

Solving the Schrödinger equation with use of $1/N$ perturbation theory

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The large N expansion provides a powerful new tool for solving the Schrödinger equation. In this paper, we present simple recursion formulas which facilitate the calculation. We do some numerical calculations which illustrate the speed and accuracy of the technique

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I. INTRODUCTION

The large N expansion provides an approximation to the low-lying spectrum and the corresponding wave functions of a quantum-mechanical system. The approximation is based on a solution of the classical equations of motion, about which a perturbation series is developed. In solid-state physics, such expansions are well known¹⁻⁴ as the "semiclassical theory of spin systems," where the expansion is formally an expansion in $1/s$, s being the spin. The generalization of those ideas to include coordinate space problems has come only recently,⁴⁻¹⁰ having been inspired by interest in similar expansions being developed for quantum field theory.⁵⁻⁷

Large N expansions are not expansions in a coupling constant (hence they are often called "nonperturbative"); rather, each coefficient in the expansion is a function of the coupling constants. Thus even the leading orders of the expansion may exhibit qualitative features of the problem that are not readily evident in coupling-constant perturbation theory. Another advantage of the large N method is that it does not depend on the Hamiltonian's being the sum of two terms, one solvable and the other relatively small. Furthermore, the calculation can be done using a simple algebraic recursion method. It is best for low-lying states, hence complementary to the WKB method.

Numerical work provides concrete evidence of the promise of large N expansions. For instance, in Ref. 11, the method was applied to the axially symmetric problem of a hydrogen atom in a uniform magnetic field; with the use of only a few terms, good results were obtained for the ground-state energy (for each subspace of fixed azimuthal angular momentum) even for strong fields where the perturbation series in e^2 diverges badly.¹²⁻¹⁴ A recursion relation derived in Ref. 11 greatly facilitated the calculation. In this paper, we show how that recursion method can be extended to allow treatment of the excited states and the calculation of the wave function.

For the sake of simplicity, we will explicitly treat the problem of a single particle in a spherically symmetric potential. The generalization to more complicated problems is discussed at the end of Sec. III. In Sec. II, we introduce and discuss the technique. The calculation is reduced to quadra-

tures. In Sec. III, we derive algebraic recursion relations (presented in detail in the Appendix) that are useful for rapidly computing the large N series for the spectrum and nodes. In Sec. IV, we examine the utility of the method in the context of a few simple problems. We obtain energies and nodes, typically correct to at least several significant figures. The calculations were performed on a VAX-11/780, essentially instantaneously. Alternatively, results accurate to within a few percent can quickly be obtained by hand.

II. LARGE N EXPANSION

We suppose that we wish to solve a given spherically symmetric Schrödinger equation with potential $V(r)$. Although we may have a specific dimensionality and angular momentum in mind, we consider the more general problem where those quantities are arbitrary.

After separating variables, we obtain the radial equation (we choose units such that $\hbar = m = 1$)

$$\left\{ -\frac{1}{2} \left(\frac{d^2}{dr^2} + \frac{N-1}{r} \frac{d}{dr} \right) + \frac{l(l+N-2)}{2r^2} + \hat{V}(r) \right\} \phi(r) = E\phi(r), \quad (2.1)$$

where $\hat{V}(r)$ is an N -dimensional potential to be defined shortly. Equation (2.1) is brought to the form of a Schrödinger equation on the half-line by setting

$$\psi(r) = r^{N-1/2} \phi(r). \quad (2.2)$$

Then ψ satisfies

$$-\frac{1}{2} \frac{d^2\psi}{dr^2} + k^2 \left[\frac{(1-1/k)(1-3/k)}{8r^2} + V(r) \right] \psi = E\psi, \quad (2.3)$$

where

$$k \equiv N + 2l, \quad (2.4)$$

and we have chosen

$$\hat{V}(r) \equiv k^2 V(r). \quad (2.5)$$

This may differ from the true potential for the number of spatial dimensions (and angular momentum) of interest, but only by a constant factor which can be absorbed in the definition of the coupling constants and reinstated at the end of the calculation. We may now develop an expansion in inverse powers of k .

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Due to definition (2.5), in the large k limit, the eigenfunctions ψ in Eq. (2.3) peak about the minimum r_0 of the effective potential $\frac{1}{8}r^{-2} + V(r)$, and the entire eigenvalue spectrum concentrates around the value¹³

$$E^{(-2)} \equiv 1/8r_0^2 + V(r_0). \quad (2.6)$$

$k^2 E^{(-2)}$ is the energy of a classical particle with angular momentum $L_{cl} = \frac{1}{2}k = l + \frac{1}{2}N$ executing circular motion in the potential $\hat{V}(r)$, and forms our “zeroth”-order approximation to the quantum eigenvalue spectrum. For finite k , the greater the radial quantum number (= the number of finite radial nodes), the greater the deviation of the wave function from r_0 , and of the quantum energy from $k^2 E^{(-2)}$. Hence our approximation is best for the low-lying states, in contrast to the WKB method.¹⁵

For the ground state, the perturbation series in powers of k^{-1} is computed as follows. Since the wave function is nodeless, we may define

$$\psi(r) \equiv e^{\mathcal{Q}(x)}, \quad (2.7)$$

where

$$x \equiv r - r_0. \quad (2.8)$$

It is also convenient to define

$$V_{\text{eff}}(x) \equiv \frac{1}{8}r(x)^{-2} + V(r(x)) - E^{(-2)}, \quad (2.9)$$

which differs from the above-mentioned effective potential only by a constant term, chosen so that the minimum of $V_{\text{eff}}(x)$ is zero. Using Eq. (2.3), we now find

$$\begin{aligned} -\frac{1}{2}(\mathcal{Q}''(x) + \mathcal{Q}'(x)\mathcal{Q}'(x)) + k^2 V_{\text{eff}}(x) \\ + (-\frac{1}{2}k + \frac{3}{8})r(x)^{-2} = \mathcal{E}, \\ \mathcal{E} = E - E^{(-2)}k^2, \quad \mathcal{Q}'(x) \equiv \frac{d\mathcal{Q}(x)}{dx}. \end{aligned} \quad (2.10)$$

The recursive solution is obtained by expanding the energy and wave function,

$$\mathcal{E} = \sum_{n=-1}^{\infty} E^{(n)}k^{-n}, \quad \mathcal{Q}'(x) \equiv \sum_{n=-1}^{\infty} u^{(n)}(x)k^{-n}, \quad (2.11)$$

and collecting terms of like order in k . Thus we obtain

$$u^{(-1)}(x) = -\sqrt{2V_{\text{eff}}(x)}, \quad (2.12a)$$

$$\sqrt{2V_{\text{eff}}(x)}u^{(0)}(x) = E^{(-1)} + \frac{1}{2}r(x)^{-2} + \frac{1}{2}u^{(-1)'}(x), \quad (2.12b)$$

$$\begin{aligned} \sqrt{2V_{\text{eff}}(x)}u^{(1)}(x) = E^{(0)} - \frac{3}{8}r(x)^{-2} \\ + \frac{1}{2}(u^{(0)'}(x) + u^{(0)}(x)u^{(0)''}(x)), \end{aligned} \quad (2.12c)$$

and

$$\begin{aligned} \sqrt{2V_{\text{eff}}(x)}u^{(n+1)}(x) = E^{(n)} \\ + \frac{1}{2}\left(u^{(n)'}(x) + \sum_{m=0}^n u^{(m)}(x)u^{(n-m)}(x)\right); \\ n > 0. \end{aligned} \quad (2.12d)$$

We must, at this point, discuss the branch of the square root to be taken in Eqs. (2.12). Since we are interested in the normalizable wave function, the positive branch must be taken (i.e., the square root is defined to be a positive number) in the region $x \geq 0$ (corresponding to $r \geq r_0$). At $x = 0$ ($r = r_0$), the square root vanishes. In the region $-r_0 < x < 0$ ($0 < r < r_0$), we take the negative branch (i.e., the square root is defined to be

a negative number), since in the large k limit ψ peaks about $x = 0$ ($r = r_0$).

Equation (2.12a) gives the leading approximation to the wave function. Because $V_{\text{eff}}(0) = 0$ and $u^{(0)}(0) < \infty$, we find from (2.12b) that

$$E^{(-1)} = -\frac{1}{2}r_0^{-2} - \frac{1}{2}u^{(-1)'}(0). \quad (2.13a)$$

This may be substituted into Eq. (2.12b), which then defines the first-order wave function correction $u^{(0)}(x)$. Similarly, the higher-order energy corrections are given by

$$E^{(0)} = \frac{3}{8}r_0^{-2} - \frac{1}{2}(u^{(0)'}(0) + u^{(0)}(0)u^{(0)''}(0)), \quad (2.13b)$$

$$\begin{aligned} E^{(n)} = -\frac{1}{2}\left(u^{(n)'}(0) + \sum_{m=0}^n u^{(m)}(0)u^{(n-m)''}(0)\right); \\ n > 0. \end{aligned} \quad (2.13c)$$

$E^{(n)}$ is calculated after $u^{(n)}(x)$, but before $u^{(n+1)}(x)$. The (unnormalized) wave function is then given by [recall that $r = r(x)$]

$$\psi(r) = \exp\left[\int_{-1}^x \sum_{n=-1}^{\infty} u^{(n)}(y)k^{-n} dy\right]. \quad (2.14)$$

If one is not interested in the long distance behavior of the wave function, the method described in the next section is considerably more efficient than that here. It is derived by expanding the functions $u^{(n)}(x)$ themselves in a Taylor series.

Before we discuss the excited states, it is useful to treat the simple example of the Coulomb problem $V = -e^2/r$. According to our prescription, what we shall really do is to approximate the solutions to the Schrödinger equation (2.1), where

$$\hat{V}(r) \equiv -k^2 \hat{e}^2/r. \quad (2.15)$$

The solution to the problem of interest is obtained through the identification $e^2 = k^2 \hat{e}^2$. Furthermore, instead of the coordinate r , we introduce the dimensionless coordinate

$$\rho = 4\hat{e}^2 r \quad (2.16)$$

in Eq. (2.3). The number “four” in Eq. (2.16) was chosen because in these units, $r_0 = 1$. The energy is now measured in units of $16\hat{e}^4$. Thus we obtain

$$E^{(-2)} = -\frac{1}{8} \quad (2.17)$$

and

$$V_{\text{eff}}(x) = x^2/8(1+x)^2, \quad x \in [-1, \infty]. \quad (2.18)$$

From Eq. (2.12a) we find that

$$u^{(-1)}(x) = -x/2(1+x), \quad (2.19)$$

and from (2.13a),

$$E^{(-1)} = -\frac{1}{4}. \quad (2.20)$$

Next, Eq. (2.12b) yields

$$u^{(0)}(x) = -\frac{2+x}{2(1+x)}, \quad (2.21)$$

and so on. We have computed

$$\begin{aligned} E_{\text{ground}} &= -\frac{1}{8}k^2\{1 + 2k^{-1} + O(k^{-2})\} \\ &= -2\hat{e}^4 k^2\{1 + 2k^{-1} + O(k^{-2})\}, \end{aligned} \quad (2.22)$$

which upon identification of e^2 with $\hat{e}^2 k^2$, is identified as the

beginning of the expansion of the exact ground-state energy

$$E_{\text{ground}} = -2e^4/(k-1)^2. \quad (2.23)$$

For the wave function, we have found (C and C' are irrelevant constants)

$$\begin{aligned} \psi(r) &= C \exp \left\{ \left[\frac{1}{2} \ln(1+x) - \frac{1}{2}(1+x) \right] k \right. \\ &\quad \left. + \left[-\frac{1}{2} \ln(1+x) - \frac{1}{2}(1+x) \right] + O(k^{-1}) \right\} \\ &= C' r^{k-1/2} \exp \left\{ -2k\hat{e}^2 [r + rk^{-1} + O(k^{-2})] \right\}, \end{aligned} \quad (2.24)$$

the expansion of the exact (unnormalized) ground-state wave function

$$\psi(r) = r^{k-1/2} \exp \left\{ -2e^2/(k-1) \right\} r. \quad (2.25)$$

We now consider the excited states. In order to account for the n nodes of the n th excited state, we alter the ansatz of Eq. (2.7):

$$\psi_n(r) \equiv \left[\prod_{i=1}^n (r - r_i) \right] e^{\mathcal{U}_n(x)}. \quad (2.26)$$

Because as k increases the wave function increasingly concentrates about the point r_0 , we must have

$$r_i = r_0 + a_i^{(1)} k^{-1} + a_i^{(2)} k^{-2} + \dots, \quad (2.27)$$

so that Eq. (2.26) becomes

$$\begin{aligned} \psi_n(r) &= \left[\prod_i (x - A_i) \right] e^{\mathcal{U}_n(x)}, \\ A_i &= a_i^{(1)} k^{-1} + a_i^{(2)} k^{-2} + \dots \end{aligned} \quad (2.28)$$

By substituting Eq. (2.28) in Eq. (2.3), we obtain a revised version of Eq. (2.10) for the excited states, which we again solve order by order in inverse powers of k . [The expansions of \mathcal{E}_n and $\mathcal{U}_n(x)$ take the same form as before.]

To illustrate the procedure, we consider the first excited state

$$\psi_1(r) = (x - A_1) e^{\mathcal{U}_1(x)}. \quad (2.29)$$

The function $\mathcal{U}_1(x)$ satisfies

$$\begin{aligned} -\frac{1}{2} \left[\mathcal{U}_1''(x) + \mathcal{U}_1'(x) \mathcal{U}_1'(x) \right] (x - a) - \mathcal{U}_1'(x) \\ + \left[k^2 V_{\text{eff}}(x) + \left(-\frac{1}{2} k + \frac{3}{8} \right) r(x)^{-2} \right] (x - a) = (x - a) \mathcal{E}_1. \end{aligned} \quad (2.30)$$

Solving this to order k^2 , we again find (the square root is defined as before) the result of Eq. (2.12a):

$$u_1^{(1)}(x) = -\sqrt{2V_{\text{eff}}(x)}. \quad (2.31)$$

This is the leading behavior of the exponent for all states. Examining the order k terms, we find

$$\begin{aligned} x\sqrt{2V_{\text{eff}}(x)} u_1^{(0)}(x) \\ = \left[E_1^{(-1)} + \frac{1}{2} r(x) + \frac{1}{2} u_1^{(-1)'}(x) \right] x + u^{(-1)}(x). \end{aligned} \quad (2.32)$$

The energy coefficient $E^{(-1)}$ is determined by differentiating (2.32) and evaluating the result at $x = 0$:

$$E_1^{(-1)} = -\frac{1}{2} r_0^{-2} - \frac{3}{8} u^{(-1)'}(0). \quad (2.33)$$

The result for the n th excited state is

$$E_n^{(-1)} = -\frac{1}{2} r_0^{-2} - \left(n + \frac{1}{2} \right) u^{(-1)'}(0), \quad (2.34)$$

reflecting the fact that, to this order, the spectrum is har-

monic^{4,8,14} with frequency proportional to $(V_{\text{eff}}''(0))^{1/2}$ [recall that $V_{\text{eff}}(0) = V_{\text{eff}}'(0) = 0$]. The next step is to examine the order k^0 terms in Eq. (2.30). The node coefficient $a_1^{(1)}$ is found by evaluating the equation at $x = 0$, whereas the energy coefficient $E_1^{(0)}$ is again obtained by differentiating the equation once and then evaluating it at $x = 0$. $u^{(1)}(x)$ is then given by an algebraic equation similar to Eq. (2.32), and one may then proceed to order k^{-1} , and so on.

III. ALGEBRAIC RECURSION METHOD

If one is not interested in the long distance behavior of the wave function, then it is useful to expand the functions $u^{(n)}(x)$ in a Taylor series in x . This results in purely algebraic recursion relations for the quantities of interest. Toward that end, it is convenient to rescale coordinates in the radial equation (2.1):

$$r \equiv \sqrt{k} \rho. \quad (3.1)$$

This necessitates a change in the definition of \hat{V} :

$$\hat{V}(r) \equiv k V(r/\sqrt{k}). \quad (3.2)$$

As before, this amounts to a mere rescaling of coupling constants which can easily be undone at the end of the calculation. For instance, if we are interested in the potential

$$V(r) = -(\alpha/r)e^{-\beta r} + \lambda r, \quad (3.3)$$

then we consider

$$\hat{V}(r) = (-k^{3/2} \hat{\alpha}/r) e^{-k^{-1/2} \hat{\beta} r} + k^{1/2} \hat{\lambda} r \quad (3.4)$$

and identify $k^{3/2} \hat{\alpha} = \alpha$, $k^{-1/2} \hat{\beta} = \beta$, and $k^{1/2} \hat{\lambda} = \lambda$ when we are done. Equation (2.3) must now be replaced by

$$-\frac{1}{2} \frac{d^2 \psi}{d\rho^2} + k^2 \left[\frac{(1-1/k)(1-3/k)}{8\rho^2} + V(\rho) \right] \psi = Ek\psi. \quad (3.5)$$

We define

$$x = \sqrt{k}(\rho - \rho_0), \quad (3.6)$$

ρ_0 being the point where the bracketed term in Eq. (3.5) is minimized (in the large k limit). Without loss of generality, we shall set $\rho_0 = 1$. The ensuing calculation parallels that of Sec. II. Note, however, that because of the rescalings (3.1) and (3.2), the intermediate equations will exhibit a different k dependence.

For the ground state, we define $[\rho = \rho(x)]$:

$$\psi(\rho) = e^{\mathcal{U}(x)}, \quad (3.7)$$

which leads to

$$\begin{aligned} -\frac{1}{2} \left[\mathcal{U}''(x) + \mathcal{U}'(x) \mathcal{U}'(x) \right] + k V_{\text{eff}}(x) \\ + \left(-\frac{1}{2} + \frac{3}{8} k^{-1} \right) \rho(x)^{-2} = \mathcal{E}, \\ \mathcal{E} \equiv E - E^{(-2)} k, \end{aligned} \quad (3.8)$$

where $E^{(-2)}$ is given by (2.6) with r_0 replaced by ρ_0 , and V_{eff} by (2.9), with r replaced by ρ . We now expand \mathcal{E} as in Eq. (A4), and also expand \mathcal{U}' in the double power series:

$$\begin{aligned} \mathcal{U}'(x) = D_1^0 x + [C_0^0 + C_1^0 x^2] y + [D_1^1 x + D_2^1 x^3] y^2 \\ + [C_0^1 + C_1^1 x^2 + C_2^1 x^4] y^3 + \dots, \quad y \equiv k^{-1/2}. \end{aligned} \quad (3.9)$$

The expansion of the potential has the form

$$\begin{aligned} W(x) &\equiv kV_{\text{eff}}(x) + \left[-\frac{1}{2} + \frac{3}{8}k^{-1}\right]\rho(x)^{-2} \\ &= [W_0^0 + W_1^0x^2] + [W_0^1x + W_1^1x^3]y \\ &\quad + \sum_{n=2}^{\infty} [W_0^n x^{n-2} + W_1^n x^n + W_2^n x^{n+2}]y^n. \end{aligned} \quad (3.10)$$

It is because of the rescaling of coordinates that \mathcal{U} and W are polynomials in x , to each order in y . Equation (3.8) can be solved order by order in x and y , beginning with the lowest order in y , but with the highest power of x within a given order of y . The energy appears only in the even orders in y . For instance, to order y^0 we find

$$D_1^0 = -(2W_1^0)^{1/2}, \quad E^{(-1)} = -\frac{1}{2}D_1^0 + W_0^0, \quad (3.11)$$

whereas to order y , we obtain

$$C_1^0 = W_1^1/D_1^0, \quad C_0^0 = -(1/D_1^0)[C_1^0 - W_0^1], \quad (3.12)$$

and so on. In order to treat the excited states, we include factors describing the nodes, as before. For example, we write the wave function for the first excited state as $[\rho = \rho(x)]$:

$$\begin{aligned} \psi_1(\rho) &= (xy - \alpha)e^{\mathcal{U}_1(x)}, \\ \alpha &= \alpha(y) = \alpha_1 k^{-1} + \alpha_2 k^{-2} + \dots \end{aligned} \quad (3.13)$$

Finally, although we have considered problems with spherical symmetry, more complicated problems can also be considered. For the ground state, application of the method to problems lacking spherical symmetry is straightforward. The function $\mathcal{U}(x)$ in Eq. (3.7) is merely replaced by a new function of as many coordinates as are required.

For example, for a problem with axial symmetry, $\mathcal{U}(x)$ becomes $\mathcal{U}(x, z)$ and Eq. (3.8) becomes (subscripts of x and z are used to denote the derivative)

$$-\frac{1}{2}(\mathcal{U}_{xx} + \mathcal{U}_x \mathcal{U}_x + \mathcal{U}_{zz} + \mathcal{U}_z \mathcal{U}_z) + W = \epsilon, \quad (3.14)$$

where W now has the form

$$\begin{aligned} W(x, z) &= [W_{00}^0 + W_{20}^0 x^2 + W_{02}^0 z^2] \\ &\quad + [W_{30}^1 x^3 + W_{21}^1 x^2 z + W_{12}^1 x z^2 \\ &\quad + W_{03}^1 z^3]y + \dots \end{aligned} \quad (3.15)$$

[It may be necessary to rotate coordinates to eliminate a possible $W_{11}^0 xz$ term in Eq. (3.15). If so, that should be done. Such a rotation affects the numerical value of the coefficients W_{ij}^n , but leaves the form of Eq. (3.15) invariant, except that it eliminates the undesired term.] A calculation of the ground-state energies for an axially symmetric problem using this method can be found in Ref. 11.

The excited states require a little further explanation. Let us consider the first excited state, and for concreteness again consider a potential with axial symmetry. To leading order in y , the Schrödinger equation (3.5) becomes

$$\begin{aligned} -\frac{1}{2} \frac{d^2 \psi}{dx^2} - \frac{1}{2} \frac{d^2 \psi}{dz^2} \\ + k(W_{20}^0 x^2 + W_{02}^0 z^2 + W_{00}^0) + O(k^{-1/2}) = \epsilon k. \end{aligned} \quad (3.16)$$

This equation is separable; in particular, it is the equation for uncoupled harmonic oscillators: just two copies of what we obtain in the spherically symmetric case. To leading order, we determine the position of the node as before, considering separately the case of excitation in the x and z directions. In higher orders there is mixing between the directions. That is, the expansion for the node, which to leading order corresponds to an excitation in the x direction, also depends on z . To be precise, Eq. (3.13) is replaced by

$$\psi_1^{(x)}(x, z) = \left\{ xy - \sum_{n=1}^{\infty} \sum_{m=0}^n y^{2n} (f_{nm} z^{2m} + y g_{nm} z^{2m+1}) \right\} e^{\mathcal{U}(x, z)}, \quad (3.17)$$

and an analogous expression for the other state, with x and z changing roles. In Eq. (3.17), y is given by¹¹

$$y = (N - 1 + 2|m|)^{-1/2}. \quad (3.18)$$

IV. DISCUSSION

We used the formulas given in the Appendix to calculate the energies and nodes of the three lowest-lying states (in each l sector) for several potentials. The results are displayed in Tables I–III. In Table I, we exhibit the energies of the low-lying states for various spherically symmetric potentials. We compare our results with the numerical calculations of Refs. 16 and 17. Tables II and III display the first ten partial sums and the first ten Shanks extrapolated partial sums, for the energies and nodes of the three lowest-lying states of the exactly solvable problem of the linear potential with $N = 3$, $l = 0$.

In computing Table I, we calculated the first 14 partial sums of the series for the energy. For the ground state and first excited state, we then determined the two successive partial sums with the smallest difference and kept as many significant figures as coincided. The results for the second excited state ($n = 2$) were obtained in the same way, except that we used the Shanks extrapolated partial sums.^{11,18}

We obtain values for the nodes to about four decimal places accuracy. That is an indication that the behavior of the wave function near the classical orbit is good. The behavior of the wave function near the origin and at large distances is not apparent from its Taylor expansion, calculated in Sec. III; therefore it should be investigated using the methods of Sec. II.

The difference between the methods of Secs. II and III is that in Sec. III the coordinate is rescaled by a power of the coupling constant ($k^{-1/2}$). This has the effect of reordering the $1/k$ expansion of the wave function, but does not effect the expansion of the energy, which is coordinate-independent. This rescaling is done because it makes the calculation of the energy much easier. It is apparent from Eqs. (2.13) that only certain derivatives of the wave function at the origin ($x = 0$) contribute to a given coefficient in the expansion for the energy. When the method of Sec. III is employed, the only information about the wave function that is calculated at a given order is that relevant to the calculation of the energy to that order. Calculation of the rest is postponed. Although this method therefore makes calculation of the

TABLE I. Energies of the low-lying states for various spherically symmetric potentials ($N = 3$). The numbers in parentheses were calculated in Refs. 16 and 17. $C_1 = 2^{1.7}$, $C_2 = 2^{0.8}$, and $\tau_0 = 2^{-1/2}$.

l	n	$\ln(\tau/\tau_0)$	$C_1 \tau^{-0.2}$	$V(r)$	$C_2 \tau^{-0.8}$
$l = 0$	0	1.044 33 (1.044 3) 1.847 44	- 2.680 3 (- 2.686) - 2.253		- 1.2187 (- 1.218) - 0.462
	1	(1.847 4) 2.289	(- 2.253) - 2.044		(- 0.462) - 0.26
	2	(2.289 7)	(- 2.044)		(- 0.265)
$l = 1$	0	1.641 141 33 (1.643) 2.150 947	- 2.344 946 1 (- 2.345) - 2.100 738		- 0.500 439 (- 0.500) - 0.280 64
	1	(2.151) 2.490 942	(- 2.101) - 1.950 72		(- 0.281) - 0.187 3
	2	(2.491)	(- 1.951)		(- 0.187)
$l = 2$	0	2.013 308 64 (2.015) 2.387 432 8	- 2.156 260 884 (- 2.156) - 1.990 055 5		- 0.294 695 9 (- 0.295) - 0.194 911
	1	(2.388) 2.662 492 0	(- 1.990) - 1.875 032		(- 0.195) - 0.141 979
	2	(2.663)	(- 1.875)		(- 0.142)
$l = 3$	0	2.284 141 353 37 (2.286) 2.579 783 312 93	- 2.029 064 889 5 (- 2.029) - 1.904 866 7		- 0.201 913 656 6 (- 0.202) - 0.146 342 0
	1	(2.581) 2.810 445 386	(- 1.905) - 1.812 502 0		(- 0.146) - 0.112 787
	2	(2.811)	(- 1.812)		(- 0.113)

TABLE II. Spectrum of the linear potential $V = \lambda r$. We treat the three lowest states in the case $N = 3$, $l = 0$, $\lambda = 2^{7/2}$. For each state the left column displays the first ten partial sums, and the one to its right, the first ten Shanks extrapolated partial sums. For the second excited state, we also display a second Shanks extrapolation. The exact energies, E_n , calculated from Ref. 18, are also given.

$n = 0$ $E_0 = 9.352\ 430$	$n = 1$ $E_1 = 16.351\ 80$	$n = 2$ $E_2 = 22.082\ 24$
9.905 78	9.346 29	9.905 78
9.315 95	16.2888	16.2888
9.347 93	16.3558	16.3558
9.353 75	16.3514	16.3514
9.352 91	16.3519	16.3519
9.352 24	16.3517	16.3517
9.352 29	16.3518	16.3518
9.352 48	16.3518	16.3518
9.352 50	16.3518	16.3518
9.352 40	16.3518	16.3518
9.346 29	16.3518	16.3518
9.355 04	16.3518	16.3518
9.353 01	16.3518	16.3518
9.349 64	16.3518	16.3518
9.352 29	16.3518	16.3518
9.352 22	16.3518	16.3518
9.352 50	16.3518	16.3518
9.352 49	16.3518	16.3518
9.352 34	16.3518	16.3518
9.352 39	16.3518	16.3518
21.4760	21.4760	21.4760
22.1774	22.1774	22.1774
22.0523	22.0523	22.0523
22.0953	22.0953	22.0953
22.0754	22.0754	22.0754
22.0863	22.0863	22.0863
22.0796	22.0796	22.0796
22.0841	22.0841	22.0841
22.0809	22.0809	22.0809
22.0832	22.0832	22.0832

TABLE III. Nodes of the wave functions of the first two excited states of the linear potential ($N = 3$, $l = 0$, $\lambda = 2^{7/2}$). α , β , and γ are defined in Eq. (A2). The exact answer was calculated from Ref. 18. The columns on the left display the first ten partial sums; those on the right, the Shanks extrapolated partial sums. The second line of the table displays the exact answers.

α 0.020 183 5	β - 0.013 933 6	γ - 0.268 043
0.023 171	- 0.021 857	- 0.305 77
0.019 537	- 0.010 452	- 0.251 67
0.020 336	- 0.016 033	- 0.278 28
0.020 151	- 0.012 423	- 0.260 46
0.020 189	- 0.015 135	- 0.274 15
0.020 180	- 0.012 920	- 0.262 89
0.020 186	- 0.014 820	- 0.272 52
0.020 183	- 0.013 141	- 0.264 07
0.020 182	- 0.014 654	- 0.271 61
0.020 183	- 0.013 271	- 0.264 79
0.020 029	- 0.014 362	- 0.259 80
0.020 192	- 0.014 199	- 0.269 51
0.020 186	- 0.013 841	- 0.267 61
0.020 183	- 0.013 972	- 0.268 20
0.020 182	- 0.013 916	- 0.267 97
0.020 184	- 0.013 943	- 0.268 08
0.020 184	- 0.013 928	- 0.268 02
0.020 181	- 0.013 937	- 0.268 06
0.020 183	- 0.013 931	- 0.268 03
0.020 180	- 0.013 935	- 0.268 05

energy easier, it has a detrimental effect on the approximation of the wave function, especially far away from the classical minimum ($x = 0$).

We also obtained the eigenvalues of the three lowest-lying states to about four decimal places accuracy when $l = 0$. For $l = 3$, we obtained 6–12 place accuracy. The series, although asymptotic,¹⁹ is, in general, divergent. The sequence of partial sums does not stabilize so well for the more highly excited states. For these states the Shanks transformed sequence is more stable, which allows one to obtain

TABLE IVa. Analytic expressions for the coefficients in the large N expansion of the ground state of the potential $V = e^2 r^{2\nu}$, $e^2 = k^{1-\nu}/(8\nu)$. f is the positive root of $4f^2 - 2 = 2\nu$. The expansion is defined in Eq. (A4).

n	$E_0^{(n)}$
-2	$\frac{1}{8} + \frac{1}{4(4f^2 - 2)}$
-1	$(f-1)/2$
0	$(-4f^6 + 23f^4 - 36f^3 - f^2 + 36f - 18)/(36f^2)$
1	$(16f^{11} - 40f^9 + 81f^7 - 48f^6 - 142f^5 + 276f^4 - 131f^3 - 156f^2 + 216f - 72)/(216f^4)$
2	$(-20288f^{16} + 25392f^{14} + 43200f^{13} - 21036f^{12} - 64800f^{11} + 18121f^{10} + 110700f^9 - 96609f^8 - 164700f^7 + 405687f^6 - 348300f^5 + 45133f^4 + 229500f^3 - 307800f^2 + 194400f - 48600)/(291600f^6)$

TABLE IVb. Analytic expressions for the coefficients in the large N expansion for the energy of the first excited state for power potentials. For the notation, see Table IVa.

n	$E_1^{(n)}$
-2	$\frac{1}{8} + \frac{1}{4(4f^2 - 2)}$
-1	$(3f-1)/2$
0	$(-52f^6 + 227f^4 - 108f^3 - 157f^2 + 108f - 18)/(36f^2)$
1	$(176f^{11} - 632f^9 + 1227f^7 - 208f^6 - 1586f^5 + 908f^4 + 599f^3 - 676f^2 + 216f - 24)/(72f^4)$
2	$(-897728f^{16} + 2572752f^{14} + 1425600f^{13} - 5267316f^{12} - 3693600f^{11} + 8713351f^{10} + 4819500f^9 - 12116379f^8 - 2907900f^7 + 15177297f^6 - 6828300f^5 - 5298377f^4 + 6601500f^3 - 2835000f^2 + 583200f - 48600)/(291600f^6)$

TABLE IVc. Analytic expressions for the coefficients in the large N expansion for the energy of the second excited state for power potentials. For the notation see Table IVa.

n	$E_2^{(n)}$
-2	$\frac{1}{8} + \frac{1}{4(4f^2 - 2)}$
-1	$(5f-1)/2$
0	$(-148f^6 + 635f^4 - 180f^3 - 469f^2 + 180f - 18)/(36f^2)$
1	$(2480f^{11} - 9080f^9 + 17595f^7 - 1776f^6 - 22370f^5 + 7620f^4 + 10295f^3 - 5772f^2 + 1080f - 72)/(216f^4)$
2	$(-6362048f^{16} + 19711632f^{14} + 6696000f^{13} - 42669156f^{12} - 17820000f^{11} + 71965291f^{10} + 22990500f^9 - 94852839f^8 - 12892500f^7 + 105866877f^6 - 30658500f^5 - 45721757f^4 + 30712500f^3 - 7889400f^2 + 972000f - 48600)/(291600f^6)$

more accurate results. Perhaps other summation techniques, which have been successfully applied to divergent coupling-constant perturbation series,²⁰ are also useful here.

The computations were done on a VAX 11/780, using double precision arithmetic. For a given state, the entire calculation (energy, nodes, wave function expansion) took less CPU time than the system clock could measure. We warn the reader, however, that if one is not careful, significant roundoff error can occur as early as the eighth term. Roundoff error became significant in our calculation at about the 15th term. Presumably, it could be further forestalled by working on a larger machine. Another way to avoid roundoff error is to employ a symbolic manipulation program, such as MACSYMA. Comparison of our results with those obtained using MACSYMA confirmed that Tables I–III are not affected by roundoff error. We also used MACSYMA to compute Tables IV–V, which exhibit analytic expressions for the first several coefficients of the $1/N$ expansion for the energy and nodes of the low-lying states of power potentials. The coefficients are given as functions of the power.

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TABLE Va. Analytic expressions for the coefficients in the large N expansion of the node for the first excited state of power potentials. α is defined in Eq. (A2). For the notation see Table IVa.

n	α_n
1	$(-4f^3 + 7f - 3)/(3f^2)$
2	$(16f^8 + 880f^6 - 720f^5 - 1581f^4 + 1620f^3 + 272f^2 - 630f + 135)/(270f^4)$
3	$(21824f^{13} - 87760f^{11} + 8064f^{10} - 148180f^9 + 445536f^8 + 218125f^7 - 908712f^6 + 258796f^5 + 427014f^4 - 234455f^3 - 34272f^2 + 39690f - 5670)/(34020f^6)$

TABLE Vb. Analytic expressions for the coefficients in the large N expansion of the nodes for the second excited state of power potentials. β and γ are defined in Eq. (A2). For the notation see Table IVa.

n	β_n	γ_n
1	$-1/(2f)$	$(28f^3 - 49f + 12)/(6f^2)$
2	$(592f^6 - 1976f^4 + 528f^3 + 1789f^2 - 1032f + 144)/(144f^4)$	$(-128f^8 - 14544f^6 + 6720f^5 + 26328f^4 - 15120f^3 - 7831f^2 + 5880f - 720)/(720f^4)$
3	$(-896f^{11} - 858880f^9 + 421632f^8 + 3057720f^7 - 2159424f^6 - 2967460f^5 + 2947248f^4 + 211021f^3 - 925956f^2 + 291600f - 25920)/(25920f^6)$	$(-4647424f^{13} + 16066688f^{11} - 387072f^{10} + 26367968f^9 - 43884288f^8 - 64789016f^7 + 90611131f^6 + 13777996f^5 - 46487952f^4 + 9025153f^3 + 5920236f^2 - 2222640f + 181440)/(544320f^6)$

Massachusetts Institute of Technology for allowing us the use of MACSYMA to perform algebraic manipulations.

APPENDIX

We present the recursion relations discussed in Sec. III of the paper. We wish to solve the differential equation

$$(-\frac{1}{2}\partial_x^2 + W - \mathcal{E})\psi = 0. \quad (\text{A1})$$

For the first three states we try the ansätze

$$\begin{aligned} \psi_1 &= e^{\mathcal{Q}(x)}, \\ \psi_2 &= (xy - \alpha(y))e^{\mathcal{Q}(x)}, \\ \psi_3 &= (x^2y^2 + xy\gamma(y) + \beta(y))e^{\mathcal{Q}(x)}. \end{aligned} \quad (\text{A2})$$

(Although the \mathcal{Q} 's are not the same for the three states, we do not write an index to distinguish them; no confusion should result.) and

This leads to the following differential equations for the ground state, and first and second excited states, respectively:

$$\begin{aligned} (\mathcal{Q}'^2 + \mathcal{Q}'' - 2W + 2\mathcal{E}) &= 0, \\ (xy - \alpha)(\mathcal{Q}'^2 + \mathcal{Q}'' - 2W + 2\mathcal{E}) + 2y\mathcal{Q}' &= 0, \\ (x^2y^2 + xy\gamma(y) + \beta(y))(\mathcal{Q}'^2 + \mathcal{Q}'' - 2W + 2\mathcal{E}) \\ + 2y^2 + 2(2x^2y + y\gamma(y))\mathcal{Q}' &= 0. \end{aligned} \quad (\text{A3})$$

We expand W , \mathcal{E} , γ , β , α , and \mathcal{Q} in power series as follows:

$$\begin{aligned} \mathcal{E} &= \sum_{n=0}^{\infty} E^{(n-1)} k^{-n}, \\ \alpha &= \sum_{n=1}^{\infty} \alpha_n k^{-n}, \\ \beta &= \sum_{n=1}^{\infty} \beta_n k^{-n}, \end{aligned} \quad (\text{A4})$$

$$\begin{aligned} \gamma &= \sum_{n=1}^{\infty} \gamma_n k^{-n}, \\ W &= E^{(-2)}k + \sum_{n=0}^{\infty} \sum_{m=0}^{n+2} W_{n,m} x^m (\sqrt{k})^{-n}, \\ \mathcal{Q} &= \sum_{n=0}^{\infty} \sum_{m=0}^{n+1} \left\{ \frac{D_m^n}{2m} x^{2m} + \frac{C_m^n k^{-1/2} x^{2m+1}}{2m+1} \right\} k^{-n}, \\ D_0^n &= 0. \end{aligned}$$

The combination $\mathcal{Q}'^2 + \mathcal{Q}'' - 2W + 2\mathcal{E}$ occurs for all states, and it is convenient to expand it in a power series as well:

$$\begin{aligned} \mathcal{Q}'^2 + \mathcal{Q}'' - 2W + 2\mathcal{E} &= \sum_{n=0}^{\infty} \sum_{m=0}^n \{ T^{nm} k^{-n} x^{2m} + S^{nm} k^{-(n+1/2)} x^{2m+1} \}. \end{aligned} \quad (\text{A5})$$

For all three states, the coefficients in \mathcal{Q} and \mathcal{E} are determined from T^{nm} , S^{nm} by the following relations:

$$\begin{aligned}
D^{nm} &= \frac{1}{2D_1^0} \left\{ T^{nm} + 2W_{2n,2m} - (2m+1)D_{m+1}^n \right. \\
&\quad \left. - \sum_{\nu=1}^{n-1} \sum_{\mu} D_{\mu}^{\nu} D_{m+1-\mu}^{n-\nu} - \sum_{\nu=0}^{n-1} \sum_{\mu} C_{\mu}^{\nu} C_{m-\mu}^{n-\nu-1} \right\}, \\
C^{nm} &= \frac{1}{2D_1^0} \left\{ S^{nm} + 2W_{2n+1,2m+1} - 2(m+1)C_{m+1}^n \right. \\
&\quad \left. - 2 \sum_{\nu=1}^n \sum_{\mu} D_{\mu}^{\nu} C_{m+1-\mu}^{n-\nu} \right\}, \\
C_{n+2}^n &\equiv D_{n+2}^n \equiv 0, \\
E^{(n-1)} &= \frac{1}{2} \left(T^{n0} - D_1^n + 2W_{2n,0} - \sum_{\nu=0}^{n-1} C_0^{n-1-\nu} C_0^{\nu} \right), \\
D_1^0 &= -\sqrt{2W_{02}}.
\end{aligned} \tag{A6}$$

For the second excited state,

$$\begin{aligned}
T^{mm} &= - \sum_{k=1}^{n-m} (2\gamma_k C_{m+1}^{n-k} + \beta_k T^{n-k+1,m+1} + \gamma_k S^{n-k,m}) - 4D_{m+1}^n, \\
S^{nm} &= - \sum_{k=1}^{n-m} \{ 2\gamma_k D_{m+2}^{n-k+1} + \gamma_k T^{n-k+1,m+1} + \beta_k S^{n-k+1,m+1} \} - 4C_{m+1}^n, \\
\beta_k &= \frac{- \sum_{k=1}^{n-1} (2\gamma_k C_0^{n-k-1} + \beta_k T^{n-k,0}) - 2\delta_{n,1}}{T^{00}}, \quad \gamma_k = \frac{- \sum_{k=1}^{n-1} (2D^{n-k} + T^{n-k,0})\gamma_k - \sum_{k=1}^n \beta_k S^{n-k,0} - 4C_0^{n-1}}{T^{00} + 2D_1^0}.
\end{aligned} \tag{A9}$$

The limits on the sums over μ in Eq. (A6) are such that only those coefficients defined in Eq. (A4) appear. The T^{nm} and S^{nm} depend on the state. For the ground state

$$T^{nm} = S^{nm} = 0. \tag{A7}$$

For the first excited state,

$$\begin{aligned}
T^{nm} &= \sum_{k=1}^{n-m} \alpha_k S^{n-k,m} - 2D_{m+1}^n, \\
S^{nm} &= \sum_{k=1}^{n-m} \alpha_k T^{n-k+1,m+1} - 2C_{m+1}^n, \\
\alpha_n &= \frac{\left(2C_0^{n-1} - \sum_{k=1}^{n-1} \alpha_k T^{n-k,0} \right)}{T^{00}}.
\end{aligned} \tag{A8}$$

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