$1/N$ expansion for the exponential-cosine-screened Coulomb potential

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The large-N expansion has been used for solving the Schrödinger equation for the exponential-cosine-screened Coulomb potential. The eigenvalues of the ground state and the first excited state and the corresponding wave functions are obtained analytically up to 14 terms.

I. INTRODUCTION

In recent years some quantum-mechanical problems have been solved by Large-N expansion,[1-8] which also has many important applications in other fields such as solid state[9,10] physics and quantum-field theory.[11-13]

The problem of the exponential-cosine-screened Coulomb potential (ECSC) is of great importance in atomic phenomena. It has been studied using numerical[14-16] and analytical[17-20] methods.

In the present work we apply the large-N expansion by following the method of Mlodinow and Shatz to obtain energies of the ground state and the first excited state and the corresponding wave functions. Analytical expressions are obtained for the first 14 terms. The results are consistent with those obtained by using different methods.

II. THE METHOD AND CALCULATIONS

We wish to solve the Schrödinger equation for the ECSC potential

$$V(r)=-\frac{a}{r}e^{-\lambda r}\cos(\lambda r)\ . \tag{1}$$

Following the method introduced by Moreno and Zepeda, the potential may be written in N dimensions as

$$V_N(r)=-\frac{a}{r}\exp\left[-\frac{9\lambda r}{N^2}\right]\cos\left[\frac{9\lambda r}{N^2}\right]\ . \tag{2}$$

The radial part of the Schrödinger equation in N dimensions (with $m=\hbar=1$) is given by

$$\left[-\frac{1}{2}\left[\frac{d^2}{dr^2}+\frac{N-1}{r}\frac{d}{dr}\right]+\frac{l(l+N-2)}{2r^2}+V_N(r)\right]R(r)=ER(r)\ . \tag{3}$$

Defining $R(r)=r^{-(N-1)/2}u(r)$ the equation reduces to

$$-\frac{1}{2}\frac{d^2}{dr^2}u(r)+k^2\left[\frac{(1-1/k)(1-3/k)}{8r^2}-\frac{\tilde{a}}{r}\exp\left[-\frac{9\lambda r}{N^2}\right]\cos\left[\frac{9\lambda r}{N^2}\right]\right]u(r)=Eu(r)\ , \tag{4}$$

where $\tilde{a}=a/k^2$, $k=N+2l$. For simplicity, we solve Eq. (4) for the $l=0$ case.

Ground state: In the large-N limit, the leading term of the energy eigenvalue becomes

$$E_\infty=k^2E^{(-2)}=k^2\left[\frac{1}{8r_0^2}-\frac{\tilde{a}}{r_0}\right]\ , \tag{5}$$

where r_0 is to be obtained by minimizing the potential $(1/8r^2-\tilde{a}/r)$. A simple calculation yields

$$r_0=1/4\tilde{a} \tag{6}$$

and

$$E^{(-2)}=-2\tilde{a}^2\ . \tag{7}$$

To calculate the higher-order corrections to the ground-state energy, we define $x=r-r_0$ and transform Eq. (4) into a Riccati equation by means of

$$u_0(x)=e^{\Phi_0(x)} \tag{8}$$

to obtain

$$-\tfrac{1}{2}[\Phi_0''(x)+\Phi_0'^2(x)]+k^2V_{\text{eff}}(x)+\left[-\frac{k}{2}+\frac{3}{8}\right]r^{-2}(x)+\omega(x)=\epsilon_0\ , \tag{9}$$

where

$$V_{\text{eff}}(x)=1/[8r^2(x)]-\tilde{a}/[r(x)]+2\tilde{a}^2\ , \tag{10}$$

$$\epsilon_0=E_0-k^2E^{(-2)}\ , \tag{11}$$

and

$$\omega(x)=(9\lambda)\tilde{a}-\frac{1}{3}\frac{(9\lambda)^3}{k^4}\tilde{a}r^2(x)+\frac{1}{6}\frac{(9\lambda)^4}{k^6}\tilde{a}r^3(x)+\cdots\ , \tag{12}$$

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

$$\epsilon_0=\sum_{n=-1}^{\infty} E_0^{(n)}(1/k)^n \tag{13}$$

and

$$\Phi_0'(x)=\sum_{n=-1}^{\infty} \Phi_0^{(n)}(x)(1/k)^n . \tag{14}$$

Substituting these expansions into Eq. (9), we obtain

$$-\tfrac{1}{2}\sum_{n=-1}^{\infty}\Phi_0^{(n)'}(x)k^{-n}-\tfrac{1}{2}\sum_{m,n=-1}^{\infty}\Phi_0^{(m)}(x)\Phi_0^{(n)}(x)k^{-(m+n)}+k^2V_{\rm eff}(x)+\left[-\frac{k}{2}+\frac{3}{8}\right]r^{-2}(x)$$
$$+(9\lambda)\tilde{a}-\frac{1}{3}\frac{(9\lambda)^3}{k^4}\tilde{a}r^2(x)+\frac{1}{6}\frac{(9\lambda)^4}{k^6}\tilde{a}r^3(x)+\cdots=\sum_{n=-1}^{\infty}E_0^{(n)}k^{-n} . \tag{15}$$

Combining the terms of the same order in $(1/k)$, one can obtain recurrence relations for $E_0^{(n)}$ and $\Phi_0^{(n)}$. Since the effective potential $V_{\rm eff}(x)$ vanishes at the minimum $(r=r_0)$, the equations are solved first for $(r=r_0)$ to obtain $E_0^{(n)}$'s and then for any r to obtain $\Phi_0^{(n)}$'s.

First excited state: Using the same definition for x and assuming that the wave function for the first excited state is of the form

$$u_1(x)=(x-c)e^{\Phi_1(x)} . \tag{16}$$

We obtain from Eq. (4)

$$[-\tfrac{1}{2}\Phi_1''(x)+\Phi_1'^2(x)](x-c)-\Phi_1'(x)+\left[k^2V_{\rm eff}(x)+\left[-\frac{k}{2}+\frac{3}{8}\right]r^{-2}(x)\right](x-c)$$
$$+\left[(9\lambda)\tilde{a}-\frac{1}{3}\frac{(9\lambda)^3}{k^4}\tilde{a}r^2(x)+\frac{1}{6}\frac{(9\lambda)^4}{k^6}\tilde{a}r^3(x)+\cdots\right](x-c)=(x-c)\epsilon_1 , \tag{17}$$

where

$$\epsilon_1=E_1-k^2E^{(-2)} , \tag{18}$$

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

$$\Phi_1'(x)=\sum_{n=-1}^{\infty}\Phi_1^{(n)}(x)(1/k)^n , \tag{19}$$

$$\epsilon_1=\sum_{n=-1}^{\infty}E_1^{(n)}(1/k)^n , \tag{20}$$

and

$$c=\sum_{n=1}^{\infty}C^{(n)}(1/k)^n . \tag{21}$$

Substituting these into Eq. (17), we obtain

$$\left[-\tfrac{1}{2}\sum_{n=-1}^{\infty}\Phi_1^{(n)'}(x)k^{-n}-\tfrac{1}{2}\sum_{m,n=-1}^{\infty}\Phi_1^{(m)}(x)\Phi_1^{(n)}(x)k^{-(m+n)}\right]\left[x-\sum_{n=1}^{\infty}C^{(n)}k^{-n}\right]$$
$$-\sum_{n=-1}^{\infty}\Phi_1^{(n)}(x)k^{-n}+\left[k^2V_{\rm eff}(x)+\left[-\frac{k}{2}+\frac{3}{8}\right]r^{-2}(x)\right]\left[x-\sum_{n=1}^{\infty}C^{(n)}k^{-n}\right]$$
$$+\left[(9\lambda)\tilde{a}-\frac{1}{3}\frac{(9\lambda)^3}{k^4}\tilde{a}r^2(x)+\frac{1}{6}\frac{(9\lambda)^4}{k^6}\tilde{a}r^3(x)+\cdots\right]\left[x-\sum_{n=1}^{\infty}C^{(n)}k^{-n}\right]=\left[x-\sum_{n=1}^{\infty}C^{(n)}k^{-n}\right]\sum_{n=-1}^{\infty}E_1^{(n)}k^{-n} . \tag{22}$$

TABLE I. Comparison of the energy eigenvalues for $0\le\beta\le0.1$ as calculated from the dynamical approach (Ref. 16) with those to order β^4 of the present work.

β	E_0/a^2	$E_{1,0}$	E_1/a^2	$E_{2,0}$
0.01	−0.490 001	−0.490 001 0	−0.115 013	−0.115 013 5
0.02	−0.480 008	−0.480 007 8	−0.105 103	−0.105 103 6
0.03	−0.470 026	−0.470 026 0	−0.095 334	−0.095 336 6
0.04	−0.460 061	−0.460 060 9	−0.085 755	−0.085 769 0
0.05	−0.450 117	−0.450 117 4	−0.076 406	−0.076 449 7
0.06	−0.440 200	−0.440 200 4	−0.067 311	−0.067 421 7
0.07	−0.430 313		−0.058 482	
0.08	−0.420 461	−0.420 463 6	−0.049 915	−0.050 392 2
0.09	−0.410 647		−0.041 598	
0.1	−0.400 875	−0.400 883 9	−0.033 500	−0.034 967 7

Combining the terms of the same order in $(1/k)$, one can again obtain recurrence relations for $E_1^{(n)}$, $\Phi_1^{(n)}$, and $C^{(n)}$. The equations are solved one by one to obtain the node coefficients $C^{(n)}$'s and the higher-order corrections to the eigenvalues of the first excited states.

III. RESULTS AND CONCLUSIONS

Ground state: Defining $C=9\lambda$, we write the solutions

$$\begin{aligned}
&E_0^{(-1)}=-4\tilde{a}^2,\ E_0^{(0)}=-6\tilde{a}^2+C\tilde{a},\ E_0^{(1)}=-8\tilde{a}^2,\ E_0^{(2)}=-10\tilde{a}^2,\ E_0^{(3)}=-12\tilde{a}^2,\\
&E_0^{(4)}=-14\tilde{a}^2-C^3/48\tilde{a},\ E_0^{(5)}=-16\tilde{a}^2+C^3/48\tilde{a},\ E_0^{(6)}=-18\tilde{a}^2+C^3/48\tilde{a}+C^4/384\tilde{a}^2,\ E_0^{(7)}=-20\tilde{a}^2-C^3/48\tilde{a},\\
&E_0^{(8)}=-22\tilde{a}^2-C^4/96\tilde{a}^2-C^5/7680\tilde{a}^3,\ E_0^{(9)}=-24\tilde{a}^2+C^4/192\tilde{a}^2-C^5/3840\tilde{a}^3,\\
&E_0^{(10)}=-26\tilde{a}^2+C^4/128\tilde{a}^2+7C^5/7680\tilde{a}^3-C^6/4608\tilde{a}^4,\ E_0^{(11)}=-28\tilde{a}^2-C^4/192\tilde{a}^2+C^5/1280\tilde{a}^3+7C^6/18\,432\tilde{a}^4,\\
&E_0^{(12)}=-30\tilde{a}^2-19C^5/7680\tilde{a}^3+C^6/1024\tilde{a}^4+211C^7/2\,580\,480\tilde{a}^5,
\end{aligned}\tag{23}$$

and

$$\begin{aligned}
&\Phi_0^{(-1)}=-2\tilde{a}+1/2r(x),\ \Phi_0^{(0)}=-2\tilde{a}-1/2r(x),\ \Phi_0^{(1)}=-2\tilde{a},\ \Phi_0^{(2)}=-2\tilde{a},\ \Phi_0^{(3)}=-2\tilde{a},\\
&\Phi_0^{(4)}=-2\tilde{a},\ \Phi_0^{(5)}=-2\tilde{a}+[C^3/24\tilde{a}]r(x)+[C^3/6]r^2(x),\ \Phi_0^{(6)}=-2\tilde{a}-[C^3/24\tilde{a}]r(x)-[C^3/6]r^2(x),\\
&\Phi_0^{(7)}=-2\tilde{a}-[C^3/24\tilde{a}+C^4/192\tilde{a}^2]r(x)-[C^4/48\tilde{a}]r^2(x)-[C^4/12]r^3(x),\\
&\Phi_0^{(8)}=-2\tilde{a}+[C^3/24\tilde{a}]r(x)+[C^4/12]r^3(x),\\
&\Phi^{(9)}=-2\tilde{a}+[C^4/48\tilde{a}^2+C^5/3840\tilde{a}^3]r(x)+[C^4/16\tilde{a}+C^5/960\tilde{a}^2]r^2(x)+[C^5/240\tilde{a}]r^3(x)+[C^5/60]r^4(x),\\
&\Phi_0^{(10)}=-2\tilde{a}+[-C^4/96\tilde{a}^2+C^5/1920\tilde{a}^3]r(x)+[-C^4/24\tilde{a}+C^5/480\tilde{a}^2]r^2(x)+[C^5/240\tilde{a}]r^3(x)-[C^5/60]r^4(x),\\
&\Phi_0^{(11)}=-2\tilde{a}-[C^4/64\tilde{a}^2+7C^5/3840\tilde{a}^3-C^6/2304\tilde{a}^4]r(x)+[-C^5/160\tilde{a}^2+C^6/576\tilde{a}^3]r^2(x)\\
&\qquad+[-C^5/48\tilde{a}+C^6/192\tilde{a}^2]r^3(x)+[C^6/144\tilde{a}]r^4(x),\\
&\Phi_0^{(12)}=-2\tilde{a}+[C^4/96\tilde{a}^2-C^5/640\tilde{a}^3-7C^6/9216a^4]r(x)-[C^5/240\tilde{a}^2+7C^6/2304\tilde{a}^3]r^2(x)\\
&\qquad+[C^5/80\tilde{a}-7C^6/576\tilde{a}^2]r^3(x)-[C^6/48\tilde{a}]r^4(x).
\end{aligned}\tag{24}$$

First excited state: We write the solutions

$$\begin{aligned}
&E_1^{(-1)}=4\tilde{a}^2,\ E_1^{(0)}=-6\tilde{a}^2+C\tilde{a},\ E_1^{(1)}=8\tilde{a}^2,\ E_1^{(2)}=-10\tilde{a}^2,\ E_1^{(3)}=12\tilde{a}^2,\\
&E_1^{(4)}=-14\tilde{a}^2-C^3/48\tilde{a},\ E_1^{(5)}=16\tilde{a}^2-13C^3/48\tilde{a},\ E_1^{(6)}=-18\tilde{a}^2-23C^3/48\tilde{a}+C^4/384\tilde{a}^2,\\
&E_1^{(7)}=20\tilde{a}^2-11C^3/48\tilde{a}+C^4/16\tilde{a}^2,\ E_1^{(8)}=-22\tilde{a}^2+13C^4/48\tilde{a}^2-C^5/7680\tilde{a}^3,\\
&E_1^{(9)}=24\tilde{a}^2+89C^4/192\tilde{a}^2-19C^5/3840\tilde{a}^3,\ E_1^{(10)}=-26\tilde{a}^2+45C^4/128\tilde{a}^2-293C^5/7680\tilde{a}^3-C^6/4608\tilde{a}^4,\\
&E_1^{(11)}=28\tilde{a}^2+19C^4/192\tilde{a}^2-493C^5/3840\tilde{a}^3-203C^6/18\,432\tilde{a}^4,\\
&E_1^{(12)}=-30\tilde{a}^2-1739C^5/7680\tilde{a}^3-445C^6/9216\tilde{a}^4+179C^7/286\,720\tilde{a}^5,
\end{aligned}\tag{25}$$

and

$$\begin{aligned}
&\Phi_1^{(-1)}=-2\tilde{a}+1/2r(x),\ \Phi_1^{(0)}=2\tilde{a}-1/2r(x),\ \Phi_1^{(1)}=-2\tilde{a},\ \Phi_1^{(2)}=2\tilde{a},\ \Phi_1^{(3)}=-2\tilde{a},\ \Phi_1^{(4)}=2\tilde{a},\\
&\Phi_1^{(5)}=-2\tilde{a}+[C^3/24\tilde{a}]r(x)+[C^3/6]r^2(x),\ \Phi_1^{(6)}=2\tilde{a}-C^3/24\tilde{a}^2+[5C^3/24\tilde{a}]r(x)+[C^3/6]r^2(x),\\
&\Phi_1^{(7)}=-2\tilde{a}-C^3/12\tilde{a}^2+[7C^3/24\tilde{a}-C^4/192\tilde{a}^2]r(x)-[C^4/48\tilde{a}]r^2(x)-[C^4/12]r^3(x),\\
&\Phi_1^{(8)}=2\tilde{a}+C^4/128\tilde{a}^3+[C^3/8\tilde{a}-C^4/16\tilde{a}^2]r(x)-[C^4/8\tilde{a}]r^2(x)-[C^4/12]r^3(x),
\end{aligned}$$

TABLE II. Improvement in energy with respect to orders of β.

β	$(E_0/a^2)_0$	$(E_0/a^2)_1$	$(E_0/a^2)_3$	$(E_0/a^2)_4$	$(E_1/a^2)_0$	$(E_1/a^2)_1$	$(E_1/a^2)_3$	$(E_1/a^2)^4$
0.02	−0.5	−0.48	−0.480 008	−0.480 007 8	−0.125	−0.105	−0.105 112	−0.105 103 2
0.05	−0.5	−0.45	−0.450 125	−0.450 117 2	−0.125	−0.075	−0.076 750	−0.076 406 3
0.08	−0.5	−0.42	−0.420 512	−0.420 640 8	−0.125	−0.045	−0.052 168	−0.049 915 2

$$\Phi_1^{(9)}=-2\tilde{a}+C^3/12\tilde{a}^2+C^4/24\tilde{a}^3+[-5C^4/24\tilde{a}^2+C^5/3840\tilde{a}^3]r(x)$$
$$+[-3C^4/16\tilde{a}+C^5/960\tilde{a}^2]r^2(x)+[C^5/240\tilde{a}]r^3(x)+[C^5/60]r^4(x)\ , \quad (26)$$
$$\Phi_1^{(10)}=2\tilde{a}+C^3/24\tilde{a}^2+9C^4/128\tilde{a}^3-C^5/1920\tilde{a}^4+[29C^4/96\tilde{a}^2+11C^5/1920\tilde{a}^3]r(x)$$
$$+[-C^4/12\tilde{a}+7C^5/480\tilde{a}^2]r^2(x)+[7C^5/240\tilde{a}]r^3(x)+[C^5/60]r^4(x)\ ,$$
$$\Phi_1^{(11)}=-2\tilde{a}+C^4/48\tilde{a}^3-C^5/192\tilde{a}^4+[-13C^4/64\tilde{a}^2+133C^5/3840\tilde{a}^3+C^6/2304\tilde{a}^4]r(x)$$
$$+[9C^5/160\tilde{a}^2+C^6/576\tilde{a}^3]r^2(x)+[11C^5/240\tilde{a}+C^6/192\tilde{a}^2]r^3(x)+[C^6/144\tilde{a}]r^4(x)$$
$$\Phi_1^{(12)}=2\tilde{a}-23C^4/384\tilde{a}^3-37C^5/1920\tilde{a}^4-13C^6/4608\tilde{a}^5+[-5C^4/96\tilde{a}^2+63C^5/640\tilde{a}^3+59C^6/9216\tilde{a}^4]r(x)$$
$$+[11C^5/120\tilde{a}^2+43C^6/2304\tilde{a}^3]r^2(x)+[C^5/48\tilde{a}+23C^6/576\tilde{a}^2]r^3(x)+[C^6/48\tilde{a}]r^4(x)\ ,$$

and also

$$C^{(1)}=0,\ C^{(2)}=-1/4\tilde{a},\ C^{(3)}=0,\ C^{(4)}=0,\ C^{(5)}=0,\ C^{(6)}=C^3/384\tilde{a}^4,\ C^{(7)}=C^3/192\tilde{a}^4\ ,$$
$$C^{(8)}=-C^3/192\tilde{a}^4-C^4/2048\tilde{a}^5,\ C^{(9)}=-C^3/64\tilde{a}^4-C^4/384\tilde{a}^5\ ,\ C^{(10)}=-7C^4/2048\tilde{a}^5+C^5/30\,720\tilde{a}^6, \quad (27)$$
$$C^{(11)}=C^3/64\tilde{a}^4+C^4/256\tilde{a}^5+C^5/3072\tilde{a}^6\ ,\ C^{(12)}=C^3/128\tilde{a}^4+37C^4/3072\tilde{a}^5+7C^5/6144\tilde{a}^6+17C^6/73\,728\tilde{a}^7\ .$$

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

$$E_0=k^2E^{(-2)}+\sum_{n=-1}^{\infty}k^{-n}E_0^{(n)} \quad (28)$$

and

$$E_1=k^2E^{(-2)}+\sum_{n=-1}^{\infty}k^{-n}E_1^{(n)}\ , \quad (29)$$

respectively. Substituting $k=3$ for three space in Eqs. (28) and (29) and defining $\beta=\lambda/a$, we obtain

$$E_0/a^2=-\tfrac{1}{2}+\beta-\beta^3+\tfrac{5}{4}\beta^4+\cdots \quad (30)$$

and

$$E_1/a^2=-\tfrac{1}{8}+\beta-14\beta^3+55\beta^4+\cdots\ . \quad (31)$$

Some numerical values of energies in the atomic units for different values of the parameter β in the range $0\leq\beta\leq0.1$ are given in Table I.

Our results are consistent to order β^4 with earlier results obtained by applying different methods.[15–18] We finally illustrate the improvement of energy with respect to orders of β in Table II.

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