1/*n* expansion for wave functions

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Using the $1/n$ expansion, analytical formulas for wave functions (and in particular for the asymptotic coefficients c_{lp} at zero) in an arbitrary potential $V(r)$ are obtained, valid in both the classically permitted and sub-barrier regions. Comparison with the exact solutions and numerical calculations for power and short-range potentials shows that the region of applicability of the formulas can be stretched to small quantum numbers $n\sim 1$ (for states with $p=0$ and 1, where p is the number of nodes in the radial wave function). With increasing p the accuracy of the formulas decreases, but in this case the WKB method may be applied, and as a result $\psi(0)$ for states with arbitrary quantum numbers can be calculated. When using WKB, a generalization of the turning-point matching conditions for quasiclassical wave functions is essential. © *1994 American Institute of Physics.*

1. INTRODUCTION

At the present time the $1/N$ expansion is widely used in theoretical physics (see, e.g., Refs. 1–20). In quantum mechanics and in atomic physics it is useful in obtaining the energies of both discrete[4–8] and quasistationary[9–12] levels. The attractive features of the method are its close relation to classical mechanics and its applicability to many-dimensional nonseparable problems[11–13] and to the many-body problem.[11,14,15] It should also be noted that, for potentials commonly found in physics, the first two or three terms of this expansion suffice to determine energy eigenvalues reasonably accurately even in the case of small quantum numbers $n\sim 1$ (see Refs. 9–12 for examples).

There are several versions of the $1/N$ expansion differing in the choice of the parameter N, the "shifted" $1/N$ expansion being an example.[16,17] We will be concerned with the version which has been suggested in Ref. 9 and applies to both discrete and quasistationary states. In this case $N\equiv n=l+p+1$, where $p=0,1,2,...$ is the radial quantum number (also frequently denoted by n_r) and l is the orbital angular momentum, it being understood that p is fixed and $l\to\infty$. Therefore in what follows we will speak of the $1/n$ expansion (in the case of the Coulomb field n is the principal quantum number of the state).

In the present work the $1/n$ expansion method is applied to the calculation of wave functions. Over most of the range within which the motion of the particle is finite, this poses no problems of principle since higher $1/n$ corrections to $\psi^{(0)}\times(\mathbf{r})$ are in fact anharmonic ones, for which effective calculation methods have been developed.[1,2,4,18]

On the other hand, there are many problems in which the wave function deep under the barrier and, in particular, the asymptotic coefficients for $r\to 0$ and $r\to\infty$, are important:

$$\chi_{lp}=(r)\begin{cases} c_{lp}r^{l+1}+\ldots, & r\to 0,\\ a_{lp}(2\kappa)^{1/2}e^{-\kappa r}+\ldots, & r\to\infty,\end{cases} \tag{1}$$

where $\kappa=(-2mE)^{1/2}/\hbar$. The values of $\psi^2(0)$ (or more precisely the $|c_{lp}|^2$) give the probability of finding particles close together and are particularly important parameters for systems having interactions involving two very different radii (for example, the nuclear and Coulomb interactions). Thus, they are crucial in calculating the decay widths of charmonium[21] and bottomonium[22] or in finding the finite-nucleus Lamb shift correction. Examples from another area of physics include the nuclear fusion reaction rate for the mesomolecules ddμ and dtμ (see Refs. 23 and 24), and the probability of muon attachment to an α particle in the course of a nuclear reaction.[25]

For level shifts in short-range atomic systems (such as the hadron atoms $\bar{p}p$, $\bar{K}K$, $\bar{K}\alpha$, etc.), there is a perturbation formula in the scattering length,

$$\Delta E_{lp}\approx\frac{\hbar^2}{2m}[(2l+1)!!]^2|c_{lp}|^2a_l^{(s)},$$

where $a_l^{(s)}$ is the l-scattering length at a short-range ("strong") potential $V_s(r)$, and where the coefficient c_{lp} corresponds to the wave function in the long-range potential $V(r)$, i.e. with no account for the perturbation from the potential V_s. If the potential is $V(r)=-1/r$, the coefficients c_{lp} are given by Eq. (25), and the above formula[1)] recovers the well-known results of Ref. 26 (for $l=0$) and Refs. 27 and 28 (for any l).

The asymptotic form of the wave function at infinity[2)] is needed in the calculation of the effective radius $r_l^{(s)}$ (see Ref. 33) used in the low energy scattering theory;[34] in the treatment of the long-range interaction in atomic systems; in the theory of atomic and ionic ionization,[35] etc. Examples of this kind could be multiplied easily.

We briefly outline the contents of the work. In Sec. 2 analytical formulas (9) and (10) are presented for the asymptotic coefficient at zero, valid for states with $p=0$ and 1 in an arbitrary smooth potential $V(r)$. Section 3 discusses their

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accuracy for the cases of power and short-range potentials. It is shown that even for small angular momentum l the formulas give $\psi(0)$ with sufficient accuracy for most physical problems. The conclusion (Sec. 4) gives a comparison between the $1/n$ expansion and the WKB approximation corrected for the small r region. In Appendix A, higher corrections and the associated divergence of the $1/n$ expansion are discussed using exactly solvable potentials as examples. In Appendix B, a generalization of the turning point matching conditions for quasiclassical wave functions is obtained, markedly improves on WKB accuracy for small l.

2. ASYMPTOTIC COEFFICIENT AT ZERO

We write the interaction potential as

$$V(r)=n^2 g\frac{\hbar^2}{mR^2}v(r/R), \tag{2}$$

where $v(x)$ is a dimensionless function determining the shape of the potential; from now on we take $\hbar=m=R=1$. We express the energy E and the effective potential (incorporating the centrifugal energy) in the form

$$E_{np}=n^2\left(\varepsilon^{(0)}+\frac{\varepsilon^{(1)}}{n}+\frac{\varepsilon^{(2)}}{n^2}+\ldots\right),$$

$$V_{\text{eff}}=n^2\left(\frac{1}{2r^2}-\frac{2p+1}{2nr^2}+\frac{p(p+1)}{2n^2r^2}+gv(r)\right) \tag{3}$$

$(n=l+p+1)$ and expand the Schrödinger equation in terms of the parameter $1/n$:

$$\chi''-n^2Q^2\chi=0,\quad Q^2(r)=Q_0^2+Q_1^2n^{-1}+Q_2^2n^{-2}+\ldots,$$
$$Q_0^2=r^{-2}+2gv(r)-2\varepsilon^{(0)},\quad Q_1^2=-(2p+1)r^{-2}-2\varepsilon^{(1)}, \tag{4}$$
$$Q_2^2=p(p+1)r^{-2}-2\varepsilon^{(2)}.$$

For $n\to\infty$ the particle is localized near the classical equilibrium point r_0 (the effective potential minimum position), which gives[9]

$$gr_0^3v'(r_0)=1,\quad \varepsilon^{(0)}=\tfrac{1}{2}r_0^{-2}+gv(r_0). \tag{5}$$

To next order in $1/n$ the expressions (4) near the point r_0 reduce to the Schrödinger equation for a harmonic oscillator of frequency $n\omega$, where

$$\omega=[3r_0^{-4}+gv''(r_0)]^{1/2}. \tag{6}$$

Introducing the variable

$$\xi=(n\omega)^{1/2}(r-r_0), \tag{7}$$

which remains of order unity as $n\to\infty$, to a first approximation we have

$$\varepsilon^{(1)}=(p+1/2)(\omega-r_0^{-2}),$$
$$\chi_{lp}^{(0)}=(n\omega/2^{2p}\pi(p!)^2)^{1/4}H_p(\xi)e^{-\xi^2/2}. \tag{8}$$

The basic idea of the subsequent calculations is as follows. For ξ within the main localization region of the particle, the anharmonic corrections of order $n^{-1/2}\xi, n^{-1/2}\xi^3$, and $n^{-1}\xi^4$ in the potential are treated as perturbations (the same region determines, up to and including terms of order $1/n$, the normalization of the wave function). In the subbarrier region, the WKB wave function, including the first-order correction in the quasiclassical parameter,[36] is employed, with $1/n$ playing the role of the formal expansion parameter $\hbar$. These two expressions overlap in the region $1\ll\xi\ll n^{1/2}$. Their matching yields the required formula[3)] for the asymptotic coefficient at zero,

$$c_{lp}^{(1)}=c_{lp}^{(0)}(1+d(p)/n), \tag{9}$$

accurate to terms $\sim 1/n^2$ (upper indices, 0 or 1, indicate the number of terms retained in the $1/n$ expansion). Here[4)]

$$c_{lp}^{(0)}=\left[\frac{n\omega^3r_0^4}{\pi(p!)^2}\right]^{1/4}(2n\omega r_0^4)^{p/2}\exp\{-[nJ_c+(2p+1)J_1]\}, \tag{10}$$

$$d(p)=-(J_2+J_3), \tag{11}$$

where

$$J_0=\ln r_0+\int_0^{r_0}dr\left[Q_0(r)-\frac{1}{r}\right],$$

$$J_1=\frac{1}{2}\int_0^{r_0}dr\left[\frac{r_0}{r(r_0-r)}-\frac{P_0(r)}{Q_0(r)}\right],$$

$$J_2=\int_0^{r_0}dr\left\{\frac{1}{8}\left[\frac{1}{r^4}+\frac{1}{3}gv''(r)-(1+s)P_0^2(r)\right]Q_0^{-3}\right.$$
$$-\left(\varepsilon^{(2)}-\frac{s}{8r^2}\right)Q_0^{-1}+\frac{1+3s/2}{12\omega(r_0-r)^3}$$
$$\left.+\frac{1}{2(r_0-r)^2}\left[\frac{1+s}{\omega^2r_0^3}+\left(1+\frac{3}{4}s\right)\omega^{-1/2}A\right]\right\}, \tag{12}$$

$$s=4p(p+1),\quad P_0(r)=r^{-2}-r_0^{-2}+\omega,$$

$$\varepsilon^{(2)}=\left\{\frac{s}{8}-\frac{15}{16}\left(\frac{22}{15}+s\right)A^2+\frac{3}{8}(2+s)B-\frac{1}{4}(1+s)\right.$$
$$\left.\times[6AC^{3/2}+2C^3+3C^2]\right\}\omega, \tag{13}$$

$$J_3=k_0+k_1A^2+k_2B+k_3C+k_4C^2+k_5C^3+k_6AC^{1/2}$$
$$+k_7AC^{1/2}, \tag{14}$$

and the quantities ω, r_0, and $Q_0(r)$ have been defined above. We have introduced the dimensionless quantities

$$A=\alpha\omega^{-5/2}=\frac{1}{6}g\omega^{-5/2}v'''(r_0)-2C^{5/2},$$
$$B=\beta\omega^{-3}=\frac{1}{24}g\omega^{-3}v^{(IV)}(r_0)+\frac{5}{2}C^3,\quad C=1/\omega r_0^2, \tag{15}$$

the first two of which are associated with the anharmonic corrections ($n^{-1/2}\alpha\omega^{-3/2}\xi^3$ and $n^{-1}\beta\omega^{-2}\xi^4$) in the effective potential in (3) near the equilibrium point r_0, and $C=n(r_q/r_0)^2$, where $r_q=(n\omega)^{-1/2}$ is the amplitude of the zero-point oscillations of the particle near the equilibrium point.[5)] Finally, thecoefficients k_i in Eq. (14) are determined by matching the quasiclassical wave function (with correc-

TABLE I. Coefficients k_i in Eq. (14).

p	i							
	0	1	2	3	4	5	6	7
0	−1/24	293/96	−61/48	1/24	13/8	1/2	1/2	11/4
1	−13/24	1217/96	−217/48	13/24	81/8	9/2	7/2	63/4

tions of order $1/n$) with the anharmonic oscillator wave function; their numerical values for $p=0$ and 1 are given in Table I. Note that while for an arbitrary p the structure of Eq. (14) remains, to find the coefficients k_i requires more involved calculations.[6)]

Equations (9)–(15) determine the value of $\psi(0)$ in explicit analytical form for an arbitrary smooth potential $V(r)$. Although somewhat unwieldy, calculation of the c_{lp} requires only single integrals and can easily be carried out numerically. We emphasize that although the integrands in J_1 and J_2 contain power-law-singular terms as $r\to r_0$, these latter completely cancel and so the integrals do converge (as a result of the regularization procedure). For the Coulomb potential and for the harmonic oscillator, the integrals in (12) are all done analytically; see Eqs. (23) and (26) below.

Note that expressions (9) and (10) are asymptotically exact for $l\to\infty$ (and the number of nodes p fixed). In applications, however, one often encounters states with small quantum numbers, for which the accuracy of the above formulas is not *a priori* obvious. In order to elucidate this question, we now turn to specific examples.

3. ACCURACY OF ASYMPTOTIC FORMULAS

We consider the power-law attractive potentials[7)]

$$v(r)=r^N/N, \quad N>-2 \tag{16}$$

and short-range potentials, for which we take as prototypes the Yukawa and exponential potentials

$$v(r)=-e^{-r}/r, -e^{-r}. \tag{17}$$

Figures 1 and 2 give the values of the quantities

$$\rho_{lp}^0=c_{lp}^{(0)}/c_{lp}-1, \quad \rho_{lp}^{(1)}=c_{lp}^{(1)}/c_{lp}-1 \tag{18}$$

for the power potentials, where the c_{lp} are the exact asymptotic coefficients at zero obtained by numerical integration of the Schrödinger equation, and where the $c_{lp}^{(0,1)}$ are the approximate forms (9) and (10). From the figures it is seen that for nodeless states (including the ground state) even the "zeroth" approximation (10) is accurate to a few percent. At the same time, for the states with $p=1$ the accuracy of this approximation is clearly not sufficient. This is because the coefficients $d(p)$ increase dramatically with increasing p (see the Appendix). Nevertheless, for one-node states ($p=1$) a correction $\propto 1/n$ ensures quite a satisfactory accuracy for the coefficients c_{lp}, especially for $l\geqslant 1$.

We emphasize that the coefficients themselves change by many orders of magnitude, as seen from Fig. 2. Their decrease with l is due to the centrifugal barrier, whereas the decrease in changing from $N=4$ (anharmonic oscillator) to $N=-1$ (Coulomb potential) is explained by the "swelling" of the bound state:

$$\langle r\rangle_{nl}\sim n^{2/(N+2)}, \quad E_{nl}\sim n^{2N/(N+2)}. \tag{19}$$

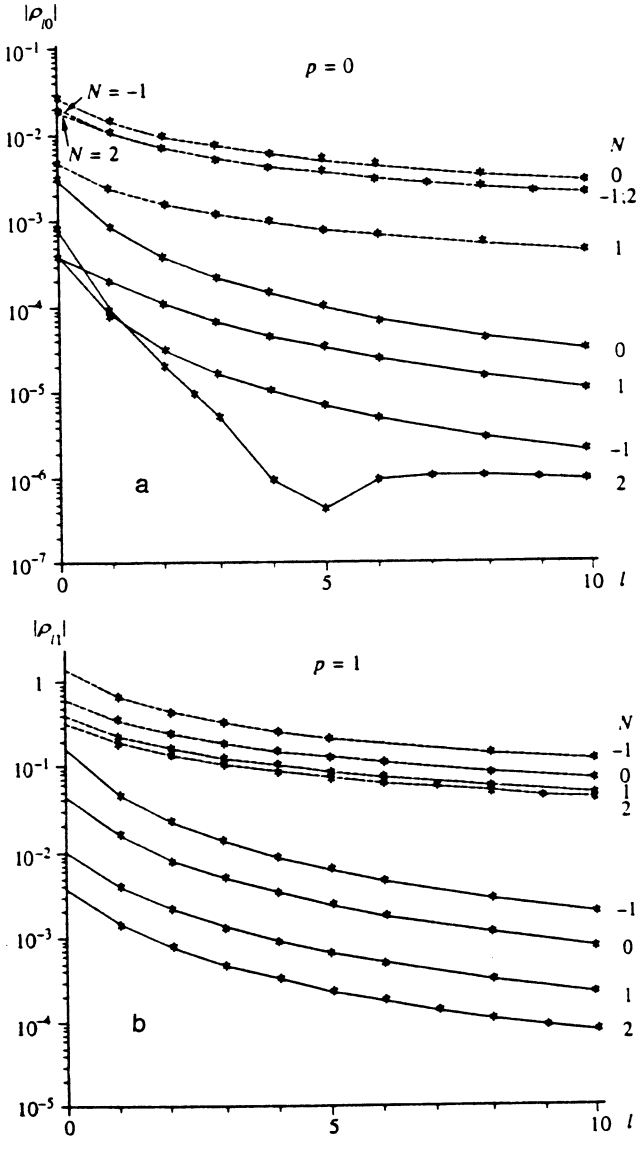

FIG. 1. Accuracy of the $1/n$ expansion for $\psi(0)$ with power potentials: a) nodeless states, $p=0$; b) $p=1$. Dashed lines correspond to the asymptotic form (10), solid curves are constructed from (9), i.e., by including the correction $\sim 1/n$. The curves are marked by the values of the exponent N.

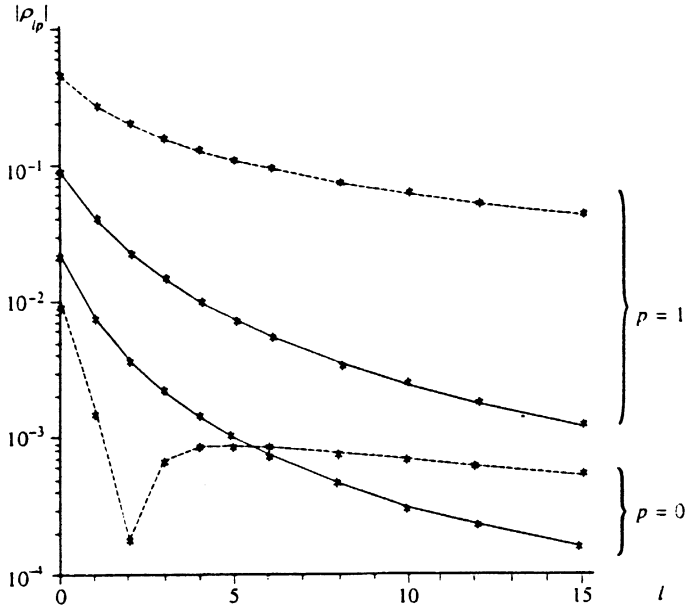

FIG. 2. Same as in Fig. 1, for the anharmonic oscillator ($N=4$).

As seen from Table II, the coefficients c_{lp} fall off especially sharply (for $l \gg 1$) in the case of the Coulomb potential. This is explained by the fact that in this case $E_n = -1/2n^2 \to 0$ for $n \to \infty$, and the penetrability of the centrifugal barrier for such slow particles is of order $D_l \propto \exp(-4l \ln l) \sim [(2l)!]^{-2}$; accordingly, $c_{lp} \propto D_l^{1/2} \propto 1/(2l)!$.

For large l, the numerical calculation of the asymptotic coefficients runs into difficulties since they fall off factorially,[8]

$$c_{lp} \propto a^l l^{\nu+p/2}/(\mu l)!, \tag{20}$$

whereas $1/n$ expansion formulas become more accurate with increasing l. Here $\mu = 2/(N+2)$, $\nu = 3(N-2)/4(N+2)$, and the parameter

$$a + -J_0 + \mu \ln(\mu/e)$$

is a rather insensitive function of the exponent N, varying from $a = 4/e = 1.472$ for $N = -1$ to $a = e/2 = 1.359$ for $N \gg 1$. The asymptotic form (20) is nontrivial but follows readily from Eqs. (9) and (10).

In general, with increasing angular momentum l the values of the $|\rho_{lp}|$ decrease monotonically $\propto 1/n$ and $\propto 1/n^2$ for the approximations (10) and (9), respectively. Sometimes, though, nonmonotonic behavior shows up (see curves with $p=0$ for the harmonic and anharmonic oscillators). This has to do with the fact that the first two corrections in the expansion

$$\rho_{lp} = C_{lp}^{(1)}/c_{lp} - 1 = d_2/n^2 + d_3/n^3 + \ldots, \tag{21}$$

cancel, the necessary condition for this being that the first coefficient be small. In the case of a harmonic oscillator $d_2 = -2.17 \cdot 10^{-4}$, $d_3 = 1.22 \cdot 10^{-3}$ for $p=0$ (see Appendix A), so that $|d_2| \ll d_3$. Accordingly, $|\rho_{l0}|$ has a minimum at $n = -d_3/d_2 \approx 5.6$, in perfect agreement with Fig. 1a.

For the short-range potentials the situation is similar except for the shallow level case $g \approx g_{lp}$, where g_{lp} is the value of the coupling constant when the lp level appears (the numerical values of the g_{lp} are given in Table III). This is illustrated in Table IV for states with $p=0$ and in Fig. 3 for $p=1$. The correction $\propto 1/n$ improves the accuracy of the asymptotics considerably, especially in the case $p=1$, and for $g/g_{lp} \gtrsim 2$ ensures accuracy to within at least a few percent for the c_{lp} for all l, including $l=0$.

TABLE II. Coefficients at zero for power potentials.

l	$N=-1$	$N=0$	$N=1$	$N=2$	$N=4$
0	2.000	1.397	1.414	1.502	1.702
	7.071(−1)	9.980(−1)	1.414	1.840	2.604
1	2.041(−1)	5.827(−1)	9.237(−1)	1.227	1.749
	1.210(−1)	5.716(−1)	1.205	1.939	3.513
2	9.016(−3)	1.535(−1)	4.367(−1)	7.758(−1)	1.483
	6.988(−3)	1.831(−1)	6.774(−1)	1.451	3.563
3	2.201(−4)	2.957(−2)	1.663(−1)	4.147(−1)	1.114
	2.040(−4)	4.064(−2)	2.934(−1)	8.796(−1)	3.055
4	3.400(−6)	4.492(−3)	5.380(−2)	1.955(−1)	7.650(−1)
	3.600(−6)	6.897(−3)	1.052(−1)	4.584(−1)	2.332
5	3.619(−8)	5.635(−4)	1.527(−2)	8.335(−2)	4.897(−1)
	4.261(−8)	9.473(−4)	3.250(−2)	2.125(−1)	1.629
10	9.129(−20)	2.285(−9)	7.082(−6)	4.100(−4)	2.540(−2)
	1.507(−19)	5.200(−9)	2.012(−5)	1.390(−3)	1.136(−1)
20	2.955(−48)	7.880(−23)	2.386(−14)	4.248(−10)	7.970(−6)
	6.882(−48)	2.478(−22)	9.290(−14)	1.970(−9)	4.910(−5)

Note. For given l and N, the first row refers to states with $p=0$ and the second, to those with $p=1$. The coefficients c_{lp} correspond to the potential $V(r) = r^N/N$, i.e., to $g = n^{-2}$ in Eq. (2).

TABLE III. Coupling constants g_{lp} at the instant the level emerges.

l	$V(r)=-gr^{-1}\exp(-r)$		$V(r)=-g\exp(-r)$	
	$p=0$	$p=1$	$p=0$	$p=1$
0	0.8399	3.2236	0.7229	3.8089
1	4.5410	8.8723	3.5245	8.4606
2	10.947	17.210	8.1358	14.940
3	20.068	28.257	14.629	23.259
4	31.904	42.018	22.946	33.423
5	46.459	58.496	33.109	45.432
10	160.00	181.65	111.62	133.18

Note that in the case $g=g_{lp}$ one can develop a modification of the $1/n$ expansion specifically for zero-energy states by setting $E=0$ in the Schrödinger equation and expanding the wave function and the coupling constant g_{lp} in a power series in $1/n$. In this way one can obtain a formula determining the coefficients c_{lp} and a_{lp} at the instant when the level appears. This question (including the effective-radius calculation) will be treated separately.

4. QUASICLASSICAL APPROXIMATION FOR $\phi(0)$

As noted, the accuracy of the $1/n$ expansion diminishes with the number of nodes. In the case $p\geqslant 2$ the approximation (9) fails at small values of l. On the other hand, for states with $p\geqslant 1$ one can employ the WKB method, whose range of applicability usually extends[38] to values $p\sim 1$. One therefore expects that the $1/n$ expansion and WKB combined should solve the problem of the analytical calculation of the wave functions and $\psi(0)$. Here we will consider this question by using the examples of the oscillator and Coulomb potentials, for which exact solutions are known.

In the case of the harmonic oscillator, $V(r)=r^2/2$, from the exact solution of the Schrödinger equation we obtain

$$c_{lp}=[2\Gamma(n+1/2)/\Gamma(n-l)\Gamma^2(l+3/2)]^{1/2}. \tag{22}$$

The parameters in Eqs. (9) and (10) are $\omega=2$, $r_0=1$, $\alpha=-2$, and $\beta=5/2$, and the integrals in (12) are evaluated in elementary fashion to give

$$J_0=-1/2,\quad J_1=(1/2)\ln 2,\quad J_2(p)=(10p(p+1)+1)/64,$$
$$J_3(0)=-7/192,\quad J_3(1)=29/192. \tag{23}$$

The $1/n$ expansion takes the form

$$c_{lp}=\left(\frac{2}{\pi}\right)^{1/4}\left(\frac{e}{n}\right)^{1/2}\frac{n^p}{(p!)^{1/2}}\left[1-\frac{p^2-1/24}{2n}+O\left(\frac{1}{n^2}\right)\right]. \tag{24}$$

Similarly, for the Coulomb potential $V(r)=-1/r$ we have

$$c_{lp}=\frac{2^{l+1}}{(2l+1)!n^{3/2}}\left\{\prod_{j=1}^{l}(1-j^2/n^2)\right\}^{1/2}, \tag{25}$$

$$\omega=1,\quad r_0=1,\quad \alpha=-1,\quad \beta=3/2,$$
$$J_0=1,\quad J_1=0,\quad J_2(p)=0,\quad J_3(0)=1/48,$$

TABLE IV. Accuracy of the $1/n$ expansion for short-range potentials (nodeless states).

g/g_{l0}	$l=0$	1	2	3	5
1.10	—	−8.5 (−2)	−1.1 (−2)	−4.6 (−3)	−1.5 (−3)
	—	9.1 (−3)	1.1 (−2)	3.5 (−3)	1.6 (−3)
1.20	—	−1.7 (−2)	−4.5 (−3)	−1.8 (−3)	−7.4 (−4)
	—	4.1 (−3)	2.8 (−3)	1.7 (−3)	8.0 (−4)
1.50	−0.135	−3.6 (−3)	−1.1 (−3)	−5.7 (−4)	−2.3 (−4)
	−2.1 (−2)	1.8 (−3)	9.6 (−4)	5.8 (−4)	2.7 (−4)
2	−1.3 (−2)	−1.2 (−3)	−4.1 (−4)	−2.2 (−4)	−8.7 (−5)
	−2.7 (−4)	8.5 (−4)	4.0 (−4)	2.3 (−4)	1.0 (−4)
3	−3.3 (−3)	−3.8 (−4)	−1.5 (−4)	−7.7 (−5)	−3.2 (−5)
	1.3 (−3)	2.5 (−4)	9.6 (−5)	5.0 (−5)	2.1 (−5)
5	−1.1 (−3)	−1.5 (−4)	−6.0 (−5)	−3.3 (−5)	−1.3 (−5)
	2.3 (−4)	−9.4 (−5)	−6.1 (−5)	−3.9 (−5)	−2.0 (−5)
10	−5.0 (−4)	−8.4 (−5)	−3.7 (−5)	−1.8 (−5)	−8.0 (−6)
	−5.6 (−4)	−2.7 (−4)	−1.4 (−4)	−8.6 (−5)	−3.9 (−5)

Note. Values of $\rho_{l0}^{(1)}$ are presented [see Eq. (18)]. In cases in which the error due to a given approximation exceeds 15%, dashes are indicated. The first row refers to the Yukawa potential, the second to the exponential potential.

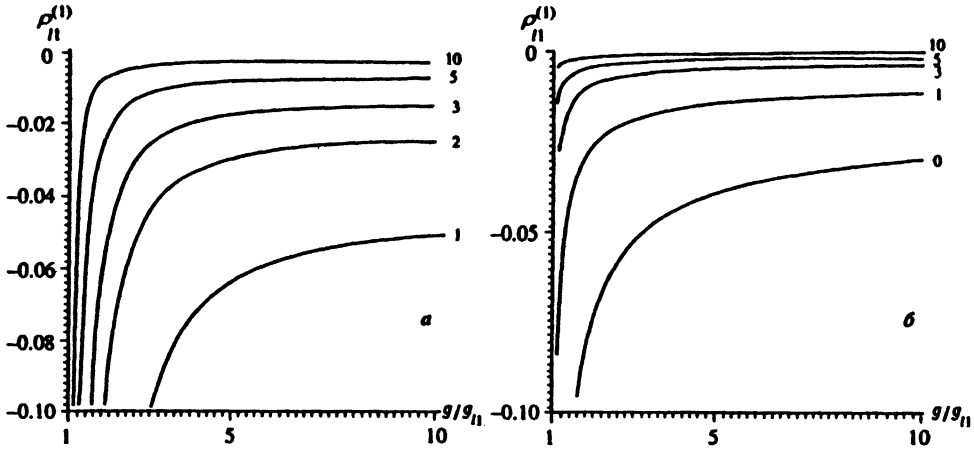

FIG. 3. Accuracy of the $1/n$ expansion for short-range potentials ($p=1$): a) Yukawa potential; b) exponential potential. The curves are marked by the values of the orbital angular momentum l.

$$J_3(1)=61/48, \tag{26}$$

giving

$$c_{lp}=(\pi n^3)^{-1/4}\left(\frac{e}{n^2}\right)^n\frac{(2n^5)^{p/2}}{(p!)^2}\left[1-\frac{7p^2+3p+1/6}{8n}\right]+\ldots]. \tag{27}$$

In these two cases, one can also calculate further terms in the $1/n$ expansion (see Appendix A). This makes it possible to trace the role of higher corrections in the $1/n$ expansion as the number of nodes increases, and also to show that the series in Eqs. (24) and (27) are asymptotic.

It can be seen just from Eqs. (24) and (27) that the correction terms in the $1/n$ expansion increase rapidly with increasing p, so for large p it is natural to change to the WKB method. Its application to the asymptotic coefficient c_{lp} encounters certain difficulties due to the nonquasiclassical nature of centrifugal potential for $l\sim 1$ at short distances. It is commonly believed[38,39] that this problem is resolved by introducing the Langer correction, i.e., by replacing $l(l+1)$ by $(l+1/2)^2$. In the case of the Coulomb and oscillator potentials this approach leads to exact expressions for the energy levels, whereas for the asymptotic coefficients it yields the values (B2) and (B3), which we denote by $c_{lp}^{(q)}$

It turns out, however, that for l fixed these formulas are not asymptotically exact for $p\to\infty$, the Langer transformation notwithstanding. For the harmonic oscillator ($N=2$) we have

$$\eta_0=(e/2)^{1/2}=1.1658, \quad \eta_1=1.0563,$$
$$\eta_2=1.0337, \tag{28}$$

and in the Coulomb potential case ($N=-1$) we have

$$\eta_0=e(2\eta)^{-1/2}=1.0844, \quad \eta_1=1.0281,$$
$$\eta_2=1.0168, \tag{28'}$$

where $\eta_l=\lim c_{lp}^{(q)}/c_{lp}$ for $p\to\infty$. The explanation is the failure, in the present case, of the usual[36] linearized-$V(r)$ matching condition for the wave functions on either side of the turning point. For the details see Appendix B, which shows that the expressions (B2) and (B3) must both be supplemented by the factor (B8). After this, the correct quasiclassical formulas for the coefficient at zero become

$$c_{lp}^{(Q)}=\frac{2^{1/2}n^{(2l+1)/4}}{\Gamma(l+3/2)}\exp(-nf(\rho)), \quad N=2, \tag{29}$$

$$c_{lp}^{(Q)}=\frac{2^{l+1}}{(2l+1)!n^{3/2}}\exp(-ng(\rho)), \quad N=-1. \tag{30}$$

Here

$$\rho=(l+1/2)n, \quad n=l+p+1,$$

$$f(\rho)=\frac{1}{2}[\rho+(1-\rho)\ln(1-\rho)], \quad g(\rho)=f(\rho)-f(-\rho). \tag{31}$$

These formulas are free from the shortcoming mentioned above: if $p\gg 1$ and the angular momentum l is fixed, then the coefficients $c_{lp}^{(Q)}$ rapidly approach their exact values, merging into them as $p\to\infty$:

$$\delta_{lp}\equiv\frac{c_{lp}^{(Q)}}{c_{lp}}=\begin{cases}1-(2l+1)/96n^2+\ldots, & N=2,\\ 1-(21+l)/48n^2+\ldots, & N=-1.\end{cases} \tag{32}$$

The values δ_{lp} in the limiting cases $l=0,1$ and $l\gg 1$ are listed in Table V, from which it follows that the corrected quasiclassical formulas (29) and (30) provide accuracy to within a few percent for c_{lp} even if the number of nodes satisfies $p\geqslant 1$. On the other hand, for nodeless states (as well as for $p=1$ and $l\gtrsim 3$) the $1/n$ expansion, which is asymptotically exact for large l and arbitrary (but fixed) p, is preferable. Thus, using the $1/n$ expansion for $p=0$ and 1 and the WKB method for $p\geqslant 1$ provides for c_{lp} analytical formulas completely covering the range of possible values of quantum numbers.

The approach we have developed may be used in calculating wave functions for finite r and in finding asymptotic coefficients of practical interest for $r\to\infty$.

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TABLE V. Accuracy of the $1/n$ expansion and of the WKB method for $\psi(0)$.

N	l	$p=0$		$p=1$		$p=2$
		ВКБ	$1/n$	ВКБ	$1/n$	ВКБ
2	0	0.9838	1.00076	0.9967	1.0035	0.9986
	1	0.9744	1.000088	0.9934	1.0014	0.9969
	∞	0.9645	1.00000	0.9865	1.0000	0.9918
-1	0	0.9776	0.99962	0.9947	0.8508	0.9977
	1	0.9702	0.999924	0.9911	0.9537	0.9955
	∞	0.9645	1.00000	0.9865	1.0000	0.9918

Note. The ratios $c_{lp}^{(1)}/c_{lp}$ and $c_{lp}^{(Q)}/c_{lp}$ are presented [quasiclassical values for $p\to\infty$, see Eq. (32)].

APPENDIX A

Higher order $1/n$ expansion corrections for the Coulomb and oscillator potentials

Let

$$\frac{C_{lp}^{(0)}}{c_{lp}}=\exp\left(\frac{\beta_1}{n}+\frac{\beta_2}{n^2}+\ldots\right), \quad n\to\infty, \tag{A1}$$

where the β_k are coefficients dependent on the radial quantum number $p\equiv n_r$. They can be found explicitly in cases for which the exact solutions of the Schrödinger equation are known. For the Coulomb potential we have, for $p=0$,

$$c_{l0}=2^n n^{-(n+1)}[(2n-1)!]^{-1/2},$$

$$c_{l0}^0=(\pi n^3)^{-1/4}\left(\frac{e}{n^2}\right)^n. \tag{A2}$$

Using the Stirling formula, this gives

$$\beta_k=\beta_{k+1}/2^{k+1}k(k+1). \tag{A3}$$

It can be shown[11] that for an arbitrary p

$$\beta_k=\frac{1}{2^k k(k+1)}\left[B_{k+1}(2p+1)-\frac{1}{2}B_{k+1}(p+1)\right], \tag{A4}$$

where B_n and $B_n(x)$ are the Bernoulli numbers and polynomials, respectively. In particular,

$$\beta_1=\frac{1}{48}(42p^2+18p+1), \quad \beta_2=\frac{1}{32}p(10p^2+7p+1),$$

$$\beta_3=\frac{1}{24}[p^2(2p+1)^2-1/240]. \tag{A5}$$

Similarly, in the harmonic oscillator case

$$\beta_k=\frac{1}{k(k+1)}\left[B_{k+1}(p+1/2)-\frac{1}{2}B_{k+1}(1/2)\right], \tag{A6}$$

$$\beta_1=\frac{1}{2}\left(p^2-\frac{1}{24}\right), \quad \beta_2=\frac{1}{6}p\left(p^2-\frac{1}{4}\right),$$

$$\beta_3=\frac{1}{12}\left(p^4-\frac{1}{2}p^2+\frac{7}{480}\right). \tag{A7}$$

The states with $p=0$ satisfy the relation

$$\beta_k(N=2)=-(2^k-1)\beta_k(N=-1), \tag{A8}$$

where $\beta_k\equiv 0$ for k even.

Note that the coefficients in (21) relate in a simple manner to the β_k:

$$d_2=\beta_2-\tfrac{1}{2}\beta_1^2, \quad d_3=\beta_3-\tfrac{1}{3}\beta_1^3,$$

$$d_4=\beta_4+\tfrac{1}{2}\beta_2^2-\tfrac{1}{2}\beta_2\beta_1^2-\tfrac{1}{8}\beta_1^4,\ldots . \tag{A9}$$

For the harmonic oscillator this yields the values given in the bulk of the paper, and for the Coulomb potential we have $(p=0)$: $d_2=-2.170\cdot 10^{-4}$, $d_3=-1.766\cdot 10^{-4}$. In the latter case the coefficients d_2 and d_3 have the same sign, so the corresponding curve in Fig. 1a is monotonic. We also display their values for $p=1$:

$$d_2=1.020(-2), \quad d_3=6.210(-3) \quad \text{for} \quad N=2,$$

$$d_2=-0.245, \quad d_3=-0.309 \quad \text{for} \quad N=-1.$$

This agrees with the shape of the curves in Fig. 1b.

Finally, for $k\to\infty$,

$$\beta_k\approx\text{const}[1-(-1)^k]\Gamma(k)a^{-k}, \quad p=0, \tag{A10}$$

where $a=(2\pi)^{-1}$ and $(4\pi)^{-1}$ for $N=2$ and $N=-1$, respectively. Thus, the $1/n$ expansion for c_{lp} is a divergent (asymptotic) series.

APPENDIX B

Quasiclassical wave functions including the Langer correction

As is well known,[36,38] the centrifugal potential at $l\sim 1$ does not satisfy the quasiclassical condition. Therefore the quasiclassical solution yields a wrong wave function behavior for $r\to 0$, one different from Eq. (1). However, if one makes the change of variable $r=e^{-x}$ and transforms to the function $w=e^{x/2}\chi_{lp}$, the Schrödinger equation becomes

$$\frac{d^2w}{dx^2}+\left[2(E_{lp}-V(e^{-x}))e^{-2x}-\left(l+\frac{1}{2}\right)^2\right]w=0 \tag{B1}$$

[i.e., it retains its form, with energy represented by $-(2l+1)^2/8$)]. The point $r=0$ now moves to $x=\infty$ and large distances x are quasiclassical for Eq. (B1). When applying the WKB method to this equation it is found that in the Bohr–Sommerfeld quantization rule, when converted back to the original variable r, the Langer correction automatically

appears[38,39]. For the asymptotic coefficients at zero, in the case of the oscillator and Coulomb potentials we get

$$c_{lp}^{(q)}=\left(\frac{2}{\pi}\right)^{1/2}\frac{(2n)^{n/2}}{(2l+l)^{l+1}}\frac{(2e)^{(2l+1)/4}}{(2p+1)^{(2p+1)/4}},\quad N=2, \tag{B2}$$

$$c_{lp}^{(q)}=\frac{(2e)^{l+1/2}}{n^{l+2}(2l+1)^{2l+3/2}}\left[\frac{(n+l+1/2)^{n+l+1/2}}{\pi(n-l-1/2)^{n-l-1/2}}\right]^{1/2},$$

$$N=-1. \tag{B3}$$

However, in calculating the sub-barrier wave function, and in particular $\psi(0)$, some refinement is needed. An important feature of the WKB method is matching the quasiclassical solution on either side of the turning point by linearly expanding the potential. In the case of Eq. (B1) with $l\sim 1$, this approach fails and must be refined.

For this, let us discuss the matching of the quasiclassical solutions of the Schrödinger equation for a one-dimensional exponential potential $V(x)=-V_0e^{-x/a}$. Making the substitution ($m=\hbar=1$)

$$z=\xi e^{-x/2a},\quad \xi=\sqrt{8V_0a^2},\quad \nu\sqrt{-8Ea^2}, \tag{B4}$$

we obtain the solution of the Schrödinger equation in terms of the Bessel functions as

$$\psi(x)=\text{const}\,J_\nu(\xi e^{-x/2a}) \tag{B5}$$

(with the boundary condition $\psi\to 0$ as $x\to\infty$). Using the $z\gg 1$ asymptotics of $J_\nu(z)$, in the region of classical motion we obtain (b the turning point)

$$\psi(x)\sim C_1(p(x))^{1/2}\sin\left\{\int_x^b p(x)dx+\frac{\pi}{4}\right\},\quad x<b. \tag{B6}$$

The asymptotics of $J_\nu(z)$ as $z\to 0$ (i.e., $r\to 0$) leads to a quasiclassical expression for the sub-barrier wave function:

$$\psi(x)\approx C_2|p(x)|^{-1/2}\exp\left\{-\int_b^x\left|p(x)\right|dx\right\} \tag{B7}$$

($x>b$, or $r<r_0$), and

$$C_2/C_1=(\pi/2)^{1/2}\nu^{\nu+1/2}e^{-\nu}/\Gamma(\nu+1). \tag{B8}$$

Thus, it is only in the case $\nu\gg 1$ [i.e., $l\gg 1$ for Eq. (B1)] that we obtain the well known result[36] $C_2/C_1=1/2$.

Looking at Eq. (B1) near the turning point, one may neglect the term $Ve^{-2x}w$ for the oscillator and $E_{lp}e^{-2x}w$ for the Coulomb potential, which gives

$$\nu=\begin{cases} l+1/2, & N=2,\\ 2l+1, & N=-1.\end{cases} \tag{B9}$$

Using (B8) and (B9) we arrive at Eqs. (29) and (30), which are asymptotically exact for $p\to\infty$ and an arbitrary l.

In conclusion, a similar treatment goes through in a more general case when the potential $V(r)$ for $r\to 0$ has a power-law behavior

$$V(r)\propto r^\alpha,\quad \alpha>-2. \tag{B10}$$

The matching condition (B8) retains its form, and now

$$\nu=\begin{cases}(2l+1)/(2+\alpha), & -2<\alpha<0,\\ l+1/2, & \alpha>0.\end{cases} \tag{B11}$$

Thus the parameter ν involved in the matching condition for quasiclassical wave functions on either side of the turning point depends on both the exponent in (B10) and the orbital angular momentum l.

[1)] Generalization to an abnormally large scattering length, when the strong potential V_s has a shallow "nuclear" level, can be found in Refs. 29–31, in which the rearrangement of the atomic spectrum, or the Zel'dovich effect,[32,25] is discussed.

[2)] Note that as opposed to the case $r\to 0$ this asymptotic form is not universal: Eq. (1) holds if the potential falls off faster than $1/r^2$ as $r\to\infty$. For potentials with a Coulomb tail, the asymptotic form is altered.

[3)] A detailed derivation of this formula involves rather lengthy calculations, in particular the regularization of divergent quasiclassical integrals. This requires special discussion, as does the derivation of wave functions for finite r.

[4)] Formula (10) for the zeroth approximation in $1/n$ was obtained earlier.[37]

[5)] Here the following point must be made. In the present work the definition of the quantities ω and ξ differs from the earlier one,[9,37] namely: $\omega=\tilde{\omega}r_0^{-2}$, $\xi=\tilde{\omega}^{1/2}\tilde{\xi}$, the tilde denoting the quantities from Ref. 37. The frequency of small oscillations in the coordinate r is $\omega_r=n\omega$, and the frequency of those in the variable ξ is unity.

[6)] The relative simplicity of the cases $p=0$ and 1 has to do with the fact that the Hermitian polynomial in (8) reduces to just one term; this considerably simplifies the wave function matching procedure.

[7)] The case of $N=0$ corresponds to the logarithmic potential.

[8)] Here and in what follows, unlike Eq. (2), the factor n^2 is incorporated into the coupling constant g. Due to scaling, the change in the asymptotic coefficient then reduces to multiplication by $n^{-(2l+3)/(N+2)}$.

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