag{38}$$

For the higher-order corrections, the following hierarchy equation can be obtained from Eq. (31):

$$-[g_i(x-\alpha_0)^2\exp(-2G_0)]'=\alpha_i[\exp(-2G_0)]'-2E_i\rho+F_i, \tag{39}$$

where

$$F_i(x)\equiv 2\alpha_{i-1}[g_1+g_0\alpha_1/(x-\alpha_0)]\exp(-2G_0)$$

$$+\sum_{m=2}^{i-1}\left[\sum_{j=0}^{m}g_jg_{m-j}-g_m'\right](x-\alpha_0)\exp(-2G_0)-\sum_{j=1}^{i-1}g_jg_{i-j}(x-\alpha_0)^2\exp(-2G_0) \tag{40}$$

and is solvable in a hierarchical scheme.

We have made use of Eqs. (32) and (33), and the second term in equation (40) contributes only when $i\geq 3$. As is obvious from Eq. (32), the factor $g_0/(x-\alpha_0)$ in Eq. (40) is singularity free. Equation (39) can then be integrated to yield solutions for E_i, α_i, and g_i by use of the following sets of limits:

$-\infty$ to $+\infty$, $-\infty$ to α_0, and $-\infty$ to x.

Then

$$E_i=\tfrac{1}{2}\int_{-\infty}^{+\infty}F_i(x)\,dx, \tag{41}$$

$$\alpha_i=\exp[2G_0(\alpha_0)]\int_{-\infty}^{\alpha_0}[2E_i\rho(x)-F_i(x)]\,dx, \tag{42}$$

and

$$g_i(x)=[-1/\rho(x)]\{\alpha_i\exp[-2G_0(x)]-\int_{-\infty}^{x}[2E_i\rho(x')-F_i(x')]\,dx'\}. \tag{43}$$

We have thus expressed all interesting physical quantities in perturbation theory in quadrature forms. The sums over intermediate states or the Green's function are completely eliminated. The extension of the present technique to higher excited states is straightforward.

A simple example.—We now illustrate our technique by a simple example. Consider a perturbation V_1 given by

$$V_1=[\rho_1\delta(x-x_2)-\rho_2\delta(x-x_1)]/(\rho_1\rho_2), \tag{44}$$

where $\rho_1=\psi_0^2(x_1)$ and $\rho_2=\psi_0^2(x_2)$. This has a zero first-order shift for the ground state. According to Eq. (18),

$$g_1(x)=[2/\rho(x)]\ \text{for}\ x_1<x<x_2,$$
$$=0\ \text{otherwise}. \tag{45}$$

Hence according to Eq. (23) the second-order energy shift is given by

$$E_2 = -\int_{x_1}^{x_2} [2/\rho(x)]\, dx\,. \tag{46}$$

On comparing this with the second-order energy shift as calculated in the Rayleigh-Schrödinger theory we obtain the following sum rule:

$$\left[\frac{1}{\psi_0(x_1)\psi_0(x_2)}\right]^2 \sum_n \frac{[\psi_0(x_1)\psi_n(x_2) - \psi_n(x_2)\psi_n(x_1)]^2}{E_n - E_0} = \int_{x_1}^{x_2} \frac{2dx}{[\psi_0(x)]^2}\,. \tag{47}$$

We see that in Eq. (46), the magnitude of the second-order shift is large if the probability density in between x_1 and x_2 is small. We give a physical interpretation to this result in the following particular example. Consider a Hamiltonian whose unperturbed potential is given by

$$V_0 = (x - x_1)^2 (x - x_2)^2. \tag{48}$$

The height of the barrier between the two valleys is equal to $[(x_1 - x_2)/2]^4$. The higher this barrier is, the smaller the wave function in between x_1 and x_2 is. In the limit that this barrier becomes infinite, the system will decouple into two separate oscillators centered around x_1 and x_2, with identical energy levels. A finite but high barrier means that almost degenerate energy levels with the same or opposite parity exist. The perturbation as given by Eq. (44) breaks the symmetry. This parity-nonconserving perturbation connects these almost degenerate states, thereby leading to a large energy shift.

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[1]See, for example, G. Baym, *Lectures on Quantum Mechanics* (Benjamin, New York, 1969).

[2]The fact the second-order energy shift can be obtained without the use of Green's functions or sums over intermediate states have been emphasized previously by Sternheimer, Dalgarno and Lewis, and Dalgarno and Stewart [R. Sternheimer, Phys. Rev. 84, 244 (1951); A. Dalgarno and J. T. Lewis, Proc. Roy. Soc. London 233, 70 (1955); A. Dalgarno and A. L. Stewart, Proc. Roy. Soc. London 238, 269 (1969)]. However, none of these authors expressed their solutions in quadrature forms as we have done here. Instead, their methods involve the solutions of inhomogenous differential equations. Our present work also goes beyond the works of these authors in our discussion on the higher-order corrections.

Constraints on Weak-Current Angles of the Six-Quark Model from the K^0-$\bar{K}^0$ System

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From calculations of the K_L-K_S mass difference and CP nonconservation based on an effective quark Lagrangian, we limit the ranges of the charged-weak-current mixing angles θ_2 and θ_3, and phase parameter δ. The relative strength of $b \to u$ and $b \to c$ couplings is determined versus θ_3.

In the sequential six-quark $SU(2)_L \otimes U(1)$ model, the left-handed $(t, b')_L$ is added to the doublets $(u, d')_L$, $(c, s')_L$ of the standard model.[1,2] The 3×3 unitary matrix U which relates the gauge-group eigenstates $(d', s', b')_L$ to the mass eigenstates (d, s, b) contains three rotation angles θ_i and a CP-nonconserving phase δ. In the form introduced by Kobayashi-Maskawa,[3] the matrix U can be written

$$U = \begin{pmatrix} c_1 & s_1 c_3 & s_1 s_3 \\ -s_1 c_2 & c_1 c_2 c_3 + s_2 s_3 e^{i\delta} & c_1 c_2 s_3 - s_2 c_3 e^{i\delta} \\ -s_1 s_2 & c_1 s_2 c_3 - c_2 s_3 e^{i\delta} & c_1 s_2 s_3 + c_2 c_3 e^{i\delta} \end{pmatrix}, \tag{1}$$

where $c_i = \cos\theta_i$ and $s_i = \sin\theta_i$. By suitable choices

