$1/N$ expansion for a more general screened Coulomb potential

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By applying the large-N expansion to the more general case of a screened Coulomb potential, $V(r)=-(a/r)[1+(1+br)e^{-2br}]$, the energy eigenvalues of the ground state and the first excited state and the corresponding wave functions are obtained analytically up to 14 terms.

I. INTRODUCTION

Following the work of Ferrell and Scalapino,[1] the large-N expansion has recently received much attention. It has been used for solving the Schrödinger equation.[2–11] It also has many important applications in other fields such as solid-state[12,13] and quantum-field theory.[1,14,15]

Screened Coulomb potentials are known to adequately describe the effective interaction in many-body atomic phenomena. Since the Schrödinger equation for such a potential does not admit exact solutions, various approximate methods, both numerical[16–30] and analytical,[31–41] have been developed. The potential $V(r)=-(a/r)[1+(1+br)e^{-2br}]$, defined for an electron of the helium atom in the field of the other electron and the nucleus, has been studied by Gerry and Laub,[38] but the present results have not been given.

In the present work we apply the large-N expansion, following the method of Mlodinow and Shatz, to obtain the energy eigenvalues of the ground state and the first excited state and the corresponding wave functions. Analytical expressions are obtained for the first 14 terms.

II. THE METHOD AND CALCULATIONS

We want to solve the Schrödinger equation for the potential

$$V(r)=-(a/r)[1+(1+br)e^{-2br}] . \tag{1}$$

The radial part of the Schrödinger equation in N dimensions (with $m=\hbar=1$) may be written

$$\left[-\frac{1}{2}\left(\frac{d^2}{dr^2}+\frac{N-1}{r}\frac{d}{dr}\right)+\frac{l(l+N-2)}{2r^2}+V_N(r)\right]R(r)=ER(r) , \tag{2}$$

where $V_N(r)=-(a/r)[1+(1+br)\exp(-18br/N^2)]$ is the generalization of the potential to N dimensions. Substituting $R(r)=-r^{-(N-1)/2}U(r)$ into Eq. (2), we obtain

$$-\frac{1}{2}\frac{d^2}{dr^2}U(r)+k^2\left\{\frac{(1-1/k)(1-3/k)}{8r^2}-\frac{\tilde{a}}{r}\left[1+(1+br)\exp\left(-\frac{18br}{N^2}\right)\right]\right\}U(r)=EU(r) , \tag{3}$$

where $\tilde{a}=a/k^2$, $k=N+2l$. For simplicity we solve Eq. (3) for the $l=0$ case.

A. Ground state

In the large-N limit the leading term of the energy eigenvalue is given by

$$E_\infty=k^2E^{(-2)}=k^2[1/8r_0^2-\tilde{a}(2+br_0)/r_0] , \tag{4}$$

where r_0 is the value for which the potential $[1/8r^2-\tilde{a}(2+br)/r]$ attains a minimum. A simple calculation yields

$$r_0=\frac{1}{8\tilde{a}} \tag{5}$$

and

$$E^{(-2)}=-\tilde{a}(8\tilde{a}+b) . \tag{6}$$

Higher-order corrections to the ground-state energy is obtained by defining $x=r-r_0$ and assuming $U_0(r)=\exp[\phi_0(x)]$ for the ground-state wave function. We get, from Eq. (3),

$$-\tfrac{1}{2}[\phi_0''(x)+\phi_0'^2(x)]+k^2V_{\rm eff}(x)+\left(-\frac{k}{2}+\frac{3}{8}\right)r^{-2}(x)+W(x)=\epsilon_0, \tag{7}$$

where

$$V_{\rm eff}(x)=\frac{1}{8r^2}(x)-\tilde{a}[2+br(x)]/r(x)+\tilde{a}(8\tilde{a}+b), \tag{8}$$

$$\epsilon_0=E_0-k^2E^{(-2)} \tag{9}$$

and

$$W(x)=\tilde{a}[1+br(x)]\left[18b-\frac{1}{3}\frac{(18b)^3}{k^4}r^2(x)+\frac{1}{6}\frac{(18b)^4}{k^6}r^3(x)-\cdots\right], \quad (10)$$

E_0 being the ground-state energy and $\phi'(x)$ and $\phi''(x)$ representing the first and second derivatives of $\phi(x)$ with respect to x. We now expand

$$\epsilon_0=\sum_{n=1}^{\infty} E_0^{(n)}(1/k)^n \quad (11)$$

and

$$\phi_0'(x)=\sum_{n=1}^{\infty} \phi_0^{(n)}(x)(1/k)^n . \quad (12)$$

Substituting these expansions into Eq. (7) and combining the terms of the same order $(1/k)$, we obtain the following recurrence relations:

$$-\tfrac{1}{2}\phi_0^{(-1)^2}(x)+V_{\text{eff}}(x)=0 , \quad (13a)$$

$$-\tfrac{1}{2}\phi_0^{(-1)'}(x)-\phi_0^{(-1)}(x)\phi_0^{(0)}-\tfrac{1}{2}r^{-2}(x)=E_0^{(-1)} , \quad (13b)$$

$$-\tfrac{1}{2}\phi_0^{(0)'}(x)-\phi_0^{(-1)}(x)\phi_0^{(1)}(x)-\tfrac{1}{2}\phi_0^{(0)^2}(x)+\tfrac{3}{8}r^{-2}(x)+\tilde{a}(1+br)(18b)=E_0^{(0)} , \quad (13c)$$

and for $n\geq 1$,

$$-\tfrac{1}{2}\phi_0^{(n-1)'}(x)-\tfrac{1}{2}\sum_{m=0}^{n=1}\phi_0^{(m)}(x)\phi_0^{(n-m-1)}(x)+(-1)^{(n-1)/2}\tilde{a}(1+br)\frac{(18b)^{(n+1)/2}}{[(n+1)/2]!}r^{(n-1)/2}(x)\begin{cases}=E^{(n-1)} & \text{if } n \text{ is odd}\\ =0 & \text{if } n \text{ is even .}\end{cases} \quad (13d)$$

Since the effective potential $V_{\text{eff}}(x)$ vanishes at the minimum $(r=r_0)$, the equations are solved one by one first for $(r=r_0)$ to obtain $E_0^{(n)}$ and then for any r to obtain $\phi_0^{(n)}$.

B. First excited state

Using the same definition for x and noticing that the wave function for the first excited state will have node

$$U_1(x)=(x-c)e^{\phi_1(x)} , \quad (14)$$

we obtain from Eq. (3)

$$-\tfrac{1}{2}[\phi_1''(x)+\phi_1'^2(x)](x-c)-\phi_1'(x)+\left[k^2V_{\text{eff}}(x)+\left[-\frac{k}{2}+\frac{3}{8}\right]r^{-2}(x)\right](x-c)+\tilde{a}[1+br(x)]\left[18b-\frac{1}{3}\frac{(18b)^3}{k^4}r^2(x)+\frac{1}{6}\frac{(18b)^4}{k^6}r^3(x)-\cdots\right](x-c)=(x-c)\epsilon_1 , \quad (15)$$

where

$$\epsilon_1=E_1-k^2E^{(-2)} , \quad (16)$$

E_1 being the energy of the first excited state. We now make the following expansions:

$$\phi_1'(x)=\sum_{n=-1}^{\infty}\phi_1^{(n)}(x)(1/k)^n , \quad (17)$$

$$\epsilon_1=\sum_{n=-1}^{\infty}E_1^{(n)}(1/k)^n , \quad (18)$$

and

$$c=\sum_{n=1}^{\infty}C^{(n)}(1/k)^n . \quad (19)$$

Substituting these expansions into Eq. (15) and combining the terms of the same order in $(1/k)$, we obtain the following recurrence relations:

$$\phi_1^{(-1)}(x)=-[2V_{\text{eff}}(x)]^{1/2} , \quad (20a)$$

$$-x\phi_1^{(-1)}(x)\phi_1^{(0)}(x)=x[E_1^{(-1)}+\tfrac{1}{2}\phi_1^{(-1)'}(x)+\tfrac{1}{2}r^{-2}(x)]+\phi_1^{(-1)}(x) , \quad (20b)$$

$$-x\phi_1^{(-1)}(x)\phi_1^{(1)}(x)=x\{E_1^{(0)}+\tfrac{1}{2}\phi_1^{(0)'}(x)+\tfrac{1}{2}\phi_1^{(0)^2}(x)+\tfrac{3}{8}r^{-2}(x)-\tilde{a}[1+br(x)](18b)\}-C^{(1)}[E_1^{(-1)}+\tfrac{1}{2}\phi_1^{(-1)'}(x)+\phi_1^{(-1)}(x)\phi_1^{(0)}(x)+\tfrac{1}{2}r^{-2}(x)]+\phi_1^{(0)}(x) , \quad (20c)$$

$$-x\phi_1^{(-1)}(x)\phi_1^{(2)}(x)=x[E_1^{(1)}+\tfrac{1}{2}\phi_1^{(1)'}(x)+\phi_1^{(1)}(x)\phi_1^{(0)}(x)]$$
$$-C^{(1)}\{E_1^{(0)}+\tfrac{1}{2}\phi_1^{(0)'}(x)+\phi_1^{(1)}(x)\phi_1^{(-1)}(x)+\tfrac{1}{2}\phi_1^{(0)^2}(x)-\tfrac{3}{8}r^{-2}(x)-\tilde{a}[1+br(x)](18b)\}$$
$$-C^{(2)}[E_1^{(-1)}+\tfrac{1}{2}\phi_1^{(-1)'}(x)+\phi_1^{(0)}(x)\phi_1^{(-1)}(x)+\tfrac{1}{2}r^{-2}(x)]+\phi_1^{(1)}(x)\ , \tag{20d}$$

$$-x\phi_1^{(-1)}(x)\phi_1^{(n)}(x)=x\left\{E_1^{(n-1)}+\tfrac{1}{2}\phi_1^{(n-1)'}(x)+\tfrac{1}{2}\sum_{m=0}^{n-1}\phi_1^{(m)}(x)\phi_1^{(n-m-1)}(x)\right.$$
$$\left.+(-1)^{(n+1)/2}\tilde{a}[1+br(x)]\frac{(18b)^{(n+1)/2}}{[(n+1)/2]!}r^{(n-1)/2}(x)\right\}$$
$$-\sum_{m=1}^{n-2}C^{(m)}\left\{E_1^{(n-m-1)}+\tfrac{1}{2}\phi_1^{(n-m-1)'}(x)+\tfrac{1}{2}\sum_{p=0}^{n-m+1}\phi_1^{(p-1)}(x)\phi_1^{(n-m-p)}(x)\right.$$
$$\left.+(-1)^{(n-m+1)}\tilde{a}[1+br(x)]\frac{(18b)^{(n-m+1)/2}}{[(n-m+1)/2]!}r^{(n-m-1)}(x)\right\}$$
$$-C^{(n-1)}\{E_1^{(0)}+\tfrac{1}{2}\phi_1^{(0)'}(x)+\phi_1^{(1)}(x)\phi_1^{(-1)}(x)+\tfrac{1}{2}\phi_1^{(0)^2}(x)-\tfrac{3}{8}r^{-2}(x)-\tilde{a}[1+br(x)](18b)\}$$
$$-C^{(n)}[E_1^{(-1)}+\tfrac{1}{2}\phi_1^{(-1)'}(x)+\phi_1^{(-1)}(x)\phi_1^{(0)}(x)+\tfrac{1}{2}r^{-2}(x)]+\phi_1^{(n-1)}(x)\ . \tag{20e}$$

The first term in Eq. (20e) vanishes if n is even; the second term (involving a sum from $m=1$ to $m=n-2$) in Eq. (20e) vanishes if m and n are both odd or both even. These equations are solved to obtain the node coefficients $C^{(n)}$'s and the higher-order corrections to the eigenvalues of the first excited state.

III. RESULTS AND CONCLUSIONS

Defining $D=3b/4$, we write only energy eigenfunctions simply.

A. Ground state

$$\begin{aligned}
&E_0^{(-1)}=-16\tilde{a}^2,\quad E_0^{(0)}=-24\tilde{a}^2+24\tilde{a}D+4D^2\ ,\\
&E_0^{(1)}=-32\tilde{a}^2-4D^2,\quad E_0^{(2)}=-40\tilde{a}^2-6D^3/\tilde{a}-D^4/2\tilde{a}^2-36D^2\ ,\\
&E_0^{(3)}=-48\tilde{a}^2+6D^3/\tilde{a}+3D^4/2\tilde{a}^2+36D^2\ ,\\
&E_0^{(4)}=-56\tilde{a}^2+42D^3/\tilde{a}+14D^4/\tilde{a}^2+3D^5/\tilde{a}^3+D^6/4\tilde{a}^4\ ,\\
&E_0^{(5)}=-64\tilde{a}^2-42D^3/\tilde{a}-28D^4/\tilde{a}^2-15D^5/2\tilde{a}^3-9D^6/8\tilde{a}^4\ ,\\
&E_0^{(6)}=-72\tilde{a}^2-36D^3/\tilde{a}-72D^4/\tilde{a}^2-105D^5/2\tilde{a}^3-29D^6/2\tilde{a}^4-21D^7/8\tilde{a}^5-3D^8/16\tilde{a}^6\ ,\\
&E_0^{(7)}=-80\tilde{a}^2+36D^2/\tilde{a}+151D^4/\tilde{a}^2+126D^5/\tilde{a}^3+89D^6/2\tilde{a}^4+153D^7/16\tilde{a}^5+135D^8/128\tilde{a}^6\ ,\\
&E_0^{(8)}=-88\tilde{a}^2+18D^4/\tilde{a}^2+2397D^5/10\tilde{a}^3+3819D^6/20\tilde{a}^4+165D^7/2\tilde{a}^5+1205D^8/64\tilde{a}^6\\
&\qquad+45D^9/16\tilde{a}^7+11D^{10}/64\tilde{a}^8\ ,\\
&E_0^{(9)}=-96\tilde{a}^2-138D^4/\tilde{a}^2-3468D^5/5\tilde{a}^3-4445D^6/8\tilde{a}^4-4347D^7/16\tilde{a}^5-2313D^8/32\tilde{a}^6\\
&\qquad-807D^9/64\tilde{a}^7-567D^{10}/512\tilde{a}^8\ ,\\
&E_0^{(10)}=-104\tilde{a}^2+81D^4/2\tilde{a}^2-1209D^5/10\tilde{a}^3-16\,687D^6/20\tilde{a}^4-34\,497D^7/40\tilde{a}^5-28\,421D^8/64\tilde{a}^6\\
&\qquad-4479D^9/32\tilde{a}^7-6861D^{10}/256\tilde{a}^8-429D^{11}/128\tilde{a}^9-91D^{12}/512\tilde{a}^{10}\ ,\\
&E_0^{(11)}=-112\tilde{a}^2+27D^4/2\tilde{a}^2+6399D^5/5\tilde{a}^3+23\,577D^6/8\tilde{a}^4+238\,419D^7/80\tilde{a}^5+195\,153D^8/128\tilde{a}^6\\
&\qquad+34\,197D^9/64\tilde{a}^7+59\,471D^{10}/512\tilde{a}^8+17\,373D^{11}/1024\tilde{a}^9+5095D^{12}/4096\tilde{a}^{10}\ ,\\
&E_0^{(12)}=-120\tilde{a}^2-6687D^5/10\tilde{a}^3+3259D^6/5\tilde{a}^4+477\,963D^7/140\tilde{a}^5+483\,573D^8/112\tilde{a}^6\\
&\qquad+41\,313D^9/16\tilde{a}^7+125\,027D^{10}/128\tilde{a}^8+125\,181D^{11}/512\tilde{a}^9+81\,845D^{12}/2048\tilde{a}^{10}\\
&\qquad+273D^{13}/64\tilde{a}^{11}+51D^{14}/256\tilde{a}^{12}\ .
\end{aligned}\tag{21}$$

TABLE I. Comparison of the energy eigenvalues for $0<\beta<1.0$ as calculated from the numerical solution of the Schrödinger equation with those to order β^4 of the present work.

β	E_0/a^2 (to order β^4)	E_{10}	E_1/a^2 (to order β^4)	E_{20}
0.02	-1.98000	(-1.98000)	-0.48005	(-0.48000)
0.04	-1.96003	(-1.96003)	-0.46038	(-0.46033)
0.06	-1.94010	(-1.94010)	-0.44116	(-0.44115)
0.08	-1.92023	(-1.92023)	-0.4225	(-0.4221)
0.1	-1.90044	(-1.90044)	-0.4043	(-0.4048)
0.3	-1.70844	(-1.70958)	-0.312	(-0.274)
0.5	-1.523	(-1.537)		
0.7	-1.321	(-1.384)		
1.0	-0.875	(-1.194)		

B. First excited state

$$
\begin{aligned}
&E_1^{(-1)}=16\tilde{a}^2,\quad E_1^{(0)}=-24\tilde{a}^2+24\tilde{a}D+4D^2 ,\\
&E_1^{(1)}=32\tilde{a}^2+20D^2,\quad E_1^{(2)}=-40\tilde{a}^2-36D^2-6D^3/\tilde{a}-D^4/2\tilde{a}^2 ,\\
&E_1^{(3)}=48\tilde{a}^2-180D^2-78D^3/\tilde{a}-15D^4/2\tilde{a}^2 ,\\
&E_1^{(4)}=-56\tilde{a}^2-102D^3/\tilde{a}+2D^4/\tilde{a}^2+3D^5/\tilde{a}^3+D^6/4\tilde{a}^4 ,\\
&E_1^{(5)}=64\tilde{a}^2+402D^3/\tilde{a}+256D^4/\tilde{a}^2+147D^5/2\tilde{a}^3+53D^6/8\tilde{a}^4 ,\\
&E_1^{(6)}=-72\tilde{a}^2+828D^3/\tilde{a}+756D^4/\tilde{a}^2+507D^5/2\tilde{a}^3+11D^6/\tilde{a}^4-21D^7/8\tilde{a}^5-3D^8/16\tilde{a}^6 ,\\
&E_1^{(7)}=80\tilde{a}^2+396D^3/\tilde{a}+209D^4/\tilde{a}^2-516D^5/\tilde{a}^3-407D^6/\tilde{a}^4-1557D^3/16\tilde{a}^5-939D^8/128\tilde{a}^6 ,\\
&E_1^{(8)}=-88\tilde{a}^2-2430D^4/\tilde{a}^2-43\,203D^5/10\tilde{a}^3-51\,631D^6/20\tilde{a}^4-2343D^7/4\tilde{a}^5-1873D^8/64\tilde{a}^6\\
&\qquad +45D^9/16\tilde{a}^7+11D^{10}/64\tilde{a}^8 ,\\
&E_1^{(9)}=96\tilde{a}^2-6126D^4/\tilde{a}^2-48\,372D^5/5\tilde{a}^3-41\,083D^6/\tilde{a}^4+2547D^7/16\tilde{a}^5+10\,497D^8/16\tilde{a}^6\\
&\qquad +9099D^9/64\tilde{a}^7+4635D^{10}/512\tilde{a}^8 ,\\
&E_1^{(10)}=-104\tilde{a}^2-12\,879D^4/2\tilde{a}^2-62\,709D^5/10\tilde{a}^3+161\,553D^6/20\tilde{a}^4+583\,263D^7/40\tilde{a}^5\\
&\qquad +448\,513D^8/64\tilde{a}^6+40611D^9/32\tilde{a}^7+15\,441D^{10}/256\tilde{a}^8-429D^{11}/128\tilde{a}^9-91D^{12}/512\tilde{a}^{10} ,\\
&E_1^{(11)}=112\tilde{a}^2-4887D^4/2\tilde{a}^2+111\,411D^5/5\tilde{a}^3+561\,531D^6/8\tilde{a}^4+1\,053\,141D^7/16\tilde{a}^5\\
&\qquad +2\,882\,527D^8/128\tilde{a}^6-16\,593D^9/64\tilde{a}^7-801\,439D^{10}/512\tilde{a}^8-294\,201D^{11}/1024\tilde{a}^9-65\,099D^{12}/4096\tilde{a}^{10} ,\\
&E_1^{(12)}=-120\tilde{a}^2+882\,153D^5/10\tilde{a}^3+2\,204\,813D^6/10\tilde{a}^4+6\,291\,312D^7/35\tilde{a}^5+3\,015\,459D^8/1\tilde{1}2a^6\\
&\qquad -247\,659D^9/8\tilde{a}^7-1\,816\,915D^{10}/128\tilde{a}^8-932\,913D^{11}/512\tilde{a}^9+77\,983D^{12}/2048\tilde{a}^{10}\\
&\qquad +675D^{13}/32\tilde{a}^{11}+255D^{14}/256\tilde{a}^{12} .
\end{aligned}
\tag{22}
$$

Energies of the ground state and the first excited state are given by

$$E_0=k^2E^{(-2)}+\sum_{n=-1}^{\infty}k^{-n}E_0^{(n)} \tag{23}$$

and

$$E_1=k^2E^{(-2)}+\sum_{n=-1}^{\infty}k^{-n}E_1^{(n)} , \tag{24}$$

respectively. Substituting $k=3$ for three space in Eqs. (26) and (27) and defining $\beta=b/a$, we obtain

$$E_0/a^2=-2+\beta-\tfrac{1}{2}\beta^3+\tfrac{5}{8}\beta^4 \tag{25}$$

and

TABLE II. Improvement in energy with respect to orders of b/a.

β	$(E_0/a^2)0$	$(E_0/a^2)1$	$(E_0/a^2)3$	$(E_0/a^2)4$
0.02	-2.0	-1.98	-1.98000	-1.98000
0.05	-2.0	-1.95	-1.95006	-1.95006
0.08	-2.0	-1.92	-1.92026	-1.92023
0.2	-2.0	-1.8	-1.804	-1.803
0.5	-2.0	-1.5	-1.563	-1.523
0.8	-2.0	-1.2	-1.456	-1.2

β	$(E_1/a^2)0$	$(E_1/a^2)1$	$(E_1/a^2)2$	$(E_1/a^2)4$
0.02	-0.5	-0.48	-0.48006	-0.48005
0.05	-0.5	-0.45	-0.45088	-0.45070
0.08	-0.5	-0.42	-0.42358	-0.42246
0.2	-0.5	-0.3	-0.356	-0.312

$$E_1/a^2 = -\tfrac{1}{2} + \beta - 7\beta^3 + \tfrac{55}{2}\beta^4 \ . \tag{26}$$

Some numerical values of energies for different values of β are compared with those which are obtained solving the Schrödinger equation (see Table I); Numerov's method is used. For each energy eigenvalue a total of 5000 steps are taken with the step size $\Delta r = 0.001$ and tolerance 1.0×10^{-8}. Results are in agreement for small values of β. They tend to deviate more and more as β approaches 1.

We also illustrate the improvement of energy with respect to orders of β in Table II.

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