

Energy eigenstates of spherically symmetric potentials using the shifted $1/N$ expansion

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We show that an excellent analytic approximation to the energy eigenvalues and eigenfunctions of the Schrödinger equation can be obtained using the shifted $1/N$ expansion, where N is the number of spatial dimensions. This technique, which was physically motivated for power-law potentials, is extended in this paper to general spherically symmetric potentials. The calculations are carried out for states with arbitrary quantum numbers n and l using fourth-order perturbation theory in the shifted expansion parameter $1/\bar{k}$, where $\bar{k} = N + 2l - a$. We obtain very accurate agreement with numerical results for a variety of potentials for a very large range of both n and l . Our results using the shift a are consistently better than those previously obtained using the unshifted expansion parameter $1/k$, $k = N + 2l$. The shifted $1/N$ expansion is seen to be applicable to a much wider class of problems than are most other approximation methods.

I. INTRODUCTION

A large number of important physical problems require solving the Schrödinger equation for spherically symmetric potentials in order to determine the energy eigenvalues and eigenfunctions. Since only a handful of potentials is exactly solvable, in general one has to resort to numerical techniques or approximation schemes. In the past few years it has been shown that even if the results of physical interest are in three dimensions, it is advantageous to work in N dimensions and use $1/N$ as a perturbation expansion parameter.¹⁻⁵ This large- N technique provides an accurate new way of solving the Schrödinger equation. More precisely, for spherically symmetric potentials, a natural choice for the expansion parameter is $1/k$ where $k = N + 2l$, N being the number of spatial dimensions and $l(l + N - 2)\hbar^2$ the eigenvalue of the square of the N -dimensional orbital angular momentum.^{5(a)} The zeroth-order result is just a solution of the classical equations of motion—hence, large- N expansions are often called semiclassical. Furthermore, the large- N technique is not an expansion in powers of the potential. Therefore

it can be used for problems which do not manifestly involve a small coupling constant for doing perturbation theory. Thus one is not restricted only to those problems in which the Hamiltonian is the sum of two terms—one of which is solvable and the other is small enough to treat as a perturbation.

For the class of power-law potentials $V(r) = Ar^\nu$, many orders of the $1/k$ expansion have been computed¹ using logarithmic perturbation theory.⁶ This approach yields exact results for the harmonic-oscillator ($\nu = 2$) case but only an approximate solution for the Coulomb case ($\nu = -1$). Recently, we have shown that a modification of the expansion parameter can reproduce the known analytic form of the eigenvalues both for the harmonic oscillator as well as the Coulomb potential in an arbitrary number of dimensions.² This desirable modification simply consists of using $1/\bar{k}$ as an expansion parameter, where $\bar{k} = k - a = N + 2l - a$, and a is a suitable shift, which will be discussed in detail below. This approach, which we call the shifted $1/N$ or $1/\bar{k}$ method, provides remarkably accurate and simple analytic expressions for the energy eigenvalues of spherically symmetric power-law potentials $V(r) = Ar^\nu$.²

$$E_n = \bar{k}^{(\nu-2)/(\nu+2)} \left[\frac{4\nu A m}{\hbar^2} \right]^{2/(\nu+2)} \frac{\hbar^2}{m} \left\{ \frac{\bar{k}(\nu+2)}{8\nu} - \frac{(\nu+1)(\nu-2)}{12^2 \bar{k}} \left[(1+6n+6n^2) + O\left(\frac{1}{\bar{k}}\right) \right] \right\}, \quad (1)$$

where

$$a = 2 - (2n+1)\sqrt{\nu+2}, \quad (2)$$

$n = 0, 1, 2, \dots$ is the radial quantum number and the dependence of the energies on l is entirely contained in \bar{k} .

For the special case $n = 0$, the expansion has been carried out to two more orders. The result is

$$E_0 = \bar{k}^{(\nu-2)/(\nu+2)} \left[\frac{4\nu A m}{\hbar^2} \right]^{2/(\nu+2)} \frac{\hbar^2}{m} \times \left\{ \frac{\bar{k}(\nu+2)}{8\nu} - \frac{(\nu+1)(\nu-2)}{12^2 \bar{k}} \left[1 - \frac{(\nu+1)(\nu-2)}{12\bar{k}\sqrt{\nu+2}} + \frac{317\nu^4 - 166\nu^3 - 1923\nu^2 - 15364\nu - 17164}{225(12\bar{k}\sqrt{\nu+2})^2} + O\left(\frac{1}{\bar{k}^3}\right) \right] \right\}. \quad (3)$$

The purpose of this paper is to extend the above results to higher orders in $1/\bar{k}$ and to generalize the shifted- $1/N$ -expansion formalism to arbitrary spherically symmetric potentials. In Sec. II, we will develop the method and obtain general expressions for the energy eigenvalues E_n [Eqs. (8), (11)–(17) and (B5)–(B11)] and the $n=0$ eigenfunction ψ_0 [Eqs. (12)–(14) and (A19)] as expansions in $1/\bar{k}$. In order to obtain these results, fairly involved fourth-order perturbation-theory calculations are needed. These calculations can be carried out by two alternative methods—the $n=0$ calculation using logarithmic perturbation theory⁶ is described in Appendix A, whereas the more standard Rayleigh-Schrödinger calculation is given in Appendix B. Many examples and applications are given in Sec. III, including various potentials used in heavy quarkonium spectroscopy. In particular, for power-law potentials, our result [Eq. (19)] is one order in $1/\bar{k}$ better than Eq. (1). We have compared our results (using the shifted $1/N$ expansion) with “exact” results obtained by numerically integrating the Schrödinger equation for a variety of potentials in three spatial dimensions.⁷ Typically, using Eqs. (8), (11)–(17) and (B5)–(B11), the energy eigenvalues are accurate to three significant figures. Likewise, the eigenfunctions are also accurately described. We find that for fixed n the computed energies become more accurate as l increases. This is expected since the expansion parameter $1/\bar{k}$ becomes smaller as l becomes larger. On the other hand, for a given value of l , the energies in the unshifted expansion become less accurate as n increases since higher-order perturbation contributions to the energy contain powers of n in the numerator. This large- n behavior of the accuracy of the energy is much less severe in the shifted expansion than in the unshifted, since the parameter \bar{k} is proportional to n and appears in the denominator in higher-order corrections [see Eq. (1), for example]. In fact, the shifted $1/N$ expansion does extremely well for large values of n (see Table II b), whereas the unshifted expansion proves useful only for $n \leq 2$,¹ since k has no n dependence to diminish the effects of the powers of n in the numerator of the higher-order terms. Hence, the shift significantly increases the domain of applicability of large- N expansions. Moreover, the shifted $1/N$ expansion seems to be applicable to a much wider class of problems and to yield more accurate results than all other currently available approxi-

mation methods known to us for spherically symmetric potentials. Also, as conjectured previously,² for any n the first few terms in the shifted expansion indicate that the series is converging more rapidly than the unshifted series.

For convenience, we present a prescription here which allows the reader to use our results without proceeding into their derivation. Given a spherically (or to be more precise, hyperspherically) symmetric potential $V(r)$ in N spatial dimensions, the energies E_n and the $n=0$ wave function (for any choice of l) can be calculated as follows:

(a) Determine the following quantities, in the order given, for the orbital angular momentum l , number of dimensions N , and radial quantum number n of interest:

- (i) r_0 from Eq. (17),
- (ii) Q from Eq. (8),
- (iii) ω from Eq. (12),
- (iv) a from Eq. (15),
- (v) $\bar{k} = k - a = N + 2l - a$; $g = 1/\bar{k}$.

(b) Compute the quantities in Eqs. (13) and (14).

(c) Substitute the above results into Eqs. (B5)–(B11) to obtain the quantity λ_n . $\bar{k}\lambda_n/r_0^2$ is the desired energy E_n . Equation (A19) yields the $n=0$ wave function.

For power-law potentials $V(r) = Ar^v$, we may bypass the above prescription and simply use Eqs. (2), (3) and (19). Also, for $V(r) = A \ln(r/b)$ we need only use Eqs. (20)–(22). This is so since Eq. (17) yields a closed-form expression for r_0 for these two classes of potentials and one may proceed algebraically (for arbitrary n, l, N) and obtain an analytic expression for the energy eigenvalues.

II. THE SHIFTED $1/N$ EXPANSION

In this section we will formulate the shifted $1/N$ expansion for an arbitrary spherically symmetric potential $V(r)$. The radial Schrödinger equation in N spatial dimensions is^{1,3}

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{(k-1)(k-3)\hbar^2}{8mr^2} + V(r) \right] \psi(r) = E\psi(r), \quad (4)$$

where $k = N + 2l$. In terms of the shifted variable $\bar{k} = k - a$, one has

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\bar{k}^2 [1 - (1-a)/\bar{k}] [1 - (3-a)/\bar{k}] \hbar^2}{8mr^2} + V(r) \right] \psi(r) = E\psi(r). \quad (5)$$

It is well known^{1–3} that unless the large- \bar{k} limit of the potential $V(r)$ is suitably defined, one does not get useful results from a $1/\bar{k}$ expansion. Since the angular momentum barrier term goes like \bar{k}^2 at large \bar{k} , so should the potential $V(r)$. This will yield an effective potential which does not vary with \bar{k} at large values of \bar{k} , resulting in a sensible zeroth-order classical result. Hence, we consider the equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(r)}{dr^2} + \bar{k}^2 \left[\frac{\hbar^2 [1 - (1-a)/\bar{k}] [1 - (3-a)/\bar{k}]}{8mr^2} + \frac{V(r)}{Q} \right] \psi(r) = E\psi(r), \quad (6)$$

where Q is a constant which rescales the potential and will be determined below.

We now proceed to solve Eq. (6) systematically in terms of the expansion parameter $1/\bar{k}$. The leading contribution to the energy E comes from the effective potential

$$V_{\text{eff}}(r) = \frac{\hbar^2}{8mr^2} + \frac{V(r)}{Q}. \quad (7)$$

We assume $V(r)$ to be sufficiently well behaved so that $V_{\text{eff}}(r)$ has a minimum and there are well-defined bound states. Let r_0 be the location of the minimum. Then we have the relationship

$$4mr_0^3 V'(r_0) = \hbar^2 Q. \quad (8)$$

Once r_0 is determined, Eq. (8) gives Q . The leading term in E is

$$\bar{k}^2 V_{\text{eff}}(r_0) = \frac{\bar{k}^2}{r_0^2} \left[\frac{\hbar^2}{8m} + \frac{r_0^2 V(r_0)}{Q} \right]. \quad (9)$$

It is convenient to shift the origin of coordinates to $r = r_0$ by defining¹⁻³

$$x = \frac{\bar{k}^{1/2}}{r_0} (r - r_0). \quad (10)$$

Substituting in Eq. (6) and expanding about $x = 0$ in powers of x yields

$$\begin{aligned} & \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{\bar{k} \hbar^2}{8m} \left[1 + \frac{3x^2}{\bar{k}} - \frac{4x^3}{\bar{k}^{3/2}} + \frac{5x^4}{\bar{k}^2} - \dots \right] - \frac{(2-a)\hbar^2}{4m} \left[1 - \frac{2x}{\bar{k}^{1/2}} + \frac{3x^2}{\bar{k}} - \dots \right] \right. \\ & \left. + \frac{(1-a)(3-a)\hbar^2}{\bar{k} 8m} \left[1 - \frac{2x}{\bar{k}^{1/2}} + \frac{3x^2}{\bar{k}} - \dots \right] + \frac{r_0^2 \bar{k}}{Q} \left[V(r_0) + \frac{V'''(r_0)r_0^2 x^2}{2\bar{k}} + \frac{V''''(r_0)r_0^3 x^3}{6\bar{k}^{3/2}} + \dots \right] \right] \phi = \frac{Er_0^2}{\bar{k}} \phi. \end{aligned} \quad (11)$$

Equation (11) is exactly of the type solved in Appendices A and B if we make the following identifications:

$$\begin{aligned} \omega &= \left[\frac{3\hbar^2}{4m^2} + \frac{r_0^4 V'''(r_0)}{mQ} \right]^{1/2} \\ &= \frac{\hbar}{2m} \left[3 + \frac{r_0^4 V'''(r_0)}{V'(r_0)} \right]^{1/2}, \end{aligned} \quad (12)$$

$$g = \frac{1}{\bar{k}}, \quad \lambda = \frac{Er_0^2}{\bar{k}},$$

$$\begin{aligned} \epsilon_0 &= \frac{\hbar^2 \bar{k}}{8m} - \frac{(2-a)\hbar^2}{4m} + \frac{\hbar^2(1-a)(3-a)}{8m\bar{k}} \\ &\quad + \frac{r_0^2 \bar{k} V(r_0)}{Q}, \end{aligned} \quad (13a)$$

$$\epsilon_1 = \frac{(2-a)\hbar^2}{2m}, \quad (13b)$$

$$\epsilon_2 = \frac{-3\hbar^2(2-a)}{4m}, \quad (13c)$$

$$\epsilon_3 = \frac{-\hbar^2}{2m} + \frac{r_0^5 V''''(r_0)}{6Q}, \quad (13d)$$

$$\epsilon_4 = \frac{5\hbar^2}{8m} + \frac{r_0^6 V''''(r_0)}{24Q}, \quad (13e)$$

$$\delta_1 = \frac{-(1-a)(3-a)\hbar^2}{4m}, \quad (14a)$$

$$\delta_2 = \frac{3(1-a)(3-a)\hbar^2}{8m}, \quad (14b)$$

$$\delta_3 = \frac{(2-a)\hbar^2}{m}, \quad (14c)$$

$$\delta_4 = \frac{-5(2-a)\hbar^2}{4m}, \quad (14d)$$

$$\delta_5 = \frac{-3\hbar^2}{4m} + \frac{r_0^7 V''''''(r_0)}{120Q}, \quad (14e)$$

$$\delta_6 = \frac{7\hbar^2}{8m} + \frac{r_0^8 V''''''(r_0)}{720Q}. \quad (14f)$$

Substitution of the above expressions into Eqs. (B5)–(B11) and (A19) immediately gives an expression for the shifted $1/N$ expansion for the energy eigenvalues E_n and the eigenfunction ψ_0 in terms of r_0 , Q , and the shift a . As noted before, the leading contribution to the energy is $\bar{k}^2 V_{\text{eff}}(r_0)$ given in Eq. (9). The next contribution is of order \bar{k} and is given by

$$\frac{\bar{k}}{r_0^2} \left[\left(n + \frac{1}{2} \right) \hbar \omega - \frac{(2-a)\hbar^2}{4m} \right].$$

The shift a is chosen so as to make this contribution vanish. (Recall that this choice was physically motivated in Ref. 2 by requiring agreement between the $1/\bar{k}$ expansions and the exact analytic results for the harmonic-oscillator and Coulomb potentials.) Therefore,

$$a = 2 - 2(2n+1)m\omega/\hbar. \quad (15)$$

For any specific choice of n, l, N , the constant Q should be such as to make Eqs. (5) and (6) identical. This means

$$\bar{k} = \sqrt{Q} \quad (16)$$

or, using Eqs. (8), (12), and (15)

$$\begin{aligned} N + 2l - 2 + (2n+1) \left[3 + \frac{r_0 V''(r_0)}{V'(r_0)} \right]^{1/2} \\ = \left[\frac{4mr_0^3 V'(r_0)}{\hbar^2} \right]^{1/2} \end{aligned} \quad (17)$$

which is an explicit equation for determining r_0 . Then

TABLE I. Comparison of the shifted $1/N$ expansion results ($N=3$), for the ground state ($n=l=0$) of various power-law potentials using Eq. (3), with numerical results (Ref. 7) (in parentheses) ($\hbar=2m=1$).

$V(r)$	E_0	$V(r)$	E_0
$-r^{-1.5}$	-0.298 88 (-0.296 09)	r^2	3.0 (3.0)
$-r^{-1.25}$	-0.220 35 (-0.220 29)	r^3	3.451 11 (3.450 56)
$-r^{-1}$	-0.25 (-0.25)	r^4	3.801 39 (3.799 67)
r^0	1.0 (1.0)	r^5	4.091 46 (4.089 16)
$r^{0.15}$	1.327 95 (1.327 95)	r^6	4.338 01 (4.338 60)
$r^{0.5}$	1.833 41 (1.833 39)	r^7	4.546 90 (4.558 66)
$r^{0.75}$	2.108 15 (2.108 14)	r^8	4.717 72 (4.755 87)
$r^{1.5}$	2.708 06 (2.708 09)	r^{10}	4.922 20 (5.097 88)

Eq. (8) gives Q and one has all the ingredients to compute the energy eigenvalues and eigenfunctions. Note that r_0 depends on the radial quantum number n .

One might expect that the results for the energies E_n gradually gets worse when n becomes large, since all partial sums in the expression for the energy contain terms which behave at least like n for large n . Thus, consecutive contributions from partial sums may not decrease and the convergence of the series is in question. However, as discussed later, the shifted $1/N$ expansion for classes of potentials of physical interest yields remarkably good results for large values of n . Also, note that the $1/\bar{k}$ expansion for wave functions extends slightly into the region $r < 0$. This happens because the potential to any given order in $1/\bar{k}$ [Eq. (11)] has a large but not infinite barrier at $r=0$.

III. EXAMPLES AND APPLICATIONS

A. Power-law potentials $V(r)=Ar^\nu$

This class of potentials was discussed in Refs. 2 and 8. Here, we shall rederive and extend previous results [Eq.

$$E_n = \bar{k}^{(\nu-2)/(\nu+2)} \left(\frac{4\nu A m}{\hbar^2} \right)^{2/(\nu+2)} \frac{\hbar^2}{m}$$

$$\times \left[\frac{\bar{k}(\nu+2)}{8\nu} - \frac{(\nu+1)(\nu-2)}{12^2 \bar{k}} \right] \left[(1+6n+6n^2) - \frac{1}{12\bar{k}\sqrt{\nu+2}} [(\nu+1)(\nu-2) + (7\nu^2-31\nu-62)n] \right.$$

$$\left. + (5\nu^2-29\nu-58)(3n^2+2n^3) \right] + O \left[\frac{1}{\bar{k}^2} \right] \quad (19)$$

A comparison of the results of Eqs. (19) and (3) with those obtained by numerically solving the Schrödinger equation for many choices of ν is given in Tables I and II. Note that for $-1 \leq \nu \leq 2$ ($n=0$) our results are accurate to within 0.001%. From Eq. (19) we can see that as ν becomes very large, the corrections to the leading term also

(1)] to one more order in $1/\bar{k}$, using the general formalism developed in Sec. II. For power-law potentials, Eqs. (12)–(15) read

$$\omega = \frac{\hbar}{2m} \sqrt{\nu+2}, \quad Q = \bar{k}^2, \quad r_0 = \left[\frac{\hbar^2 \bar{k}^2}{4\nu A m} \right]^{1/(\nu+2)},$$

$$\bar{k} = N + 2l - a, \quad a = 2 - (2n+1)\sqrt{\nu+2},$$

$$\epsilon_0 = \frac{\bar{k} \hbar^2 (\nu+2)}{8m\nu} - \frac{\hbar^2 \sqrt{\nu+2} (2n+1)}{4m} + \frac{\hbar^2 [(2n+1)^2 (\nu+2) - 1]}{8m\bar{k}},$$

$$\epsilon_1 = \frac{\hbar^2 \sqrt{\nu+2} (2n+1)}{2m},$$

$$\epsilon_2 = \frac{-3\hbar^2 \sqrt{\nu+2} (2n+1)}{4m},$$

$$\epsilon_3 = \frac{\hbar^2 (\nu+2) (\nu-5)}{24m},$$

$$\epsilon_4 = \frac{\hbar^2 (\nu+2) (\nu^2 - 8\nu + 27)}{96m},$$

$$\delta_1 = \frac{\hbar^2 [1 - (2n+1)^2 (\nu+2)]}{4m},$$

$$\delta_2 = \frac{-3\hbar^2 [1 - (2n+1)^2 (\nu+2)]}{8m},$$

$$\delta_3 = \frac{\hbar^2 \sqrt{\nu+2} (2n+1)}{m},$$

$$\delta_4 = \frac{-5\hbar^2 \sqrt{\nu+2} (2n+1)}{4m},$$

$$\delta_5 = \frac{\hbar^2 (\nu+2)}{480m} (\nu^3 - 12\nu^2 + 59\nu - 168),$$

$$\delta_6 = \frac{\hbar^2 (\nu+2)}{2880m} (\nu^4 - 17\nu^3 + 119\nu^2 - 463\nu + 1200),$$

and considerable simplification occurs in the formula for the energy eigenvalues. After some lengthy but straightforward algebra, the final result for E_n is

become large and the perturbation expansion breaks down, a similar situation also occurs when $\nu \rightarrow -2$. However for $\nu=10$ ($n=l=0$), the shifted $1/N$ expansion, Eq. (3), yields 96.6% accuracy (see Table I), much better than the 79% obtained with the unshifted expansion to the same order, and for $\nu=-1.5$ ($n=l=0$) Eq. (3) gives 99% ac-

TABLE II. (a) Comparison of the shifted $1/N$ expansion results ($N=3$) with numerical results from Refs. 7, 8, and 15 (in parentheses), for the logarithmic potential, Eqs. (20) and (22) ($\hbar=2m=1$), and various power-law potentials, Eqs. (3) and (19) ($\hbar=m=1$) for several choices of n and l . (b) Same as (a), but for larger values of n and l with $\hbar=2m=1$.

(a)					
	n	$\ln(r)$	$-2^{1.7}r^{-0.2}$	$V(r)$ $-2^{0.8}r^{-0.8}$	$2^{7/2}r$
$l=0$	0	1.044 36	-2.686 01	-1.218 70	9.352 43
		(1.0443)	(-2.686)	(-1.218)	(9.352 43)
	1	1.844 57	-2.254 83	-0.462 82	16.326 36
		(1.8474)	(-2.253)	(-0.462)	(16.3518)
	2	2.284 17	-2.046 58	-0.265 45	22.023 19
		(2.2897)	(-2.044)	(-0.265)	(22.082 24)
$l=1$	0	1.641 14	-2.344 94	-0.500 44	
		(1.643)	(-2.345)	(-0.500)	
	1	2.150 23	-2.101 03	-0.280 71	
		(2.151)	(-2.101)	(-0.281)	
	2	2.488 97	-1.951 47	-0.187 45	
		(2.491)	(-1.951)	(-0.187)	
$l=2$	0	2.013 31	-2.156 26	-0.294 70	
		(2.015)	(-2.156)	(-0.295)	
	1	2.387 18	-1.990 15	-0.194 93	
		(2.388)	(-1.990)	(-0.195)	
	2	2.661 60	-1.875 35	-0.142 02	
		(2.663)	(-1.875)	(-0.142)	
$l=3$	0	2.284 14	-2.029 06	-0.201 91	
		(2.286)	(-2.029)	(-0.202)	
	1	2.579 67	-1.904 91	-0.146 35	
		(2.581)	(-1.905)	(-0.146)	
	2	2.809 99	-1.812 66	-0.112 80	
(b)					
	n	l	$V(r)=\ln(r)$	Percent accuracy	
	3	0	2.588 63	99.73	
			(2.5957)		
		1	2.742 44	99.94	
			(2.744)		
		2	2.877 86	99.93	
			(2.880)		
	4	3	2.998 22	99.97	
			(2.999)		
		4	3.106 29	99.98	
			(3.107)		
	4	0	2.821 76	99.71	
			(2.8299)		
		1	2.944 84	99.89	
			(2.948)		
		2	3.056 10	99.87	
			(3.060)		
	6	3	3.157 19	99.94	
			(3.159)		
		4	3.249 60	99.96	
			(3.251)		
	6	0	3.169 56	99.70	
			(3.179 11)		

TABLE II. (Continued.)

n	l	$V(r)=\ln(r)$	Percent accuracy
10	0	3.631 77 (3.642 71)	99.70
4	0	44.183 23 (43.9812)	100.46
6	0	70.595 60 (70.2524)	100.49
10	0	131.313 75 (130.642)	100.51

curacy as compared to 52.1% for the unshifted expansion. A plot of the accuracy of our results vs ν is given in Fig. 1 for the ground state. Various graphs are given corresponding to the number of orders of $1/\bar{k}$ retained in the calculation. Clearly, including one additional order in $1/\bar{k}$ increases the range of accuracy by 2 units of ν . This can be understood by noting that two more terms in the expansion of $V(r)$ [Eq. (11)] are involved in the calculation when an additional order is computed.

It is found that Eq. (19) yields remarkably good results even for large values of n . In fact, as can easily be checked by taking the ratio of successive terms, the rate of convergence of the three terms in Eq. (19) is approximately the same as $n \rightarrow \infty$ as it is for $n=0$. So, if the results for small n are accurate, one expects roughly similar accuracy for all n . As stated previously, this is far from true in the unshifted expansion which is found to be useful for $n \leq 2$. The results of Eq. (19) for $\nu=4$ and various large values of n are shown in Table II b, along with their accuracies.

The usefulness of the shifted $1/N$ expansion for small n is brought out more clearly by comparing its results with the results of the unshifted expansion^{1,3} to the same order. This is illustrated in Fig. 2 where the accuracy of both expansions is plotted vs ν . However, it should be pointed out that calculations in the shifted $1/N$ expansion are somewhat more difficult to perform numerically than in

the unshifted expansion.¹ Indeed for power-law potentials, many higher-order corrections to the energies have been numerically calculated with ease in the unshifted expansion.¹

Figure 3 shows the ground-state wave function of the harmonic oscillator ($\nu=2$) from Eq. (A19) as well as the solution obtained by a precise numerical integration of the Schrödinger equation.

B. Logarithmic potential $V(r)=A \ln(r/b)$

This is one of the potentials which has been used in heavy quarkonium spectroscopy.^{8,9} It is simple to calculate the quantities in Eqs. (12)–(14) and obtain the following result for the energy eigenvalues:

$$E_n = A \left\{ \ln \left[\frac{\bar{k}\hbar}{2b\sqrt{Am}} \right] + \frac{1}{2} + \frac{1}{18\bar{k}^2} (1+6n+6n^2) + \frac{1}{108\sqrt{2}\bar{k}^3} [1+31n+29(3n^2+2n^3)] + O\left[\frac{1}{\bar{k}^4}\right] \right\}, \quad (20)$$

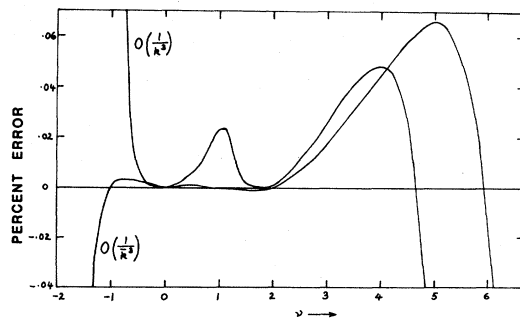


FIG. 1. A comparison of the accuracy of the $1/\bar{k}$ expansion and the unshifted $1/k$ expansion for the energy eigenvalues of the ground state ($n=l=0$) of the attractive potential $V(r) \propto r^\nu$ ($N=3$). A plot of the accuracy of the energy eigenvalues vs ν is given for each expansion.

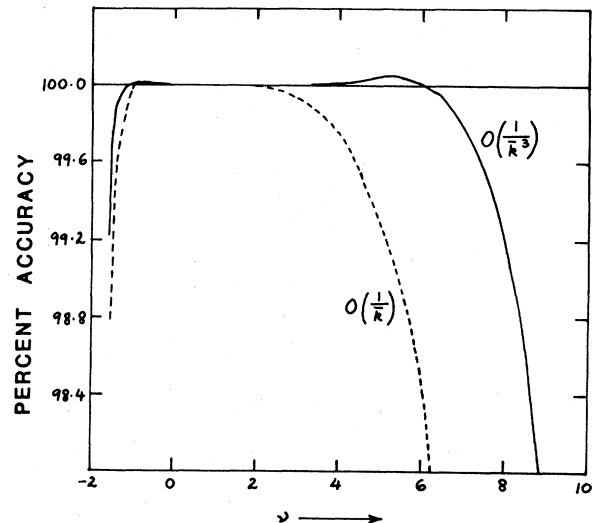


FIG. 2. A plot of the accuracy of the energy eigenvalues, computed from Eq. (3), of the ground state ($n=l=0$) of the attractive potential $V(r) \propto r^\nu$ vs ν ($N=3$).

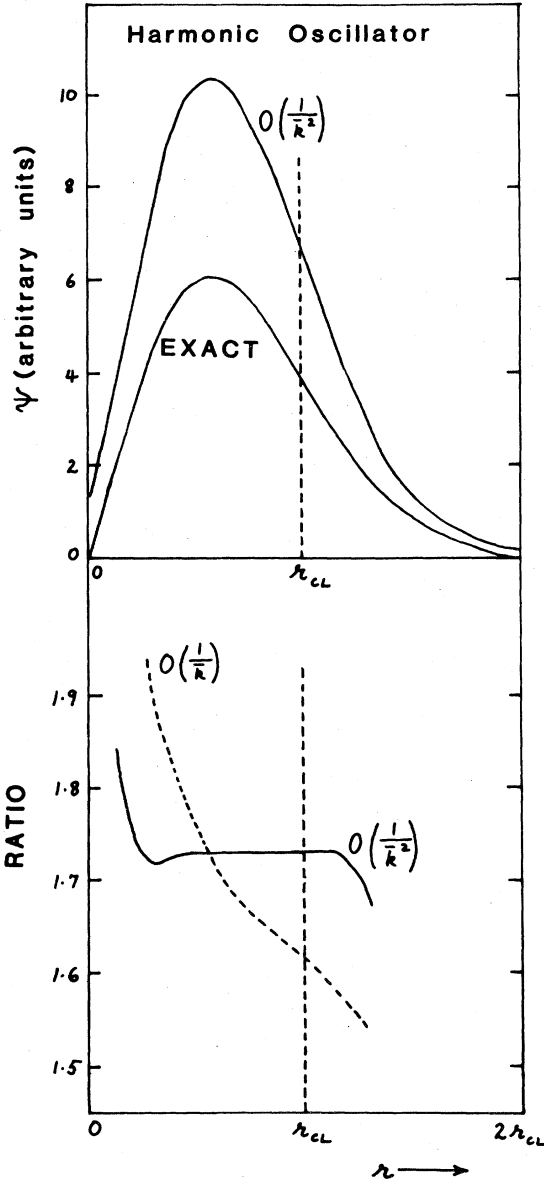


FIG. 3. A comparison of the shifted $1/N$ result for the ground-state ($n=l=0$) wave function of the three-dimensional harmonic oscillator $V(r)=r^2$, with the "exact" wave function obtained by numerical integration of the Schrödinger equation. The top figure shows both these wave functions (in arbitrary units) vs r as well as the position of the classical turning point r_{CL} . The bottom figure shows the ratio of the shifted $1/N$ wave function to the numerical wave function vs r when computed to $O(1/k)$ and $O(1/k^2)$. This ratio is a constant if the results are 100% accurate.

where

$$\bar{k} = k - a, \quad a = 2 - (2n + 1)\sqrt{2}. \quad (21)$$

Since the logarithmic potential is really a special case of the power-law potential [$\ln x = \lim_{\epsilon \rightarrow 0} (x^\epsilon - 1)/\epsilon$], one can also obtain Eq. (20) from Eq. (19) by taking the ap-

propriate limit. In particular, for the ground state the result can be carried out one order in $1/\bar{k}$ further by making use of Eq. (3). The result is

$$E_0 = A \left[\ln \left[\frac{\bar{k}\hbar}{2b\sqrt{Am}} \right] + \frac{1}{2} + \frac{1}{18\bar{k}^2} + \frac{1}{108\sqrt{2}\bar{k}^3} - \frac{4291}{291600\bar{k}^4} + O\left[\frac{1}{\bar{k}^5}\right] \right]. \quad (22)$$

Note that the spacing between energy levels is mass-independent—a property which is roughly obeyed by the low-lying ($c\bar{c}$) and ($b\bar{b}$) states, thus motivating the choice of an interquark logarithmic potential. A comparison with "exact" results is shown in Table II, and shows excellent agreement. Table II b displays the accuracy of the energies E_n for various large values of n and l . These results are in most cases superior to those calculated using the WKB approximation.⁸

C. Other potentials

In order to further test the accuracy of our $1/\bar{k}$ expansion, we have applied it to a variety of physically interesting potentials. Among these are two potentials which have been extensively used in charmonium spectroscopy:

- (i) the Martin potential¹⁰ $V(r) = 6.8698r^{0.1} - 8.064$,
- (ii) the Cornell potential¹¹ $V(r) = r/(2.34)^2 - 0.52/r$, and special cases of two potentials which have wide applications in atomic and molecular physics:
- (iii) the Morse potential¹² $V(r) = 10(e^{-2r} - 2e^{-r})$,
- (iv) the anharmonic oscillator¹³ $V(r) = r^2 + r^4$.

Results are listed in Table III.

The "exact" ground-state wave functions for (iii) and (iv) are compared with those computed from Eq. (A19) in Figs. 4 and 5. The comparison is clearly satisfactory.

So far, we have only considered monotonically increasing potentials which give rise to one minimum of the effective potential and an infinite number of bound states. We now consider an example in which $V(r)$ has both a minimum and a maximum; $V(r) = r^2 - (r^3/10)$, $N=3$. Application of Eqs. (12)–(14) and (B5)–(B11) yields the results displayed in Table IV. The shifted $1/N$ expansion results are compared to numerical results⁷ for $n=0, 1, 2, 3, 4$ ($l=0$), and show excellent agreement. As n increases, the leading term, Eq. (9), in the shifted expansion seems to converge to a value of $\simeq 19$ [very roughly equal to the maximum value of $V(r)$] indicating a high energy continuum of states. Below we display the value of the leading term, denoted by E_n^1 , for various value of $n \geq 5$:

$$\begin{aligned} n=5, \quad E_n^1 &= 15.18576, \\ n=10, \quad E_n^1 &= 18.57497, \\ n=20, \quad E_n^1 &= 18.94257, \\ n=40, \quad E_n^1 &= 18.96174, \\ n=100, \quad E_n^1 &= 18.96293. \end{aligned}$$

This convergence does not occur in the unshifted $1/k$ expansion where the leading term diverges as $n \rightarrow \infty$. It

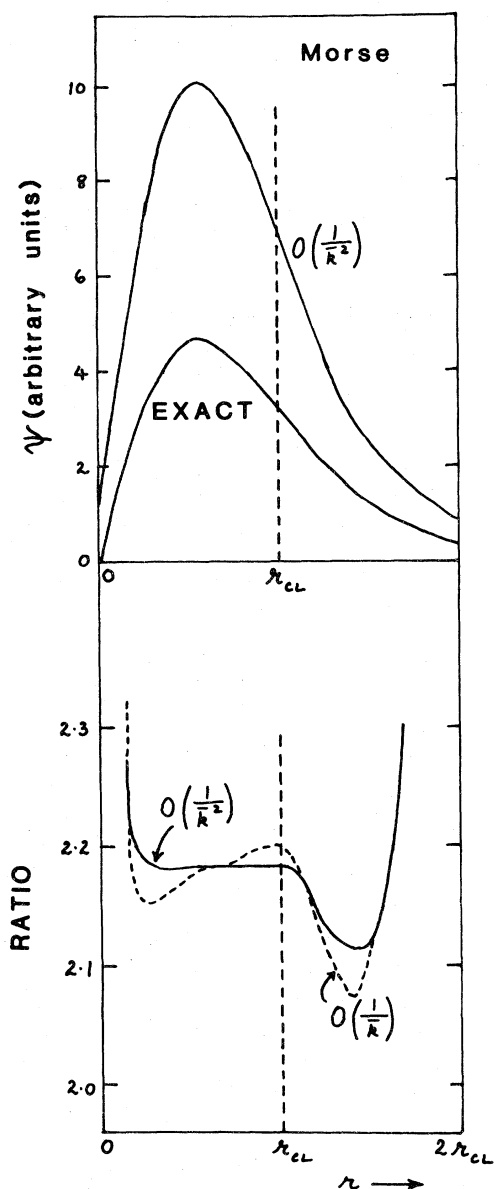


FIG. 4. A comparison of the shifted $1/N$ expansion result for the ground-state ($n=l=0$) wave function of the Morse potential $V(r)=10(e^{-2r}-2e^{-r})$, $N=3$, with the "exact" wave function. The details of the figure are explained in the caption of Fig. 3.

should also be possible to extend the above considerations to potentials with more than one minimum with an appropriate determination of r_0 for each minimum.

CONCLUSION

The shifted $1/N$ expansion for an arbitrary spherically symmetric potential which we have developed in this paper clearly gives useful and accurate analytic expressions for the energy eigenstates of the Schrödinger equation. The general results derived for excited states go much further than any previous attempts. The shifted expansion surpasses most approximation methods in its domain of

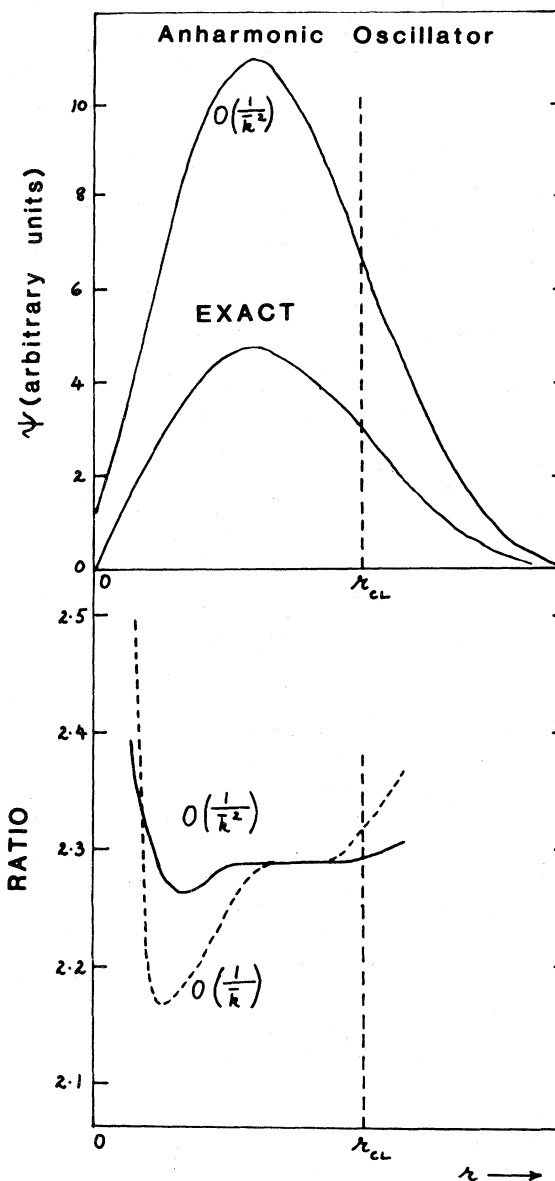


FIG. 5. A comparison of the shifted $1/N$ expansion result for the ground-state ($n=l=0$) wave function for the three-dimensional anharmonic oscillator $V(r)=r^2+r^4$, with the "exact" wave function. The details of the figure are explained in the caption of Fig. 3.

applicability and the accuracy of its results for spherically symmetric potentials. It treats nonperturbative problems on which standard coupling-constant perturbation theory cannot be performed, it also handles highly excited states which pose problems for variational methods, and it yields superior results for low-lying states where the WKB method gives only modest accuracy.

For the special case of power-law potentials we have extended our previous calculations² for excited states to one more order in $1/\bar{k}$. These results are the simplest known analytic expressions for the energy eigenvalues of power-

TABLE III. Comparison of the shifted $1/N$ expansion results with numerical results (Ref. 7) (in parentheses) for the ground state ($n=l=0$) of various spherically symmetric potentials ($N=3$). The contributions to the final energy E_0 , from each of the three partial sums computed (E_0^1, E_0^2, E_0^3 of increasing order in $1/\bar{k}$) are displayed. The Martin potential, being a power-law potential, also contains a term E_0^4 by virtue of Eq. (3) ($\hbar=2m=1$).

$V(r)$	E_0	E_0^1	E_0^2	E_0^3	E_0^4
$6.8698r^{0.1}-8.064$	-0.319 14 (-0.319 17)	-0.347 86	0.028 69	0.000 35	-0.000 32
$\frac{r}{(2.34)^2}-\frac{0.52}{r}$	0.478 80 (0.478 11)	0.489 57	-0.007 70	-0.003 07	
$10(e^{-2r}-2e^{-r})$	-4.286 18 (-4.285 92)	-4.313 25	0.035 55	-0.008 48	
r^2+r^4	4.650 61 (4.648 81)	4.727 74	-0.090 34	0.013 21	

law potentials and are incredibly accurate. The shifted $1/N$ expansion also consistently yields substantially more accurate results than the unshifted expansion¹ for every class of potential we have considered. In a sense, the shift a has provided a physically motivated resummation of the perturbation series for the energy eigenstates which improves its convergence.¹⁴ Furthermore, it has previously been stated^(5b) that unshifted $1/N$ expansions are not very useful for atomic physics calculations since they are not in very good agreement with the Coulomb-potential energy levels for $N=3$. This situation is fully remedied by our shifted expansions in $1/\bar{k}$, since they exactly give the eigenvalues of the Coulomb potential, thus providing an excellent starting point for atomic physics calculations.

ACKNOWLEDGMENTS

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APPENDIX A

In this appendix, we consider the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 + \epsilon_0 + V(x) \right] \psi(x) = \lambda \psi(x), \quad (\text{A1})$$

where the perturbation $V(x)$ is given by

$$\begin{aligned} V(x) = & g^{1/2}(\epsilon_1 x + \epsilon_3 x^3) + g(\epsilon_2 x^2 + \epsilon_4 x^4) \\ & + g^{3/2}(\delta_1 x + \delta_3 x^3 + \delta_5 x^5) \\ & + g^2(\delta_2 x^2 + \delta_4 x^4 + \delta_6 x^6). \end{aligned} \quad (\text{A2})$$

Our aim is to calculate the ground-state energy and eigenfunction as an expansion in the parameter g , correct up to and including terms in g^2 . We shall do this by using logarithmic perturbation theory (LPT),⁶ which is a highly suitable and simple technique for one-dimensional problems. LPT only requires a knowledge of the unperturbed eigenfunction, and the perturbation calculation just involves the evaluation of a small number of integrals. The calculation proceeds in a systematic, iterative manner which we outline below. A complete derivation of the formulas used can be found in Ref. 6.

The ground-state energy and wave function are given by

$$\lambda_0 = \lambda_0^{(0)} + \lambda_0^{(1)} + \lambda_0^{(2)} + \lambda_0^{(3)} + \lambda_0^{(4)} + \cdots, \quad (\text{A3})$$

$$\psi_0 = \psi_0^{(0)} + \psi_0^{(1)} + \psi_0^{(2)} + \psi_0^{(3)} + \psi_0^{(4)} + \cdots, \quad (\text{A4})$$

where $\lambda_0^{(i)}$ and $\psi_0^{(i)}$ ($i=1,2,\dots$) are corrections from i th-order perturbation theory.

The unperturbed potential is a simple harmonic oscillator. Hence,

$$\lambda_0^{(0)} = \epsilon_0 + \frac{1}{2} \hbar \omega, \quad (\text{A5})$$

$$\psi_0^{(0)}(x) = \left[\frac{\alpha}{\pi} \right]^{1/4} e^{-\alpha x^2/2}, \quad \alpha \equiv m\omega/\hbar. \quad (\text{A6})$$

TABLE IV. Comparison of the energy eigenvalues E_n , of the potential $V(r)=r^2-(r^3/10)$, $N=3$, obtained using the shifted $1/N$ expansion with numerical results (Ref. 7) E_{num} , for various values of n ($l=0$). The contribution from each partial sum in the expansion (E_n^1, E_n^2 , and E_n^3 of increasing order in $1/\bar{k}$) is displayed ($\hbar=2m=1$).

n	E_n^1	E_n^2	E_n^3	E_n	E_{num}
0	2.747 37	0.003 27	-0.000 49	2.750 15	2.750 13
1	5.980 85	0.086 55	0.004 98	6.072 38	6.073 18
2	8.840 48	0.216 97	0.013 07	9.070 52	9.072 64
3	11.339 30	0.371 86	0.025 32	11.736 48	11.739 45
4	13.462 46	0.484 35	0.034 57	13.981 38	13.950 44

The first-order correction to the energy is

$$\begin{aligned}\lambda_0^{(1)} &= \int_{-\infty}^{\infty} V(x) |\psi_0^{(0)}(x)|^2 dx \\ &= g \left[\frac{\epsilon_2}{2\alpha} + \frac{3\epsilon_4}{4\alpha^2} \right] + g^2 \left[\frac{\delta_2}{2\alpha} + \frac{3\delta_4}{4\alpha^2} + \frac{15\delta_6}{8\alpha^3} \right].\end{aligned}\quad (\text{A7})$$

The next step is to define a function $C_1(x)$ by

$$C_1(x) |\psi_0^{(0)}(x)|^2 = \frac{2m}{\hbar^2} \int_{-\infty}^x [V(x) - \lambda_0^{(1)}] |\psi_0^{(0)}(x)|^2 dx. \quad (\text{A8})$$

The integrals involved are easily computed, giving

$$\begin{aligned}-\frac{\hbar^2}{2m} C_1(x) &= g^{1/2} \left[\frac{\epsilon_1}{2\alpha} + \frac{\epsilon_3}{2\alpha^2} (1 + \alpha x^2) \right] + g \left\{ \frac{\epsilon_2}{2\alpha^{3/2}} (\alpha x^2)^{1/2} + \frac{\epsilon_4}{2\alpha^{5/2}} \left[\frac{3}{2} (\alpha x^2)^{1/2} + (\alpha x^2)^{3/2} \right] \right\} \\ &\quad + g^{3/2} \left[\frac{\delta_1}{2\alpha} + \frac{\delta_3}{2\alpha^2} (1 + \alpha x^2) + \frac{\delta_5}{2\alpha^3} (2 + 2\alpha x^2 + \alpha^2 x^4) \right] \\ &\quad + g^2 \left\{ \frac{\delta_2}{2\alpha^{3/2}} (\alpha x^2)^{1/2} + \frac{\delta_4}{2\alpha^{5/2}} \left[\frac{3}{2} (\alpha x^2)^{1/2} + (\alpha x^2)^{3/2} \right] + \frac{\delta_6}{2\alpha^{7/2}} \left[\frac{15}{4} (\alpha x^2)^{1/2} + \frac{5}{2} (\alpha x^2)^{3/2} + (\alpha x^2)^{5/2} \right] \right\}.\end{aligned}\quad (\text{A9})$$

The second-order correction to the energy is

$$\begin{aligned}\lambda_0^{(2)} &= -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} C_1^2(x) |\psi_0^{(0)}(x)|^2 dx \\ &= -\frac{2m}{\hbar^2} \left[g \left[\frac{\epsilon_1^2}{4\alpha^2} + \frac{3\epsilon_1\epsilon_3}{4\alpha^3} + \frac{11\epsilon_3^2}{16\alpha^4} \right] \right. \\ &\quad \left. + g^2 \left[\frac{\epsilon_2^2}{8\alpha^3} + \frac{6\epsilon_2\epsilon_4}{8\alpha^4} + \frac{21\epsilon_4^2}{16\alpha^5} + \frac{\epsilon_1\delta_1}{2\alpha^2} + \frac{3\epsilon_1\delta_3}{4\alpha^3} + \frac{15\epsilon_1\delta_5}{8\alpha^4} + \frac{3\epsilon_3\delta_1}{4\alpha^3} + \frac{11\epsilon_3\delta_3}{8\alpha^4} + \frac{65\epsilon_3\delta_5}{16\alpha^5} \right] \right] + O(g^3).\end{aligned}\quad (\text{A10})$$

Similarly, the subsequent corrections are computed from the equations⁶

$$C_2(x) |\psi_0^{(0)}(x)|^2 = - \int_{-\infty}^x \left[\frac{2m}{\hbar^2} \lambda_0^{(2)} + C_1^2(x) \right] |\psi_0^{(0)}(x)|^2 dx, \quad (\text{A11})$$

$$\lambda_0^{(3)} = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} 2C_1(x)C_2(x) |\psi_0^{(0)}(x)|^2 dx, \quad (\text{A12})$$

$$C_3(x) |\psi_0^{(0)}(x)|^2 = - \int_{-\infty}^x \left[\frac{2m}{\hbar^2} \lambda_0^{(3)} + 2C_1(x)C_2(x) \right] |\psi_0^{(0)}(x)|^2 dx, \quad (\text{A13})$$

$$\lambda_0^{(4)} = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} [2C_1(x)C_3(x) + C_2^2(x)] |\psi_0^{(0)}(x)|^2 dx, \quad (\text{A14})$$

$$C_4(x) |\psi_0^{(0)}(x)|^2 = - \int_{-\infty}^x \left[\frac{2m}{\hbar^2} \lambda_0^{(4)} + 2C_1(x)C_3(x) + C_2^2(x) \right] |\psi_0^{(0)}(x)|^2 dx. \quad (\text{A15})$$

The final result is

$$\begin{aligned}\lambda_0^{(3)} &= \left[\frac{2m}{\hbar^2} \right]^2 g^2 \left[\frac{9\epsilon_1\epsilon_2\epsilon_3}{8\alpha^5} + \frac{11\epsilon_2\epsilon_3^2}{8\alpha^6} + \frac{31\epsilon_1\epsilon_3\epsilon_4}{8\alpha^6} + \frac{171\epsilon_3^2\epsilon_4}{32\alpha^7} + \frac{\epsilon_1^2\epsilon_2}{4\alpha^4} + \frac{3\epsilon_1^2\epsilon_4}{4\alpha^5} \right] + O(g^3), \\ \lambda_0^{(4)} &= - \left[\frac{2m}{\hbar^2} \right]^3 g^2 \left[\frac{\epsilon_1^3\epsilon_3}{8\alpha^6} + \frac{27\epsilon_1^2\epsilon_3^2}{32\alpha^7} + \frac{132\epsilon_1\epsilon_3^3}{64\alpha^8} + \frac{465\epsilon_3^4}{256\alpha^9} \right] + O(g^3).\end{aligned}\quad (\text{A16})$$

The corrections to the unperturbed ground-state wave function are related to the quantities $C_1, C_2, C_3, C_4, \dots$, defined above. The relation is⁶

$$\psi_0(x) = \exp \left[\sum_{i=1}^{\infty} S_i(x) \right] \psi_0^{(0)}(x), \quad (\text{A17})$$

where

$$S_i(x) = \int^x C_i(x) dx, \quad i = 1, 2, \dots \quad (\text{A18})$$

The final result for the ground-state wave function up to and including $O(g^2)$ is

$$\begin{aligned} \psi_0(x) &\sim e^{-\alpha x^2/2} \left[1 + Q_1 + \frac{Q_1^2}{2!} + \frac{Q_1^3}{3!} + \frac{Q_1^4}{4!} + Q_2 + Q_3 + Q_4 + \frac{Q_2^2}{2!} + Q_1 Q_2 + Q_1 Q_3 + \frac{Q_1^2 Q_2}{2} + O(g^{5/2}) \right], \\ Q_1(x) &= g^{1/2} \left[-\frac{2m}{\hbar^2} \right] \left[\left[\frac{\epsilon_1}{2\alpha} + \frac{\epsilon_3}{2\alpha^2} \right] x + \frac{\epsilon_3}{6\alpha} x^3 \right], \\ Q_2(x) &= g \left\{ \left[-\frac{2m}{\hbar^2} \right] \left[\left[\frac{\epsilon_2}{4\alpha} + \frac{3\epsilon_4}{8\alpha^2} \right] x^2 + \frac{\epsilon_4}{8\alpha} x^4 \right] + \left[\frac{2m}{\hbar^2} \right]^2 \left[\left[\frac{\epsilon_1 \epsilon_3}{8\alpha^3} + \frac{7\epsilon_3^2}{32\alpha^4} \right] x^2 + \frac{\epsilon_3^2}{32\alpha^3} x^4 \right] \right\}, \\ Q_3(x) &= g^{3/2} \left\{ \left[-\frac{2m}{\hbar^2} \right] \left[\left[\frac{\delta_1}{2\alpha} + \frac{\delta_3}{2\alpha^2} + \frac{\delta_5}{\alpha^3} \right] x + \left[\frac{\delta_3}{6\alpha} + \frac{\delta_5}{3\alpha^2} \right] x^3 + \frac{\delta_5}{10\alpha} x^5 \right] \right. \\ &\quad + \left[\frac{2m}{\hbar^2} \right]^2 \left[\left[\frac{\epsilon_1 \epsilon_2}{4\alpha^3} + \frac{5\epsilon_1 \epsilon_4}{8\alpha^4} + \frac{\epsilon_2 \epsilon_3}{2\alpha^4} + \frac{3\epsilon_3 \epsilon_4}{2\alpha^5} \right] x + \left[\frac{\epsilon_1 \epsilon_4}{12\alpha^3} + \frac{3\epsilon_3 \epsilon_4}{8\alpha^4} + \frac{\epsilon_2 \epsilon_3}{12\alpha^3} \right] x^3 + \frac{\epsilon_3 \epsilon_4}{20\alpha^3} x^5 \right] \\ &\quad \left. - \left[\frac{2m}{\hbar^2} \right]^3 \left[\left[\frac{\epsilon_1^2 \epsilon_3}{8\alpha^5} + \frac{17\epsilon_1 \epsilon_3^2}{32\alpha^6} + \frac{5\epsilon_3^3}{8\alpha^7} \right] x + \left[\frac{\epsilon_1 \epsilon_3^2}{16\alpha^5} + \frac{13\epsilon_3^3}{96\alpha^6} \right] x^3 + \frac{\epsilon_3^3}{80\alpha^5} x^5 \right] \right\}, \\ Q_4(x) &= g^2 \left\{ \left[-\frac{2m}{\hbar^2} \right] \left[\left[\frac{\delta_2}{4\alpha} + \frac{3\delta_4}{8\alpha^2} + \frac{15\delta_6}{16\alpha^3} \right] x^2 + \left[\frac{\delta_4}{8\alpha} + \frac{5\delta_6}{16\alpha^2} \right] x^4 + \frac{\delta_6}{12\alpha} x^6 \right] \right. \\ &\quad + \left[\frac{2m}{\hbar^2} \right]^2 \left[\left[\frac{\epsilon_1 \delta_3}{8\alpha^3} + \frac{7\epsilon_1 \delta_5}{16\alpha^4} + \frac{\delta_1 \epsilon_3}{8\alpha^3} + \frac{7\epsilon_3 \delta_3}{16\alpha^4} + \frac{49\epsilon_3 \delta_5}{32\alpha^5} + \frac{\epsilon_2^2}{16\alpha^3} + \frac{3\epsilon_2 \epsilon_4}{8\alpha^4} + \frac{21\epsilon_4^2}{32\alpha^5} \right] x^2 \right. \\ &\quad + \left[\frac{\epsilon_1 \delta_5}{16\alpha^3} + \frac{\epsilon_3 \delta_3}{16\alpha^3} + \frac{11\epsilon_3 \delta_5}{32\alpha^4} + \frac{\epsilon_2 \epsilon_4}{16\alpha^3} + \frac{11\epsilon_4^2}{64\alpha^4} \right] x^4 + \left[\frac{\epsilon_3 \delta_5}{24\alpha^3} + \frac{\epsilon_4^2}{48\alpha^3} \right] x^6 \left. \right] \\ &\quad - \left[\frac{2m}{\hbar^2} \right]^3 \left[\left[\frac{3\epsilon_1 \epsilon_2 \epsilon_3}{16\alpha^5} + \frac{7\epsilon_2 \epsilon_3^2}{16\alpha^6} + \frac{7\epsilon_1 \epsilon_3 \epsilon_4}{8\alpha^6} + \frac{123\epsilon_3^2 \epsilon_4}{64\alpha^7} + \frac{\epsilon_1^2 \epsilon_4}{16\alpha^5} \right] x^2 \right. \\ &\quad + \left[\frac{3\epsilon_2 \epsilon_3^2}{64\alpha^5} + \frac{47\epsilon_3^2 \epsilon_4}{128\alpha^6} + \frac{3\epsilon_1 \epsilon_3 \epsilon_4}{32\alpha^5} \right] x^4 + \frac{\epsilon_3^2 \epsilon_4}{32\alpha^5} x^6 \left. \right] \\ &\quad \left. + \left[\frac{2m}{\hbar^2} \right]^4 \left[\left[\frac{3\epsilon_1^2 \epsilon_3^2}{32\alpha^7} + \frac{29\epsilon_1 \epsilon_3^3}{64\alpha^8} + \frac{305\epsilon_3^4}{512\alpha^9} \right] x^2 + \left[\frac{5\epsilon_1 \epsilon_3^3}{128\alpha^7} + \frac{99\epsilon_3^4}{1024\alpha^8} \right] x^4 + \frac{5\epsilon_3^4}{768\alpha^7} x^6 \right] \right\}. \end{aligned} \quad (\text{A19})$$

The above ground-state formulas for LPT can be modified to handle excited states. This modification consists of factoring out the zeros of the unperturbed wave function.^{1,6} However, we will obtain the desired results for arbitrary n by a different method in Appendix B.

APPENDIX B

Here we compute the energy eigenvalues for an arbitrary excited state for the Schrödinger equation (A1) with the perturbation potential given in Eq. (A2). The calculation is carried out to fourth order in the potential using standard Rayleigh-Schrödinger perturbation theory, and yields the energy λ_n to $O(g^2)$.

Although the perturbation formulas for the two lowest-order corrections ($\lambda_n^{(1)}$ and $\lambda_n^{(2)}$) to the unperturbed energy $\lambda_n^{(0)}$ are in most quantum mechanics textbooks, the general formulas for the third- and fourth-order corrections ($\lambda_n^{(3)}$ and $\lambda_n^{(4)}$) are easy to derive but not readily available:

$$\lambda_n^{(3)} = \sum_{i,j \neq n} \frac{V_{ni} V_{ij} V_{jn}}{\lambda_{ni} \lambda_{nj}} - V_{nn} \sum_{i \neq n} \frac{V_{ni} V_{in}}{(\lambda_{ni})^2}, \quad (\text{B1})$$

$$\lambda_n^{(4)} = \sum_{i,j,k \neq n} \frac{V_{ni} V_{ij} V_{jk} V_{kn}}{\lambda_{ni} \lambda_{nj} \lambda_{nk}} - \sum_{i,j \neq n} \frac{V_{ni} (V_{in} V_{nj} + 2V_{nn} V_{ij}) V_{jn}}{(\lambda_{ni})^2 \lambda_{nj}} + |V_{nn}|^2 \sum_{i \neq n} \frac{V_{ni} V_{in}}{(\lambda_{ni})^3}, \quad (\text{B2})$$

where

$$\lambda_{nj} \equiv \lambda_n^{(0)} - \lambda_j^{(0)} \quad (\text{B3})$$

and

$$V_{ij} \equiv \langle i | V | j \rangle \quad (\text{B4})$$

are the matrix elements of the perturbation potential between unperturbed eigenstates.

For the specific problem under consideration, $\lambda_{nj} = (n-j)\hbar\omega$, and the matrix elements V_{nj} of the perturbation potential given in Eq. (A2) can be computed using the standard formalism of harmonic-oscillator raising and lowering operators. These are the only ingredients necessary for computing energy corrections. The calculations are long and tedious, but straightforward in principle. The results are ($n=0,1,2,3,\dots$)

$$\lambda_n = \lambda_n^{(0)} + \lambda_n^{(1)} + \lambda_n^{(2)} + \lambda_n^{(3)} + \lambda_n^{(4)} + \dots, \quad (\text{B5})$$

$$\lambda_n^{(0)} = \epsilon_0 + (n + \frac{1}{2})\hbar\omega, \quad (\text{B6})$$

$$\lambda_n^{(1)} = V_{nn} = g[(1+2n)\tilde{\epsilon}_2 + 3(1+2n+2n^2)\tilde{\epsilon}_4] + g^2[(1+2n)\tilde{\delta}_2 + 3(1+2n+2n^2)\tilde{\delta}_4 + 5(3+8n+6n^2+4n^3)\tilde{\delta}_6], \quad (\text{B7})$$

$$\begin{aligned} \lambda_n^{(2)} = \sum_{i \neq n} \frac{V_{ni} V_{in}}{\lambda_{ni}} = & -\frac{g}{\hbar\omega} [\tilde{\epsilon}_1^2 + 6(1+2n)\tilde{\epsilon}_1\tilde{\epsilon}_3 + (11+30n+30n^2)\tilde{\epsilon}_3^2] \\ & - \frac{g^2}{\hbar\omega} [(1+2n)\tilde{\epsilon}_2^2 + 12(1+2n+2n^2)\tilde{\epsilon}_2\tilde{\epsilon}_4 + 2(21+59n+51n^2+34n^3)\tilde{\epsilon}_4^2 \\ & + 2\tilde{\epsilon}_1\tilde{\delta}_1 + 6(1+2n)\tilde{\epsilon}_1\tilde{\delta}_3 + 30(1+2n+2n^2)\tilde{\epsilon}_1\tilde{\delta}_5 + 6(1+2n)\tilde{\epsilon}_3\tilde{\delta}_1 \\ & + 2(11+30n+30n^2)\tilde{\epsilon}_3\tilde{\delta}_3 + 10(13+40n+42n^2+28n^3)\tilde{\epsilon}_3\tilde{\delta}_5] + O(g^3), \end{aligned} \quad (\text{B8})$$

$$\begin{aligned} \lambda_n^{(3)} = \frac{g^2}{(\hbar\omega)^2} [& 4\tilde{\epsilon}_1^2\tilde{\epsilon}_2 + 36(1+2n)\tilde{\epsilon}_1\tilde{\epsilon}_2\tilde{\epsilon}_3 + 8(11+30n+30n^2)\tilde{\epsilon}_2\tilde{\epsilon}_3^2 + 24(1+2n)\tilde{\epsilon}_1^2\tilde{\epsilon}_4 \\ & + 8(31+78n+78n^2)\tilde{\epsilon}_1\tilde{\epsilon}_3\tilde{\epsilon}_4 + 12(57+189n+225n^2+150n^3)\tilde{\epsilon}_3^2\tilde{\epsilon}_4] + O(g^3), \end{aligned} \quad (\text{B9})$$

$$\lambda_n^{(4)} = -\frac{g^2}{(\hbar\omega)^3} [8\tilde{\epsilon}_1^3\tilde{\epsilon}_3 + 108(1+2n)\tilde{\epsilon}_1^2\tilde{\epsilon}_3^2 + 48(11+30n+30n^2)\tilde{\epsilon}_1\tilde{\epsilon}_3^3 + 30(31+109n+141n^2+94n^3)\tilde{\epsilon}_3^4] + O(g^3), \quad (\text{B10})$$

$$\tilde{\epsilon}_j = \frac{\epsilon_j}{(2\alpha)^{j/2}}, \quad \tilde{\delta}_j = \frac{\delta_j}{(2\alpha)^{j/2}}, \quad (j=1,2,\dots) \quad (\text{B11})$$

where $\alpha \equiv m\omega/\hbar$. Note that for the special case $n=0$ (ground state), the results previously obtained in Appendix A are reproduced. Of course, the excited state wave functions may also be obtained using the standard Rayleigh-Schrödinger formulas.

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