Convergence of the first-order logarithmic perturbation iteration method

C. K. Au
Physics Department, University of South Carolina, Columbia, South Carolina 29208
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The ground-state wave function for a system with nonsingular potentials is free from zero except at the boundaries and hence its logarithm is regular. We show that the first-order perturbation iteration method, when applied to the logarithm of the wave function in ground-state problems, provides a systematic method in arriving at improved trial wave functions resulting in a decreasing sequence for the variational energy. In situations where the ground state truly exists, this sequence is bounded from below by the true energy and hence the decreasing sequence would converge to the true energy with the corresponding trial wave function (the logarithm of which is regular) converging to the correct wave function.

Logarithmic perturbation theory was introduced many years ago[1] and has since been rediscovered or discussed by a number of authors.[2–10] In problems reducible to one dimension, it is well known that successive perturbation corrections are obtainable in quadrature in a hierarchical form.[2,4] When the first-order logarithmic perturbation method is used iteratively, it has been shown to lead to accelerated convergence.[11] Henceforth, we shall denote the "first-order logarithmic-perturbation-iteration method" as FOLPIM. What has not been widely publicized is that FOLPIM is a *convergent* perturbative-variational method for problems where a normalizable ground state exists. Even though we have utilized this property in our previous treatment of the one-dimensional anharmonic oscillator,[12] we had neither stated nor proved this theorem explicitly. The purpose of the present Brief Report is to provide a simple proof of this theorem for the multidimensional case.[13]

Let us consider a unit-mass Schrödinger particle in a N-dimensional system acted on by a local potential $V(\mathbf{x})$. The Schrödinger equation in this case is

$$[-\tfrac{1}{2}\nabla^2+V(\mathbf{x})]\psi=E\psi\ , \tag{1}$$

where E and ψ are the eigenvalue and the eigenfunction, respectively, $\nabla^2=\nabla\cdot\nabla$, and ∇ is the N-dimensional gradient operator. For a normalizable ground state, the wave function does not have any zero except at the boundary and so its logarithm is regular. We define

$$G\equiv-\ln\psi\ . \tag{2}$$

In terms of G, the Schrödinger equation (1) becomes

$$\nabla G\cdot\nabla G-(\nabla^2 G)=2(V-E)\ . \tag{3}$$

This is a nonlinear eigenvalue equation in the Ricatti form. To restrict ourselves to ground-state solutions, G has to be regular except at the boundaries. Let G_0^0 be a regular function that satisfies the equation

$$\nabla G_0^0\cdot\nabla G_0^0-\nabla^2 G_0^0=2(V_0^0-E_0^0)\ , \tag{4}$$

such that E_0^0 is a constant that minimizes the difference

$$V_1^0\equiv V-V_0^0\ . \tag{5}$$

It is to be emphasized that one can merely invent the regular function G_0^0, set E_0^0 to be equal to zero and then solve for V_0^0 algebraically according to Eq. (4). Normally, in perturbative problems, there exists a solution ψ_0 to the Schrödinger equation (1) for a certain potential V_0 with eigenvalue E_0. For this case, one may choose $G_0^0=-\ln\psi_0$ and $E_0^0=E_0$. Then automatically $V_0^0=V_0$ according to Eqs. (1) and (3). But such a choice is neither necessary nor always desirable. Quite often it is more convenient to choose a G_0^0 that corresponds to a V_0^0 that in turn approaches V in the asymptotic region. Let us denote the kinetic energy of the particle by K and so the original Hamiltonian is

$$H\equiv K+V\ . \tag{6}$$

The wave function corresponding to G_0^0 is $\psi_0^0\equiv\exp(-G_0^0)$. Furthermore, we shall assume that the difference potential V_1^0 defined by Eq. (5) is of order λ. There is an added advantage if λ is less than unity but this is *not* a necessary requirement for the convergence of this procedure. It is then trivial to verify that E_0^0 is the expectation value of

$$H_0^0\equiv K+V_0^0\ , \tag{7}$$

for the state ψ_0^0 by using Eqs. (1) and (4)

$$E_0^0=\langle\psi_0^0\,|\,H_0^0\,|\,\psi_0^0\rangle\ . \tag{8}$$

Next we define the following:

$$E_1^0\equiv\langle\psi_0^0\,|\,V_1^0\,|\,\psi_0^0\rangle\ . \tag{9}$$

Bearing in mind that G_0^0, V_1^0, and E_1^0 are either defined or known, we next seek the regular solution G_1^0 to the following inhomogeneous linear differential equation:

$$2\nabla G_1^0\cdot\nabla G_0^0-\nabla^2 G_1^0=2(V_1^0-E_1^0)\ . \tag{10}$$

This can be regarded as a first-order differential equation in the vector function ∇G_1^0 and hence in one-dimensional systems can be solved in quadrature. We shall assume

that it is possible to solve for G_1^0 given G_0^0, V_1^0, and E_1^0 in Eq. (10). Furthermore, if V_1^0 is of order λ, then E_1^0 is also of order λ according to Eq. (9) and hence G_1^0 is necessarily of order λ. We now begin our iteration routine and define

$$G_0^{\mathrm{I}} \equiv G_0^0 + G_1^0 \equiv -\ln\psi_0^{\mathrm{I}} \tag{11}$$

and

$$E_0^{\mathrm{I}} \equiv E_0^0 + E_1^0 \ . \tag{12}$$

From Eqs. (5)—(9), it is easy to see that

$$E_0^{\mathrm{I}} = \langle \psi_0^0 \mid H \mid \psi_0^0 \rangle \ , \tag{13}$$

and hence is the variational energy of the system corresponding to the trial wave function ψ_0^0 and by the well-known theorem on variational calculations, it is bounded from below by the true energy E_{true}

$$E_0^{\mathrm{I}} \geq E_{\mathrm{true}} \ . \tag{14}$$

Knowing G_0^{I} and E_0^{I}, we define a function V_0^{I} by

$$\nabla G_0^{\mathrm{I}} \cdot \nabla G_0^{\mathrm{I}} - \nabla^2 G_0^{\mathrm{I}} \equiv 2(V_0^{\mathrm{I}} - E_0^{\mathrm{I}}) \ . \tag{15}$$

Physically, V_0^{I} is a potential for the Hamiltonian

$$H_0^{\mathrm{I}} \equiv K + V_0^{\mathrm{I}} \ , \tag{16}$$

that admits ψ_0^{I} as its eigenfunction with eigenvalue E_0^{I}. Then the effective perturbation after the first iteration is

$$V_1^{\mathrm{I}} \equiv V - V_0^{\mathrm{I}} = V_0^0 + V_1^0 - V_0^1 \ . \tag{17}$$

It is straightforward to show, using Eqs. (4), (10), and (15), that

$$V_1^{\mathrm{I}} = -\tfrac{1}{2} \nabla G_1^0 \cdot \nabla G_1^0 \ , \tag{18}$$

and since G_1^0 is of order λ, V_1^{I} is of order λ^2. More importantly, we notice that V_1^{I} is negative definite. Hence, irrespective of the nature of the initial perturbation V_1^0 (of order λ), we have succeeded in transforming the problem into one with a negative definite perturbation and of order λ^2. We next define

$$E_1^{\mathrm{I}} \equiv \langle \psi_0^{\mathrm{I}} \mid V_1^{\mathrm{I}} \mid \psi_0^{\mathrm{I}} \rangle \ , \tag{19}$$

which is the first iterated analog of Eq. (9), and then seek the regular solution G_1^{I} to the first iterated analog of Eq. (10):

$$2\nabla G_1^{\mathrm{I}} \cdot \nabla G_0^{\mathrm{I}} - \nabla^2 G_1^{\mathrm{I}} = 2(V_1^{\mathrm{I}} - E_1^{\mathrm{I}}) \ , \tag{20}$$

bearing in mind that G_0^{I}, V_1^{I}, and E_1^{I} have all been defined or known. Having obtained G_1^{I}, we can define the analogs of Eqs. (11) and (12) to be used in the second iteration step

$$G_0^{\mathrm{II}} \equiv G_0^{\mathrm{I}} + G_1^{\mathrm{I}} \equiv -\ln\psi_0^{\mathrm{II}} \tag{21}$$

and

$$E_0^{\mathrm{II}} \equiv E_0^{\mathrm{I}} + E_1^{\mathrm{I}} \ . \tag{22}$$

Again, it is easy to see that from Eqs. (15)—(19)

$$E_0^{\mathrm{II}} = \langle \psi_0^{\mathrm{I}} \mid H \mid \psi_0^{\mathrm{I}} \rangle \ , \tag{23}$$

and hence is equal to the variational energy corresponding to the trial wave function ψ_0^{I} and is therefore bounded from below by E_{true}. Moreover, because V_1^{I} is negative definite, E_1^{I} is negative definite too and hence

$$E_0^{\mathrm{I}} \geq E_0^{\mathrm{II}} \geq E_{\mathrm{true}} \ . \tag{24}$$

It is now quite evident that the iteration process can continue for having defined G_0^{II} and E_0^{II}, we can define V_0^{II} by

$$\nabla G_0^{\mathrm{II}} \cdot \nabla G_0^{\mathrm{II}} - \nabla^2 G_0^{\mathrm{II}} \equiv 2(V_0^{\mathrm{II}} - E_0^{\mathrm{II}}) \ . \tag{25}$$

In turn, this implies that ψ_0^{II} is an eigenfunction of

$$H_0^{\mathrm{II}} \equiv K + V_0^{\mathrm{II}} \tag{26}$$

with eigenvalue E_0^{II}. The effective perturbation after the second iteration is

$$V_1^{\mathrm{II}} \equiv V - V_0^{\mathrm{II}} = V_0^{\mathrm{I}} + V_1^{\mathrm{I}} - V_0^{\mathrm{II}} \ , \tag{27}$$

and using Eqs. (20), (25), and (15), we can show that

$$V_1^{\mathrm{II}} = -\tfrac{1}{2} \nabla G_1^{\mathrm{I}} \cdot \nabla G_1^{\mathrm{I}} \ , \tag{28}$$

and since G_1^{I} is of order λ^2, V_1^{II} is of order λ^4. It is now possible to generalize our procedure. At the end of the Kth iteration, one obtains the effective perturbation

$$V_1^K = -\tfrac{1}{2} \nabla G_1^{K-1} \cdot \nabla G_1^{K-1} \ , \tag{29}$$

which is of order λ^{2^K}. From this, one calculates

$$E_1^K = \langle \psi_0^K \mid V_1^K \mid \psi_0^K \rangle \leq 0 \ , \tag{30}$$

where

$$-\ln\psi_0^K \equiv G_0^K \equiv G_0^{K-1} + G_1^{K-1} \ , \tag{31}$$

is known from the previous iteration. One then solves an inhomogeneous differential equation for the regular solution G_1^K

$$2\nabla G_1^K \cdot \nabla G_0^K - \nabla^2 G_1^K = 2(V_1^K - E_1^K) \ . \tag{32}$$

Having obtained G_1^K one defines

$$-\ln\psi_0^{K+1} \equiv G_0^{K+1} \equiv G_0^K + G_1^K \ , \tag{33}$$

and

$$E_0^{K+1} \equiv E_0^K + E_1^K = \langle \psi_0^K \mid H \mid \psi_0^K \rangle \ . \tag{34}$$

The corresponding effective potential V_0^{K+1} at the $(K+1)$th iteration to the wave function ψ_0^{K+1} is defined by the algebraic equation

$$\nabla G_0^{K+1} \cdot \nabla G_0^{K+1} - \nabla^2 G_0^{K+1} \equiv 2(V_0^{K+1} - E_0^{K+1}) \ . \tag{35}$$

The effective perturbation at this stage is given by

$$V_1^{K+1} \equiv V - V_0^{K+1} \ , \tag{36}$$

which can be shown to be equal to

$$V_1^{K+1} = -\tfrac{1}{2} \nabla G_1^K \cdot \nabla G_1^K \ . \tag{37}$$

Because of the negative definiteness of E_1^K we have

$$E_0^{K+1} \leq E_0^K \ . \tag{38}$$

Because of the variational native of E_0^{K+1}, we have

$$E_0^{K+1} \geq E_{\text{true}} \ . \tag{39}$$

On combining Eqs. (38) and (39), we have

$$E_0^{\text{I}} \geq \cdots \geq E_0^K \geq E_0^{K+1} \geq \cdots E_0^{\infty} \geq E_{\text{true}} \ , \tag{40}$$

and thus we see that our procedure leads to a decreasing sequence of upper bounds on the true energy and hence this sequence would approach the true energy in its limit provided this limit is finite, i.e., the ground state truly exists. Bearing in mind that we limit ourselves to regular solutions for G, we see that our sequence of wave functions are free from zeros except at the boundaries, and hence should converge to the correct ground-state wave function. Thus we see that FOLPIM provides a systematic combination of perturbative and variational calculations for the ground-state problem in a local potential. Furthermore, we have never required that the wave function or the eigenvalue (eigenenergy) be expandable as a power series in some coupling constant. Indeed we have previously solved the one dimensional anharmonic oscillator problem with this procedure,[12] where it is well known that both the wave function and its corresponding energy are not analytic in the coupling constant in the anharmonic term.[14] This should be regarded as an added advantage of the present procedure.

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