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VARIATION-ITERATION PRINCIPLE FOR WAVE FUNCTIONS*

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ABSTRACT

A simple variation-iteration principle for the wave function is given that is stationary at every value of the coordinate r . Both analytical and numerical applications are discussed using a popular charmonium potential as an example.

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I. INTRODUCTION

It has been pointed out by Gerjuoy, Rau, and Spruch¹ that variational principles can be derived for a large class of physically interesting functionals "with little exercise in ingenuity". Their work was based on a general observation by Borowitz and Gerjuoy.² The constraints on trial functions are included in this scheme by means of Lagrange multipliers. Stationary functionals of this general form had been derived earlier for application to the Schroedinger equation,^{3,4,5,6,7} and to relativistic Bethe-Salpeter equations⁸ but the generality of the approach had not been realized.

In this short note, we would like to call attention to this general method by considering a specific problem—the construction of a variational principle for the Schroedinger wave function that is stationary at each value of the coordinate, r . Once this problem has been solved, it is then possible to use the resultant wave functions in variational estimates of arbitrary operators; two important such operators are the Hamiltonian and transition (decay) operators. We shall derive a variation-iteration scheme for the wave function and energy which is very suitable for both analytical and numerical evaluation and shall give examples of both. Our primary example is the combination of coulomb and linear potential that has been used to describe the spectrum of charmonium.⁹

First, a variational treatment of a general, first order, nonlinear differential equation will be derived and then applied to the Schroedinger equation. Both bound states and scattering states⁵ will be discussed. Finally, a very brief description of a numerical treatment of ground and excited states for the charmonium potential will be given as an illustration of the simplicity and convergence of the method.¹⁰

II. GENERAL VARIATIONAL PRINCIPLE

We wish to write down a variational solution¹¹ to the first order nonlinear equation

$$\frac{df(r)}{dr} + H(f, r) = 0 \quad (1)$$

for $0 < r < R$, with the boundary condition that $f(R)$ is fixed. We also define

$$h(f, r) \equiv \frac{d}{df} H(f, r) \quad (2)$$

for later use.

Since we wish to write down an expression for $f(r)$ which is stationary at each value of r , the simplest way to proceed is to enforce Eq. (1) by means of a Lagrange multiplier for all points between r and R . Thus consider the functional of a trial function $f_1(r)$:

$$[f] = f_1(r) + \int_r^R dz L_1(z, r) \left[\frac{df_1(z)}{dz} + H(f_1, z) \right] \quad (3)$$

Clearly if f_1 is the exact solution, then $[f] = f(r)$. The conditions that the first order error in $f_1 = f + \delta f$ vanish in Eq. (3) are

$$L_1(z, z) = 1 \quad (4)$$

and

$$\frac{d}{dz} L_1(z, r) = h(f_1(z), z) L_1(z, r) = h_1(z) L_1(z, r) \quad .$$

Thus

$$\ln L_1(z, r) = \int_r^z dw h_1(w) \quad . \quad (5)$$

Equation (3) can be written in several equivalent forms. Since it involves the derivative of the trial function $f_1(z)$, an operation that is not convenient to perform in a numerical analysis, an integration by parts yields the alternative

expression

$$[\bar{f}] = f_1(R) L_1(R, r) + \int_r^R dz L_1(z, r) [H_1 - f_1 h_1] . \quad (6)$$

Since these expressions for $[\bar{f}]$ are stationary at each value of r , they can be directly iterated. Defining the sequence (a similar procedure can be used with Eq. (6))

$$f_{n+1}(r) = f_n(r) + \int_r^R dz L_n(z, r) \left[\frac{df_n(z)}{dz} + H_n \right] , \quad (7)$$

in which L_n is to be computed from Eq. (5) using $f_n(w)$, it is straightforward to see that

$$\frac{df_{n+1}(r)}{dr} = -H_n(r) - h_n(r) (f_{n+1}(r) - f_n(r)) ,$$

and hence

$$\begin{aligned} \frac{df_{n+1}(r)}{dr} + H_{n+1}(r) &= H_{n+1}(r) - H_n(r) - h_n(r) (f_{n+1}(r) - f_n(r)) \\ &= O(f_{n+1} - f_n)^2 . \end{aligned}$$

This illustrates clearly the variational property of Eq. (3) and allows the next iteration of Eq. (7) to be written in the form

$$f_{n+2}(r) = f_{n+1}(r) + \int_r^R dz L_{n+1}(z, r) [H_{n+1} - H_n - h_n(f_{n+1} - f_n)] , \quad (8)$$

which again does not involve derivatives of the functions f_n . It is therefore convenient for numerical analysis.

An important property of Eq. (8) is that after $(f_{n+1} - f_n)$ becomes sufficiently small, depending on the concavity of $H(f)$, the iteration sequence becomes monotonic; the sign of the approach depends upon the second derivative of H with

with respect to f .¹¹ For example, if H is quadratic in f , $H = \lambda f^2 + g(r)$, then

$$\frac{d}{dr} f_{n+1} + H_{n+1} = \lambda (f_{n+1} - f_n)^2$$

which has a definite sign, as does the integral $L_{n+1}(z, r)$. Thus the sequence is monotonic at every stage.

III. SCHROEDINGER EQUATION—BOUND STATES

It is convenient to apply the previous treatment to the second order bound state equation by writing the wave function as

$$\psi(r) = P(r) \exp\left(-\int_0^r dw f(w)\right), \quad (9)$$

and hence

$$\psi'/\psi = P'/P - f(r) \quad .$$

The polynomial $P(r)$ contains the zeroes of the wave function at finite r and its behavior at the origin, $r^{\ell+1}$. The Schrodinger equation takes the form

$$\frac{df}{dr} - f^2 + 2f \frac{P'}{P} + \left(V(r) - \frac{P''}{P}\right) - E = 0 \quad , \quad (10)$$

where $V(r)$ is the effective potential, including the centripetal term. Now

$$h(f, r) = -2f(r) + 2P'/P$$

and hence

$$L(z, r) = \frac{P^2(z)}{P^2(r)} e^{-2\int_r^z dw f(w)} \equiv \frac{P^2(z)}{P^2(r)} \ell(z, r) \quad . \quad (11)$$

The variational expression for f is (using Eq. (6))

$$[f] = f(R) L(R, r) + \int_r^R dz L(z, r) \left[f^2(z) + V(z) - \frac{P''}{P} - E \right] \quad . \quad (12)$$

It is convenient to choose $R=\infty$ for formal arguments (but not for numerical analysis since the upper limit must of necessity be finite). The iteration procedure

discussed earlier then becomes

$$f_{n+1}(r) = \frac{1}{P_n^2(r)} \int_r^\infty dz \ell_n(z, r) P_n^2(z) \left[f_n^2 + V(z) - \frac{P_n''}{P_n} - E \right]. \quad (13)$$

Since $f_{n+1}(r)$ is finite, in particular at the zeroes of $P_n(r)$, their values are determined by the requirement that the integral over z vanishes at these points. Since the integrand also vanishes automatically because of the explicit factor of $P_n(z)$, these zeroes are of second order, as required. The value of the eigen-energy E is determined by the requirement that the integral be zero at the origin.

There are several ways to proceed at this point. One can fix E , iterate until $f(r)$ converges and then repeat with different E values until the integral vanishes at $r=0$ and $f(0)$ is finite. A more efficient procedure is to choose E at each stage to satisfy the boundary condition at the origin:

$$E_n \equiv \frac{\int_0^\infty dz \ell_n(z, 0) \left[P_n^2(z) \left(V(z) + f_n^2(z) \right) - P_n(z) P_n''(z) \right]}{\int_0^\infty dz \ell_n(z, 0) P_n^2(z)}. \quad (14)$$

This is, of course, just the Rayleigh-Ritz stationary estimate of E using the trial function $\psi_n(r)$ given in terms of $P_n(r)$ and $f_n(r)$. Thus, if f_1 is in error of order ϵ , then f_n is in error of order ϵ to the power 2^{n-1} , and the error in E_n is of order ϵ to the power 2^n ; clearly if ϵ is small, the convergence can be quite rapid. Explicit numerical examples of this procedure will be given in a later section.

Finally note that if $V(r)$ grows as $r \rightarrow \infty$, $f(r) \sim \sqrt{V(r)}$ for large r and this can be used in Eq. (12) as the boundary condition on $f(R)$. This boundary condition can be used to improve the accuracy of numerical treatments of the

equation (with a finite upper limit R) since one does not require the wave function to vanish at this finite point.

IV. CHARMONIUM EXAMPLE

We will now give an analytical treatment of the ground state in the coulomb plus linear potential used to describe the bound states of charmonium⁹:

$$V = -\frac{\alpha}{r} + ar \quad . \quad (15)$$

For a trial function f_1 , we will choose a constant $f_1 = \alpha_1/2$, and $P(r)=r$. This corresponds to an simple exponential trial wave function and is the exact solution to the potential $V_1 = -\alpha_1/r$.

The stationary principle for f then treats the difference $V-V_1$ as a perturbation and corrects $f(r)$ to first order in this difference. Using Eqs. (13) and (14), one finds

$$f_2(r) = \frac{1}{2}r + \frac{ar}{\alpha_1} \quad (16)$$

and

$$E_1 = \frac{1}{4} \alpha_1 (\alpha_1 - 2a) + \frac{3a}{\alpha_1} \quad . \quad (17)$$

Any value of α_1 can be used in the above formula, but to make the perturbation ($V-V_1$) as small as possible, it may be convenient to choose the optimum α_1 in the Rayleigh-Ritz sense, i.e., $dE/d\alpha_1 = 0$. In this case, α , is the solution to the equation

$$\alpha_1^2 (\alpha_1 - a) = 6a \quad . \quad (18)$$

Now $f_2(r)$ is completely determined and

$$\psi_2(r) = rN_2 \exp \left[-\frac{1}{2}\alpha r - \frac{a}{2\alpha_1} r^2 \right] \quad (19)$$

is the first order corrected wave function. This wave function can now be used to compute matrix elements involving the ground state. These will have the

same accuracy as the Rayleigh-Ritz value of the energy E_1 given by Eq. (17). For example, in the estimation of certain decay rates, the value of the wave function at the origin is of interest. One easily finds to first order

$$|N_2|^2 = |N_1|^2 \left[1 + \frac{3}{\alpha_1} \left(\alpha_1 - \alpha - \frac{4a}{\alpha_1^2} \right) \right]^{-1},$$

where $|N_1|^2 = \alpha_1^3/2$. A similar analysis can be carried out for excited states of interest. A numerical test of this approach for interesting values of α and a will be given later.

Finally, note that the improvement in f is directly related to the $F(r)$ function introduced by Dalgarno and Lewis³ and Schwartz⁴:

$$f_2(r) - f_1(r) = \frac{dF(r)}{dr}.$$

The function $F(r)$ is the ratio of the first order correction to the wave function to its zero order value.

V. PHASE SHIFTS

In this section we shall apply the Lagrange multiplier method to derive a variational principle for the phase shift given first by Calogero.⁵ The wave function is written as

$$\psi(r) = A(r) \sin B(r), \quad (20)$$

where $B(0) = 0$ and the phase shift δ is then given by

$$B(r) \sim kr + \delta$$

as $r \rightarrow \infty$. If the relation between A and B is fixed by demanding that $\psi' = kA \cos B$, then the Schrödinger equation is equivalent to the first order equations

$$\frac{dB(r)}{dr} = k - \frac{V(r)}{k} \sin^2 B(r) \quad (21)$$

and

$$\frac{dA}{dr} / A(r) = \frac{V}{2k} \sin 2B(r) \quad (22)$$

The variational expression for $B(r)$ is written in the canonical form (3) with $f=B$ and

$$H(B, r) = -k + \frac{V(r)}{k} \sin^2 B$$

$$h(B, r) = \frac{V(r)}{k} \sin 2B$$

The equation satisfied by $L(z, r)$ is then

$$\frac{dL(z, r)}{dz} = \frac{V(z)}{k} \sin 2B(z) \cdot L(z, r)$$

which can be directly integrated. A comparison with Eq. (22) shows that

$$L(z, r) = A^2(z)/A^2(r) \quad .$$

The variational principle is completely determined and is equal to that given by Calogero.

VI. NUMERICAL EXAMPLES

A. There are two exactly solvable examples that can be used as illustrations for this variational analysis, the coulomb potential and the simple harmonic oscillator. In the former case, one has $V = -\alpha/r$, and $f(r) = \alpha/2 = \text{constant}$. Since V vanishes at large r , $E = -f^2(\infty) = -\alpha^2/4$. Choosing $\alpha = 2$ and the initial trial function to be $f_1(r) = r$, a rather poor choice, we find that after 3 iterations, the energy and the function $f(r)$ have converged to within 0.1% of the exact values.

The second solvable example is the harmonic oscillator with $V = c^2 r^2$, $f(r) = cr$, and $C = 3c$. Choosing $c = .312$ and the initial trial function to be $f_1(r) = 1$, again a poor choice, the energy and the function $f(r)$ converged to better than 0.01% of the exact values after 3 iterations.

B. A more interesting case is that of the charmonium potential, Eq. (15), with $\alpha = 0.32$ and $a = 0.363$ that are typical of the values that have been used in

physical applications.⁹ The final ground state energy for these values is 0.989. Starting with the choice discussed in Section IV, $f_1(r) = \alpha_1/2$, where $\alpha_1 = 1.412$ as determined from Eq. (18), the iterations converge to 0.1% for E and f(r) in four iterations. If one starts with the harmonic oscillator choice $f_1(r) = cr$, with the Rayleigh-Ritz choice $c = 0.312$, the sequence converges to the same accuracy in three iterations.

The energy given by Eq. (17) is $\sim 5\%$ high, and thus the trial wave function given by f_1 is in error by roughly $\sqrt{.05} = 23\%$. The error in the function $f_2(r)$ given by (19) is then estimated to be $\sim 5\%$ both from the above energy estimate and our direct numerical iterations. One also finds that the value of the wave function at the origin is changed by $N_2^2/N_1^2 \cong 0.88$, which is consistent with the above estimates. As one would expect, the simple harmonic oscillator choice is more accurate, the simple gaussian choice being in error by only $\sim 10\%$.

C. The excited states for the charmonium potential are also easy to discuss. The lowest P-state has no radial nodes and can be treated by choosing $P=r^2$. We have tested two choices for the trial function, $f_1(r) = cr$ with $c = 0.312$ as before, and also the choice $f_1(r) = c\sqrt{r}$. The final energy turns out to be $1.59 \pm .01$ after 3 iterations for both choices.

The first excited S-state has one radial node, at d say, so some discussion on the procedure for determining its position is in order. Rewriting Eq. (13) in the form

$$P_n^2(r) f_{n+1}(r) = I_n(r, d) \ell_n(0, r) \quad ,$$

and

$$\begin{aligned} I_n(r, d) &= \int_r^\infty dz \ell_n(z, 0) P_n^2(z) \left[f_n^2(z) + V(z) - \frac{P''}{P} - E_n \right] \\ &\equiv \sum_0^2 d^i J_i(r) - E_n \sum_0^2 d^i K_i(r) \quad . \end{aligned}$$

The J_i and K_i are simple integrals over $\ell_n(z, 0)$ that do not involve the unknown parameter d . The energy E_n is, of course, given by

$$E_n = \sum d^i J_i(0) / \sum d^i K_i(0) \quad .$$

It is a simple matter to form the function $I_n(r, r)$ and to search for its (double) zero. This zero is defined to be at $r=d$. Now that d is known, the function $I_n(r, d)$ can be formed and finally, $f_{n+1}(r)$ can be computed.

For the charmonium example, we found that for $f_1(r) = c\sqrt{r}$, $c=0.312$, the sequence converged after three iterations and the values achieved were $d=2.29$, and $E=1.94$.

VII. CONCLUSION

A simple variational principle for the wave function is given that is stationary for each value of the coordinate r . It is suitable to both analytic and numerical evaluation and improvement of approximate wave functions, energies, and arbitrary matrix elements.

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