The matching conditions in the WKB method

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The modified matching condition for quasiclassical wave functions on the two sides of a turning point has been obtained for the radial Schrödinger equation. It differs essentially from the usual Kramers condition which holds for one-dimensional problems. Comparison with exact and numerical solutions of the Schrödinger equation shows that the modified matching condition not only makes the quasiclassical approximation in the subbarrier region asymptotically exact in the limit $n\to\infty$, but also considerably enhances its accuracy even in the case of small quantum numbers, $n\sim 1$. Power-law and short-range potentials are considered in detail. It is shown that for zero-energy states in a short-range attractive potential (i.e., at the point when the bound l-state occurs, $l\geqslant 1$) the normalization condition generally used in the WKB method should also be modified. © *1995 American Institute of Physics.*

1. INTRODUCTION

An important point in the WKB method is the matching (or boundary[1]) condition for quasiclassical wave functions defined on either side of a turning point $x=a$:

$$\psi(x)=\begin{cases} Cp^{-1/2}(x)\cos\left(\int_a^x p\,dx-\gamma\right), & x>a,\\ C'|p(x)|^{-1/2}\exp\left(-\int_x^a|p|\,dx\right), & x<a,\end{cases} \tag{1}$$

where[1,2]

$$C'/C=1/2,\quad \gamma=\pi/4. \tag{2}$$

In the one-dimensional case the Kramers boundary condition (2) usually holds for smooth potentials. However, as will be shown below, for three-dimensional problems expression (2) is incorrect in general: the coefficient ratio C'/C is no longer a universal constant, but depends on the orbital angular momentum l and on the behavior of the potential $V(r)$ at short distances [see Eqs. (7), (8), and (8′) below], and only in the limit $l\gg 1$ does it go over to Eq. (2).

2. MODIFIED MATCHING CONDITION

The centrifugal potential for angular momenta $l\sim 1$ does not satisfy the quasiclassical condition at short distances.[1,2] In particular, the quasiclassical treatment leads to incorrect behavior of the wave function in the limit $r\to 0$: it goes as $\chi_l(r)\propto r^s$ with $s=1/2+\sqrt{l(l+1)}$ $(l\neq 0)$, rather than the correct value $s=l+1$. As is well known,[2,3] this difficulty can be overcome by using the Langer transformation:

$$r=e^x,\quad \psi(x)=e^{-x/2}\chi_l(e^x), \tag{3}$$

after which the radial Schrödinger equation assumes the form ($\hbar=m=1$)

$$\frac{d^2\psi}{dx^2}+k^2(x)\psi=0,$$

$$k=\sqrt{-\left(l+\frac{1}{2}\right)^2+2[E_{nl}-V(e^x)]e^{2x}}. \tag{4}$$

Here $-(2l+1)^2/8$ plays the role of the energy, the point $r=0$ maps into to $x=-\infty$, and as follows from (4) in the region of large $|x|$ the quasiclassical condition is satisfied automatically for $x\to-\infty$:

$$\left|\frac{d}{dx}\left(\frac{1}{k(x)}\right)\right|=0(e^{\sigma x})\to 0,$$

$$\sigma=\begin{cases}2, & \alpha>0,\\ \alpha+2, & -2<\alpha<0.\end{cases}$$

[Here α is an exponent that determines the behavior of $V(r)$ in the limit $r\to 0$; see Eq. (5). The condition $\alpha>-2$ or $\sigma>0$ excludes "falling into the center" in quantum mechanics.[1]].

For attractive potentials with power-law behavior at short distances ($r\to 0$),

$$V(r)=\frac{g}{\alpha}r^\alpha, \tag{5}$$

for $\alpha>0$ and sufficiently large values of the energy E we can omit the term with the potential V in Eq. (4), after which it can be solved in terms of Bessel functions:

$$\psi(x)=\text{const}\cdot J_{l+1/2}(\sqrt{2E}e^x). \tag{6}$$

This solution makes it possible to pass through the turning point by matching it with the quasiclassical asymptotic forms (1); after some calculations we find

$$\frac{C'}{C}=\frac{1}{2}\,\xi(\nu),\quad \xi(\nu)=\frac{\sqrt{2\pi}\nu^{\nu+1/2}e^{-\nu}}{\Gamma(\nu+1)}, \tag{7}$$

$$\nu=l+1/2\quad \text{for } \alpha>0. \tag{8}$$

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TABLE I. Values of the function $\xi(\nu)$.

ν	$\xi(\nu)$	ν	$\xi(\nu)$
0.5	0.85776	5	0.98349
1.0	0.92214	5.5	0.98498
1.5	0.94666	6	0.98622
2.0	0.95950	7	0.98817
2.5	0.96738	8	0.98964
3.0	0.97270	9	0.99079
3.5	0.97653	10	0.99170
4.0	0.97942	12	0.99308
4.5	0.98168	20	0.99584

Note. For large ν this function can be calculated using the asymptotic formula (9), in which case the error for $\nu \geqslant 10$ is less than 10^{-5}.

In the case $\alpha<0$ the energy levels usually crowd toward the boundary of the continuum,[1] so that in contrast to the above, in (4) the term $E\exp(-2x)$ should be neglected but the potential (5) should be retained. Ultimately we arrive again at condition (7), in which, however,

$$\nu=(2l+1)/(2+\alpha), \quad -2<\alpha<0. \tag{8'}$$

Note that the function $\xi(\nu)$ is numerically close to unity;[2] see Table I. Thus, we have $\xi(1/2)=\sqrt{2/e}=0.8578$, $\xi(1)=\sqrt{2\pi e^{-1}}=0.9221$, while in the limit $\nu\to\infty$ we have

$$\xi(\nu)=1-\frac{1}{12\nu}+\frac{1}{288\nu^2}+\ldots. \tag{9}$$

Thus, (7) goes over to the usual Kramers matching condition (2) only in the limit $l\gg 1$, while for $l\sim 1$ these two conditions differ. The reason for this is as follows. In order that condition (2) be applicable it is necessary that the region in which the linear approximation $V(x)=V_0-F\cdot(x-a)$ holds for the potential intersect the quasiclassical region where $|(d/dx)(1/k(x)|\ll 1$ holds. In the case we are considering this requirement reduces to the inequality $(2l+1)^{-2/3}\ll 1$, and for $l\sim 1$ it is not satisfied.

3. EVALUATION OF $\psi(0)$

The matching condition (7) determines the wave function in the subbarrier region. As is well known, the value of $\psi^2(0)$ (or rather $|c_{nl}|^2$) is an important physical parameter for systems in which there are interactions with two very different radii, e.g., the strong and electromagnetic interactions (see, e.g., Ref. 4 and the work cited there). At short distances we have

$$\chi_{nl}(r)\equiv rR_{nl}(r)=c_{nl}r^{l+1}+\ldots, \quad r\to 0. \tag{10}$$

Using Eqs. (1)–(4) we can derive the quasiclassical expression for the asymptotic coefficient at zero:

$$c_{nl}^{\mathrm{WKB}}=\sqrt{\frac{2}{(2l+1)T_r}}\,r_-^{-(l+1/2)} \times\exp\left\{\int_0^{r_-}\left[\left(l+\frac{1}{2}\right)r^{-1}-\left|p(r)\right|\right]dr\right\}, \tag{11}$$

where

$$p(r)=\sqrt{2[\tilde{E}_{nl}-V(r)]-\left(l+\frac{1}{2}\right)^2 r^{-2}},$$

$$T_r=2\int_{r_-}^{r_+}\frac{dr}{p(r)}, \tag{11'}$$

$\tilde{E}_{nl}$ is the energy determined by the Bohr–Sommerfeld quantization condition $\int_{r_-}^{r_+}p(r)dr=(q+1/2)\pi$, $r_\pm$ are turning points $(0<r_-<r_+)$, T_r is the classical period of the radial oscillations of the particle, $n=l+q+1$, and $q=0,1,\ldots$ is the radial quantum number (frequently denoted in the literature by n_r). Note that the quasiclassical momentum $p(r)$ is calculated here with the Langer correction,[3] i.e., $l(l+1)$ is replaced by $(l+1/2)^2$.

We emphasize that Eq. (11) has been derived through the application of the usual matching condition (2). From (7) the correct quasiclassical approximation for the coefficient at zero is

$$\tilde{c}_{nl}=\xi(\nu)c_{nl}^{\mathrm{WKB}}. \tag{12}$$

The nontrivial point in (12) is the appearance of the factor $\xi(\nu)$. Here we do not derive Eqs. (7), (11), and (12), but compare them with the results of analytical and numerical calculations of the coefficient c_{nl} for power-law and short-range potentials.

4. EXAMPLES

The integrals that appear in Eqs. (11) and (11′) can easily be calculated for the exactly soluble models of the harmonic oscillator [$\alpha=2$ in Eq. (5)] and the hydrogen atom ($\alpha=-1$); see Appendix A. We also consider other power-law potentials,[3] where the Schrödinger equation can only be solved numerically.[4] Some of these results are shown in Tables II and III, where the following notation is used:

$$\tilde{E}_{nl}/E_{nl}=1+\epsilon_{nl}, \quad \eta_{nl}^{\mathrm{WKB}}=c_{nl}^{\mathrm{WKB}}/c_{nl}, \quad \tilde{\eta}_{nl}=\tilde{c}_{nl}/c_{nl}. \tag{13}$$

Here E_{nl} and c_{nl} are the exact values of the energy and the coefficient at zero, and $\tilde{E}_{nl}$, c_{nl}^{WKB}, and $\tilde{c}_{nl}$ are defined above. For particular values of the quantum numbers n,l (or q,l) in Table III two numbers are given: (A) corresponds to (11), i.e., to the usual matching rule (2) for a turning point; (B) is calculated from Eq. (12), including the factor $\xi(\nu)$.

Let us discuss the results of the calculations. As can be seen from Table III, the modified matching rule (7) in practically all cases, including the ground state ($q=l=0$), substantially increases the accuracy of the quasiclassical approximation for $\psi(0)$. Note the exceptionally high accuracy of Eq. (12) in the case of the anharmonic oscillator ($\alpha=4$).

It should be emphasized that for $n\to\infty$ and fixed l the ratios η_{nl}^{WKB} do not approach unity,[5]

$$\eta_l=\lim_{n\to\infty}\eta_{nl}^{\mathrm{WKB}}=\begin{cases}[\xi(l+1/2)]^{-1}, & \alpha>0\\ \left[\xi\left(\dfrac{2l+1}{\alpha+2}\right)\right]^{-1}, & \alpha<0.\end{cases} \tag{14}$$

Thus, expression (11) is not asymptotically correct, even if the number of nodes satisfies $q\gg 1$. Only after the introduction of the correction $\xi(\nu)$ does Eq. (12) become asymptoti-

TABLE II. Energies E_{nl} for attractive power-law potentials.

α	l , q	E_{nl}	ϵ_{nl}	α	l , q	E_{nl}	ϵ_{nl}
0	0 , 0	0.69776	1.31(−2)	4	0 , 0	1.50790	−2.80(−2)
	0 , 1	1.50087	2.24(−3)		0 , 1	4.62122	−5.73(−3)
	0 , 2	1.94304	9.48(−4)		0 , 2	8.42845	−2.33(−3)
	1 , 0	1.29457	1.56(−3)		0 , 3	1.27383(1)	−1.26(−3)
	1 , 1	1.80437	6.28(−4)		1 , 0	2.82099	−9.19(−3)
	1 , 2	2.14437	3.47(−4)		1 , 1	6.36257	−3.29(−3)
	2 , 0	1.66674	5.13(−4)		1 , 2	1.04570(1)	−1.63(−3)
	2 , 1	2.04086	2.79(−4)		1 , 3	1.49907	−9.63(−4)
	10 , 0	2.91666	2.03(−5)		2 , 0	4.30282	−4.46(−3)
	10 , 1	3.03660	1.73(−5)		2 , 1	8.19236	−2.10(−3)
					2 , 2	1.25463(1)	−1.19(−3)
1	0 , 0	1.85576	4.94(−3)		10 , 0	1.99638(1)	−3.71(−4)
	0 , 1	3.24461	1.60(−3)		10 , 1	2.55651(1)	−2.94(−4)
	0 , 2	4.38167	8.10(−4)		10 , 2	3.13926(1)	−2.37(−4)
	1 , 0	2.66783	1.22(−3)				
	1 , 1	3.87679	6.21(−4)	8	0 , 0	1.80214	−9.66(−2)
	1 , 2	4.92699	3.82(−4)		0 , 1	6.57180	−1.65(−2)
	2 , 0	3.37178	5.37(−4)		0 , 2	1.34512(1)	−6.75(−3)
	2 , 1	4.46830	3.31(−4)		1 , 0	3.58452	−4.07(−2)
	10 , 0	7.58336	3.88(−5)		1 , 1	9.54346	−1.07(−2)
	10 , 1	8.34111	3.35(−5)		10 , 0	3.35398(1)	−2.24(−3)

Note. Here we have set $g=1$; $\alpha=0$ corresponds to the logarithmic potential $V(r)=\ln r$. The quantities ϵ_{nl} characterize the accuracy of the WKB method and are defined in Eq. (13). Here and in what follows the numbers in parentheses give the order of the exponent: $1.31(-2)\equiv 1.31\cdot 10^{-2}$, etc.

cally correct in the limit $q\equiv n_r\to\infty$ (this is a necessary condition for the quasiclassical expression to be correct).

Similar calculations were carried out for short-range Yukawa and Hulthén potentials,

$$V(r)=-g\frac{e^{-r}}{r},\quad uV(r)=-\frac{g}{e^r-1}. \tag{15}$$

Table IV shows the values of the binding constants $g_{nl}^{(cr)}$ and $\tilde{g}_{nl}$ corresponding to $E_{nl}=0$ and $\tilde{E}_{nl}=0$, respectively, i.e., those for which the nl level appears. It is clear that even in this case (which is less favorable for the quasiclassical treatment) the WKB method is accurate to a few percent, except for the s-states.

A more detailed investigation was performed for several s- and p-states in the Yukawa potential. As an example, Table V shows the values of the energy, the coefficient at zero, and the ratios $\tilde{E}_{nl}/E_{nl}$ and η_{nl} for the $2s$ level. The notation for columns (A) and (B) is the same as in Table III. The entries in Tables IV and V show that (except for a relatively narrow region near $g=g_{nl}^{cr}$, i.e., the case of shallow levels) the quasiclassical formula (12) is accurate to a few percent even for $n=2$ and 3 (here n is the principal quantum number of a state).

Generally speaking, the modified matching condition (7) significantly increases the accuracy of the quasiclassical approximation for the wave functions [compare columns (A) and (B) for $g\geqslant 1.5g_{2s}^{cr}$]. For large values of g the nl state is localized in the region of small r where the Yukawa potential goes over to the Coulomb potential. By virtue of this the limiting values c_{nl}, η_{nl} for $g\to\infty$ agree with the corresponding coefficients c_{nl} from Table III for $\alpha=-1$.

5. ZERO-ENERGY STATES

This case requires special treatment, since the asymptotic form of a bound-state ($l\geqslant 1$) wave function changes: $\chi_l(r,E=0)$ falls off as r^{-1} rather than exponentially in the limit $r\to\infty$. We consider this point for the example of the Tietz potential:

$$V(r)=-\frac{Z}{r(1+\mu r)^2},\quad \hbar=m=e=1, \tag{16}$$

which is often used in atomic physics.[5,6] The "critical" values of the effective binding constant $g=Z/\mu$ corresponding to when the nl state appears can be found explicitly either from the exact solution of the Schrödinger equation ($g_{nl}=Z/\mu_{nl}^{cr}$) or from the Bohr–Sommerfeld quantization condition ($\tilde{g}_{nl}$):

$$g_{nl}=\frac{1}{2}(n+l)(n+l+1),\quad \tilde{g}_{nl}=\frac{1}{2}\left(n+l+\frac{1}{2}\right)^2. \tag{17}$$

Thus, in the limit $n\to\infty$ we have

$$\frac{\tilde{g}_{nl}}{g_{nl}}=1+\frac{1}{4(1+\rho)^2n^2}+\ldots\to 1.$$

Equation (11) in this case reduces to the following form:

$$c_{nl}^{\mathrm{WKB}}=\frac{\exp\{(l+1/2)[(z+1)\ln(z+1)-(z-1)\ln(z-1)]\}}{\sqrt{4\pi z^2(3z^2-2)}}, \tag{18}$$

where

TABLE III. Accuracy of the quasiclassical treatment for the coefficients at zero (power-law potentials).

ns-levels, $n=q+1$						
q	$\alpha=-1$		$\alpha=0$		$\alpha=1$	
	(A)	(B)	(A)	(B)	(A)	(B)
0	1.0602	0.9776	1.0900	0.9350	1.1234	0.9636
1	1.0787	0.9947	1.1221	0.9625	1.1494	0.9859
2	1.0819	0.9977	1.1312	0.9703	1.1558	0.9914
3	1.0830	0.9987	1.1357	0.9742	1.1587	0.9939
10	1.0843	0.9998	1.1450	0.9821	1.1635	0.9980
15	1.0843	0.99992	1.1471	0.9839	1.1642	0.9986
∞	1.0844	1	1.1658	1	1.1658	1
q	$\alpha=2$		$\alpha=4$		$\alpha=8$	
	(A)	(B)	(A)	(B)	(A)	(B)
0	1.1469	0.9838	1.1675	1.00145	1.1581	0.9934
1	1.1620	0.9967	1.1661	1.00022	1.1635	0.9980
2	1.1642	0.9986	1.16586	1.000 035	1.1648	0.9992
3	1.1650	0.99927	1.16583	1.000 010	1.1653	0.9995
10	1.1657	0.99991	1.16582	1.000 0002	1.16577	0.99995
∞	1.1658	1	1.16582	1	1.16582	1
states with $l\neq 0$						
q	$\alpha=0$, $l=1$		$\alpha=2$, $l=1$		$\alpha=2$, $l=3$	
	(A)	(B)	(A)	(B)	(A)	(B)
0	1.0069	0.9532	1.0293	0.9744	0.9928	0.9695
1	1.0312	0.9762	1.0493	0.9934	1.0144	0.9906
2	1.0375	0.9822	1.0531	0.9969	1.0191	0.9952
3	1.0405	0.9850	1.0545	0.9982	1.0210	0.9971
10	1.0464	0.9906	1.0561	0.9998	1.0235	0.9995
∞	1.0563	1	1.0563	1	1.0240	1
q	$\alpha=4$, $l=1$		$\alpha=4$, $l=2$		$\alpha=8$, $l=1$	
	(A)	(B)	(A)	(B)	(A)	(B)
0	1.0406	0.9851	1.0119	0.9789	1.0348	0.9796
1	1.0536	0.9974	1.0291	0.9956	1.0495	0.9935
2	1.0553	0.9990	1.0318	0.9982	1.0531	0.9969
3	1.0558	0.9994	1.0327	0.9990	1.0545	0.9982
10	1.0562	0.9999	1.0335	0.9998	1.0561	0.9997
∞	1.0563	1	1.0337	1	1.0563	1

Note. Columns (A) and (B) give the ratios η_{nl}^{WKB} and $\tilde{\eta}_{nl}$; cf. Eq. (13). For the exact values of the coefficients at zero (c_{nl}) see Table II of Ref. 4.

$$z=\sqrt{\frac{2\tilde{g}_{nl}}{\nu^2}}=\frac{1+\rho}{2\rho}>1, \quad \nu=2l+1, \quad \rho=\frac{(l+1/2)}{n}.$$

The results of the calculations using these formulas are given in Table VI, from which it is clear (cf. the column for $\rho_{nl}=\tilde{g}_{nl}/g_{nl}$) that the quasiclassical treatment determines the critical values g_{nl} to within a few percent, just as it does the energies E_{nl} for power-law potentials (compare Table II). On the other hand, the coefficients c_{nl}^{WKB} in this case have a fairly large error [column (A)], which only grows as $q\to\infty$. Introducing the factor $\xi(2l+1)$ in Eq. (18) following Sec. 2 does not eliminate this flaw.

It is found that because of the slow (power-law, not exponential!) dropoff in $\chi_l(r)$ in the subbarrier region the usual quasiclassical normalization condition[2,7]

$$C=2T_r^{-1/2} \tag{19}$$

must also be modified.

For potentials with an algebraic "tail" at infinity

$$V(r)\simeq -gr^{-\beta}, \quad (\beta>2), \quad r\to\infty, \tag{20}$$

a finite contribution to the normalization comes from the subbarrier region $r>r_+$ (except for the case $E<0$). The Schrödinger equation with the potential (20) and energy $E=0$ can be solved in terms of Bessel functions. Using this solution we find in place of (19)

$$C=2d_l(\beta)T_r^{-1/2}, \tag{21}$$

$$d_l(\beta)=\left\{\left(\frac{\beta-2}{2l+1}\right)^{\beta+2/\beta-2}\Gamma\left(\frac{2l+1+\beta}{\beta-2}\right)\Big/\Gamma\left(\frac{2l-1}{\beta-2}\right)\right\}^{1/2} \tag{22}$$

(here we have $l\geqslant 1$, since for $l=0$ the wave function at the point where the level appears is not normalizable). In particular, for the Tietz potential ($\beta=3$) we have

$$d_l(3)=\left[\left(1-\frac{1}{\nu^2}\right)\left(1-\frac{4}{\nu^2}\right)\right]^{1/2}, \quad \nu=2l+1. \tag{23}$$

In column (B) of Table VI the values of the ratios $\tilde{\eta}_{nl}=\tilde{c}_{nl}/c_{nl}$ are given, where c_{nl} are the exact coefficients at zero and $\tilde{c}_{nl}$ is the quasiclassical approximation for them (including the modification of both the matching rule and the normalization):

$$\tilde{c}_{nl}=\xi(2l+1)d_l(3)c_{nl}^{\mathrm{WKB}}. \tag{24}$$

After introducing these corrections we find that the ratios satisfy $\tilde{\eta}_{nl}\to 1$ in the limit $q\to\infty$, i.e., the quasiclassical treatment yields the exact asymptotic form for the coefficients in zero. Note that the principal role in (24), especially in the case of the p-states, is played by the correction d_l given in Eq. (3), which is associated with the change in the quasiclassical normalization condition. It can readily be seen that for $l\gg 1$

$$d_l(\beta)=1-\frac{\beta(\beta+2)}{24(\beta-2)l^2}+\ldots, \tag{25}$$

so that for large values of l the ratio (21) goes over to the usual normalization condition.[7]

TABLE IV. Short-range potentials (at the point when the nl level appears).

State	l, q	Yukawa potential		Hulthén potential	
		$g_{nl}^{(cr)}$	ρ_{nl}	$g_{nl}^{(cr)}$	ρ_{nl}
$1s$	0, 0	0.8399	1.199	0.5	1.221
$2s$	0, 1	3.2236	1.082	2.0	1.090
$3s$	0, 2	7.171	1.049	4.5	1.053
$2p$	1, 0	4.5410	1.032	2.7486	1.036
$3p$	1, 1	8.872	1.022	5.3623	1.025
$4p$	1, 2	14.731	1.016	9.0505	1.018

Note. Here $n=l+q+1$ and $\rho_{nl}=\tilde{g}_{nl}/g_{nl}^{(cr)}$.

TABLE V. Results of calculations for the $2s$ level in the Yukawa potential.

$g/g_{2s}^{(cr)}$	$-E_{2s}$	$\tilde{E}_{2s}/E_{2s}$	c_{2s}	(A)	(B)
1.10	8.9933(−3)	0.251	1.6393	0.9614	0.8865
1.25	5.8677(−2)	0.819	2.9529	1.0455	0.9641
1.50	2.4711(−1)	0.939	4.9966	1.0644	0.9816
1.75	5.7670(−1)	0.968	7.0962	1.0700	0.9867
2	1.0538	0.9795	9.3011	1.0727	0.9892
2.5	2.4652	0.9894	1.4055(1)	1.0752	0.9915
3	4.4997	0.9934	1.9258(1)	1.0764	0.9926
5	1.9007(1)	0.9980	4.4050(1)	1.0779	0.9940
10	1.0042(2)	0.9995	1.2810(2)	1.0785	0.9945
$g\to\infty$	$g^2/8$	1	$2^{-1/2}g^{3/4}$	1.0787	0.9947

Here we have restricted ourselves to treating the asymptotic coefficient c_{nl} [cf. Eq. (10)]. The same corrections should be taken into account, however, in calculating the wave functions for finite r in the subbarrier region, the matrix elements, etc.

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APPENDIX A

Here we present formulas for the exactly soluble power-law potentials, specifically, the cases $\alpha = 2, -1$, and 1 in Eq. (5).

In the first case we have

$$V(r)=\frac{\omega^2 r^2}{2},\quad E_{lq}=\tilde{E}_{lq}=\left(l+2q+\frac{3}{2}\right)\omega,\quad T_r=\frac{\pi}{\omega}$$

and Eq. (11) yields

$$c_{lq}^{\mathrm{WKB}}=\left\{\frac{1}{\pi}\,\frac{n^n e^{l+1/2}}{(q+1/2)^{q+1/2}}\left(l+\frac{1}{2}\right)^{l+1/2}\right\}^{1/2}\omega^{2l+3/4}, \tag{A1}$$

whereas the exact value of the coefficient at zero is

$$c_{lq}=\frac{[2\Gamma(n+1/2)/q!]^{1/2}}{\Gamma(l+3/2)}\,\omega^{2l+3/4}, \tag{A2}$$

$n=l+q+1$. Hence

$$\eta_{lq}^{\mathrm{WKB}}\equiv\frac{c_{lq}^{\mathrm{WKB}}}{c_{lq}}=\frac{\lambda(q+l+1/2)}{\lambda(q)\xi(l+1/2)}, \tag{A3}$$

where

$$\lambda(x)=\left\{\sqrt{2\pi}\,\frac{[(x+1/2)e^{-1}]^{x+1/2}}{\Gamma(x+1)}\right\}^{1/2}, \tag{A4}$$

and the function $\xi(x)$ is defined in Eq. (7). Using the duplication formula for the gamma function we can readily establish the identity

$$\lambda(x)=\left(1+\frac{1}{2x}\right)^{1/4}\xi(x)\left[\frac{\xi(x+1/2)}{\xi(2x)}\right]^{1/2}, \tag{A5}$$

which enables us to evaluate the function $\lambda(x)$ for the data in Table I. In the limit $x\gg 1$ we have

$$\lambda(x)=1+\frac{1}{48x}-\frac{47}{4608x^2}+O(x^{-3}) \tag{A6}$$

[cf. the expansion (9)].

Similarly, in the case of the Coulomb potential ($\alpha=-1$) we find

$$\eta_{lq}^{\mathrm{WKB}}=\frac{\lambda(q+2l+1)}{\lambda(q)\xi(2l+1)}\,. \tag{A7}$$

TABLE VI. The Tietz potential ($E_{nl}=0$).

q	$l=1$			$l=2$			$l=3$		
	(A)	(B)	ρ_{nl}	(A)	(B)	ρ_{nl}	(A)	(B)	ρ_{nl}
0	1.4469	0.9890	1.0208	1.1062	0.9770	1.0083	1.0372	0.9721	1.0045
1	1.4592	0.9974	1.0125	1.1248	0.9934	1.0060	1.0577	0.9913	1.0035
2	1.4609	0.9986	1.0083	1.1282	0.9964	1.0045	1.0618	0.9952	1.0028
3	1.4615	0.9990	1.0060	1.1296	0.9976	1.0035	1.0635	0.9968	1.0023
5	1.4621	0.9994	1.0035	1.1307	0.9986	1.0023	1.0650	0.9982	1.0016
10	1.4626	0.9998	1.0014	1.1316	0.9994	1.0010	1.0661	0.9992	1.0008
∞	1.4630	1	1	1.1323	1	1	1.0669	1	1
$d_l(3)$	$\sqrt{40/81}=0.7027$			$\sqrt{504/625}=0.8980$			0.9485		

Note: Here $\rho_{nl}=\tilde{g}_{nl}/g_{nl}=\mu_{nl}^{(cr)}/\tilde{\mu}_{nl}$.

From (A3) and (A7) it is immediately apparent that in the limit $q\to\infty$ (i.e., for states with a large number of nodes in the radial wave function) the ratios η_{lq}^{WKB} approach a limit which differs from unity:

$$\lim_{q\to\infty}\eta_{lq}^{\mathrm{WKB}}=[\xi(\nu)]^{-1},\quad \nu=\begin{cases}l+1/2, & \alpha=2\\ 2l+1, & \alpha=-1\end{cases}. \tag{A8}$$

Thus, the quasiclassical approximation with the matching rule (2) does not yield the correct values of $\psi^2(0)$ for $l\sim 1$ (this is also evident from Table III). This contradiction is removed by using the modified matching rule (7), by means of which we find

$$\tilde{\eta}_{lq}\equiv\frac{\tilde{c}_{lq}}{c_{lq}}=\frac{\lambda(q+\nu)}{\lambda(q)}=1-\frac{\nu}{48q^2}+O(q^{-3}),\quad q\to\infty, \tag{A9}$$

where ν is defined in (A8). On the other hand, if both quantum numbers q and l are large, then it follows from (A3) and (A7) that

$$\eta_{lq}^{\mathrm{WKB}}=1+\frac{c(\rho,\alpha)}{12\rho(1-\rho)}\,\frac{1}{n}+\ldots\ldots\to 1,\quad \rho=\frac{l+1/2}{n}, \tag{A10}$$

where

$$c(\rho,2)=1-\rho-\frac{1}{4}\rho^2,\quad c(\rho-1)=\frac{1-2\rho^2}{2(1+\rho)},\quad 0<\rho<1.$$

Of course, this expansion is invalid in the limit $\rho\to 0$ or $\rho\to 1$, when one of the quantum numbers (l or q) is of order unity.

Finally, the Schrödinger equation can also be solved exactly for the s-states in a linear potential ($\alpha=1$):

$$E_{ns}=2^{-1/3}\zeta_n,\quad \chi_{ns}(r)=N_n\mathrm{Ai}(2^{1/3}r-\zeta_n), \tag{A11}$$

where $z=-\zeta_n$ is the nth real root of the Airy function $\mathrm{Ai}(z)$, and it follows from the normalization condition that $N_n^2=2^{1/3}[\mathrm{Ai}'(-\zeta_n)]^{-2}$. Hence

$$c_{ns}=\sqrt{2},\quad n=1,2,3,\ldots \tag{A12}$$

(thus, the coefficient c_{ns} in this case does not depend on n in general).

APPENDIX B

For power-law potentials the following scaling relation holds:

$$E_{nl}(g,m)=g^{2/\alpha+2}m^{-\alpha/\alpha+2}E_{nl},$$
$$c_{nl}(g,m)=(gm)^{l+3/2/\alpha+2}c_{nl}, \tag{B1}$$

whose validity can be verified by means of a scale transformation in the radial Schrödinger equation:

$$r\to\lambda r,\quad \lambda=(gm)^{-1/\alpha+2}$$

(cf. also Ref. 8). Likewise, for the logarithmic potential $V(r)=g\ ln\ r$ we have

$$E_{nl}(g,m)=g\left[E_{nl}-\frac{1}{2}\ln(gm)\right],$$
$$c_{nl}(g,m)=(gm)^{2l+3/4}c_{nl}, \tag{B2}$$

where the values of these quantities for $g=m=1$ are written as E_{nl} and c_{nl}. In consequence of these relations we can restrict ourselves to the case $g=m=1$, as was done in Tables II and III. Using (B2) we can show that our calculations for the logarithmic potential are completely equivalent to the results of Quigg and Rosner[8] for ns-states.

Note that the logarithmic potential follows from (5) for $\alpha=0$:

$$\frac{r^\alpha}{\alpha}=\alpha^{-1}+\ln r+O(\alpha),\quad \alpha\to 0$$

(the infinite constant α^{-1} can be disregarded, since it only yields a general shift in the energies E_{nl} and cannot change the wave functions).

Note also that the binding constant g in (5) and the coefficient at zero have dimensions

$$[g]=L^{-(\alpha+2)},\quad [c_{nl}]=L^{-(l+3/2)}, \tag{B3}$$

where L is length and we have written $\hbar=m=1$. In particular, for $\alpha=-1$ we have $g=Z=a_B^{-1}$ (atomic units) and $c_{nl}\propto Z^{l+3/2}$, while for $\alpha=2$ we have $g=\omega^2$, $c_{nl}\propto\omega^{(2l+3)/4}$ [which is consistent with Eq. (A2)], where ω is the frequency of the oscillator.

[1)] In a power-law potential [i.e., under the condition that Eq. (5) holds for all $0<r<\infty$] elementary scaling arguments yield $E_n\propto n^{2\alpha/\alpha+2}$, $n\gg 1$. If $\alpha<0$ holds, then we have $E_n\to -0$ in the limit $n\to\infty$.

[2)] The reason for this is that the Stirling formula for the gamma-function $\Gamma(x)$ is very accurate even for $x\sim 1$.

[3)] The attractive power-law potential is defined by Eq. (5) with $g>0$ for all values of r, $0<r<\infty$. Here we set $g=1$, which can always be done in view of the scaling relations (see Appendix B).

[4)] In the numerical calculations we used the Merson method (a modification of Runge–Kutta). The calculations of the energy eigenvalues E_{nl} and the coefficients at zero were performed with an accuracy of order 10^{-6}–10^{-7}.

[5)] The limiting value of η_l does not depend on the exponent α for $\alpha>0$ (this can be seen clearly in Table III).

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