Shifted $1/N$ expansion for energy eigenvalues of the exponential cosine screened Coulomb potential

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The shifted $1/N$ expansion has been used for solving the Schrödinger equation for exponential cosine screened Coulomb potential. The analytic expressions for the energies $E_{n,l}$ yield fairly accurate results for a wide range of values of n,l and the screening parameter λ. The energy values obtained by this method have been compared and found to be in excellent agreement with the Padé-approximation calculations.

I. INTRODUCTION

Recently, the shifted $1/N$ expansion has emerged as an extremely powerful technique for determining energy eigenvalues of the Schrödinger equation with fairly good accuracy.[1-3] The shifted $1/N$ expansion differs from the ordinary large-N expansion[4] in the expression for the expansion parameter. In the former case the expansion parameter is $1/\bar{k}$ where $\bar{k}=N+2l-a$, whereas in the latter case it is $1/k$ where $k=N+2l$, N being the number of spatial dimensions, $l(l+N-2)\hbar^2$ the eigenvalue of the square of the N-dimensional orbital angular momentum, and a the shift chosen by requiring agreement between the $1/\bar{k}$ expansions and the exact analytic results for the harmonic oscillator and Coulomb potentials.[1]

One palpable advantage of choosing $1/\bar{k}$ as an expansion parameter is that unlike the ordinary Rayleigh-Schrödinger perturbation theory which requires an expansion in powers of the coupling constant, the shifted $1/N$ technique can be used for problems which do not manifestly involve a small coupling constant. Hence, 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 be treated as a perturbation.

In the present work, we shall show that the shifted $1/N$ expansion provides remarkably accurate and simple analytic expressions for the energy eigenvalues of the Schrödinger equation with the exponential-cosine screened Coulomb potential (ECSC), i.e.,

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

This potential has received much attention in recent years[5-11] because of its frequent occurrence in solid-state physics.[12]

II. THE METHOD AND CALCULATIONS

The radial Schrödinger equation in N spatial dimensions in terms of the shifted variable $\bar{k}=N+2l-a$ is

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

where $V(r)$ is given by Eq. (1)

In order to get useful results from a $1/\bar{k}$ expansion, the large-E limit of the potential should be suitably defined.[1] Since the angular-momentum barrier term behaves like $\bar{k}^2$ at large $\bar{k}$, so should the potential $V(r)$. This will give 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 following equation:

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

where Q is a constant to be specified later.

The shifted $1/N$ expansion method consists in solving Eq. (3) systematically in terms of the expansion parameter $1/\bar{k}$. The leading contribution to the energy comes from the effective potential

$$V_{\rm eff}(r)=\frac{\hbar^2}{8mr^2}+\frac{V(r)}{Q}\ . \tag{4}$$

Now it is assumed that $V(r)$ is sufficiently well behaved so that $V_{\rm eff}(r)$ has a minimum at $r=r_0$ and there are well defined bound states. Then the following relationship is valid:

$$4mr_0^3V'(r_0)=\hbar^2Q\ , \tag{5}$$

where r_0 is the root of the equation

$$N+2l-2+(2n+1)\left[3+\frac{r_0V''(r_0)}{V'(r_0)}\right]^{1/2}=\left[\frac{4mr_0^3V'(r_0)}{\hbar^2}\right]^{1/2}. \quad (6)$$

Once r_0 is determined, the leading term in E is given by

$$\bar{k}^2V_{\rm eff}(r_0)=\frac{\bar{k}^2}{r_0^2}\left[\frac{\hbar^2}{8m}+\frac{r_0^2V(r_0)}{Q}\right]. \quad (7)$$

The next contribution is of order $\bar{k}$ and is given by

$$\frac{\bar{k}}{r_0^2}\left[(n+\tfrac{1}{2})\hbar\omega-\frac{(2-a)h^2}{4m}\right]. \quad (8)$$

The shift a is chosen so that this contribution vanishes. Therefore

$$a=2-2(2n+1)m\omega/\hbar\,. \quad (9)$$

The successive contributions to the energy are determined by substituting

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

in Eq. (3) and expanding about $x=0$ in powers of x. Since the algorithm for the shifted $1/N$ expansions has been developed previously,[2] we present here only the essential steps.

The energy eigenvalues are given by an expansion in powers of $1/\bar{k}$ where $\bar{k}=N+2l-a$ as

$$E_{n,l}=\frac{\bar{k}}{r_0^2}\left[\frac{\hbar^2\bar{k}}{8m}+\frac{r_0^2\bar{k}V(r_0)}{Q}+\frac{\beta^{(1)}}{\bar{k}}+\frac{\beta^{(2)}}{\bar{k}^2}+O\left[\frac{1}{\bar{k}^3}\right]\right], \quad (11)$$

where

$$\beta^{(1)}=\frac{\hbar^2(1-a)(3-a)}{8m}+(1+2n)\tilde{\epsilon}_2+3(1+2n+2n^2)\tilde{\epsilon}_4-\frac{1}{\hbar\omega}[\tilde{\epsilon}_1^2+6(1+2n)\tilde{\epsilon}_1\tilde{\epsilon}_3+(11+30n+30n^2)\tilde{\epsilon}_3^2], \quad (12)$$

$$\begin{aligned}\beta^{(2)}=&(1+2n)\tilde{\delta}_2+3(1+2n+2n^2)\tilde{\delta}_4+5(3+8n+6n^2+4n^3)\tilde{\delta}_6\\&-\frac{1}{\hbar\omega}[(1+2n)\tilde{\epsilon}_2^2+12(1+2n+2n^2)\tilde{\epsilon}_2\tilde{\epsilon}_4+2(21+59n+51n^2+34n^3)\tilde{\epsilon}_4^2+2\tilde{\epsilon}_1\tilde{\delta}_1\\&+6(1+2n)\tilde{\epsilon}_1\tilde{\delta}_3+30(1+2n+2n^2)\tilde{\epsilon}_1\tilde{\delta}_5+6(1+2n)\tilde{\epsilon}_3\tilde{\delta}_1+2(11+30n+30n^2)\tilde{\epsilon}_3\tilde{\delta}_3\\&+10(13+40n+42n^2+28n^3)\tilde{\epsilon}_3\tilde{\delta}_5]+\frac{1}{(\hbar\omega)^2}[4\tilde{\epsilon}_1^2\tilde{\epsilon}_2+36(1+2n)\tilde{\epsilon}_1\tilde{\epsilon}_2\tilde{\epsilon}_3\\&+8(11+30n+30n^2)\tilde{\epsilon}_2\tilde{\epsilon}_3^2\\&+24(1+2n)\tilde{\epsilon}_1^2\tilde{\epsilon}_4+8(31+78n+78n^2)\tilde{\epsilon}_1\tilde{\epsilon}_3\tilde{\epsilon}_4\\&+12(57+189n+225n^2+150n^3)\tilde{\epsilon}_3^2\tilde{\epsilon}_4]\\&-\frac{1}{(\hbar\omega)^3}[8\tilde{\epsilon}_1^3\tilde{\epsilon}_3+108(1+2n)\tilde{\epsilon}_1^2\tilde{\epsilon}_3^2+48(11+30n+30n^2)\tilde{\epsilon}_1\tilde{\epsilon}_3^3+30(31+109n+141n^2+94n^3)\tilde{\epsilon}_3^4],\end{aligned} \quad (13)$$

$$\tilde{\epsilon}_j=\frac{\epsilon_j}{(2m\omega/\hbar)^{j/2}},\quad \tilde{\delta}_j=\frac{\delta_j}{(2m\omega/\hbar)^{j/2}}\quad (j=1,2,\ldots), \quad (14)$$

and where

$$\omega=\frac{\hbar}{2m}\left[3+\frac{r_0V''(r_0)}{V'(r_0)}\right]^{1/2}, \quad (15)$$

$$\epsilon_1=\frac{(2-a)\hbar^2}{2m}, \quad (16)$$

$$\epsilon_2=-\frac{3\hbar^2(2-a)}{4m}, \quad (17)$$

$$\epsilon_3=-\frac{\hbar^2}{2m}+\frac{r_0^5V'''(r_0)}{6Q}, \quad (18)$$

$$\epsilon_4=\frac{5\hbar^2}{8m}+\frac{r_0^6V^{(\rm iv)}(r_0)}{24Q}, \quad (19)$$

$$\delta_1=-\frac{(1-a)(3-a)\hbar^2}{4m}, \quad (20)$$

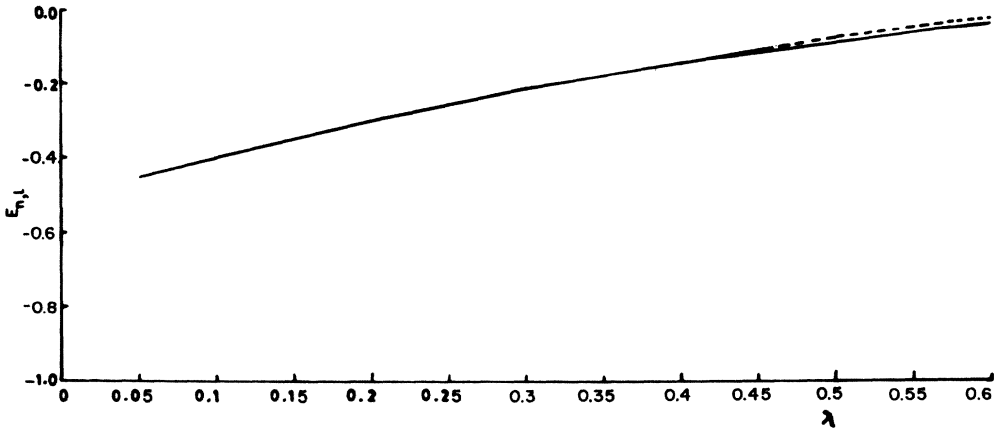

FIG. 1. The ground state ($1s$) energy as a function of the screening parameter λ. The solid line corresponds to the shifted $1/N$ expansion and the dashed line corresponds to the Padé-approximation energies. The energies are given in atomic units.

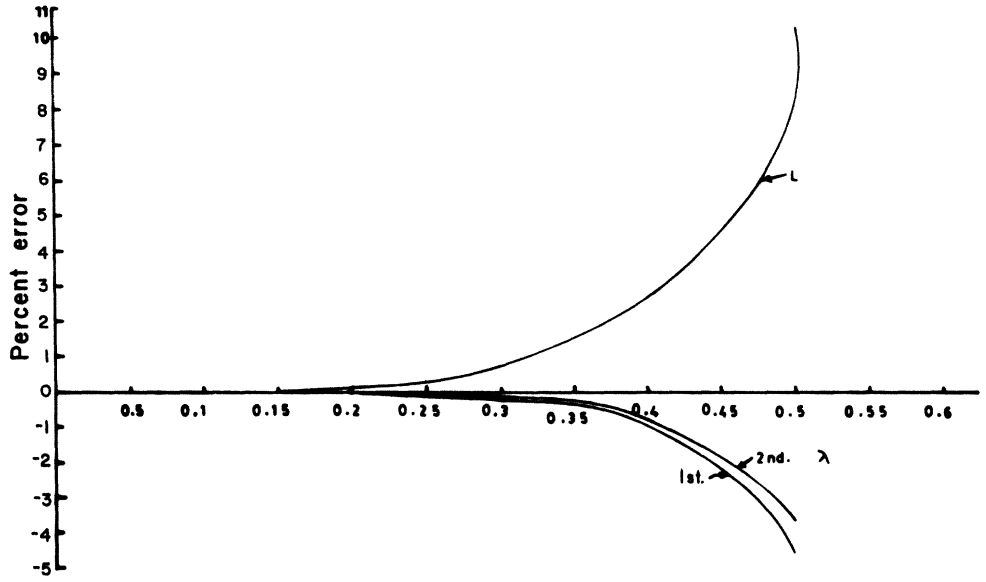

FIG. 2. The percent error in the shifted $1/N$ expansion for the ground state ($1s$) energy vs λ. The curve indicated by L corresponds to the leading-order energy values. The curve indicated by 1st (2nd) corresponds to the leading order plus one (two) corrections.

TABLE I. Energy eigenvalues for the $1s$ state in atomic units.

λ	E (Present)	E (Padé)
0.06	−0.440 201	−0.440 201
0.08	−0.420 466	−0.420 464
0.1	−0.400 891	−0.400 885
0.2	−0.306 416	−0.306 335
0.3	−0.219 751	−0.219 416
0.4	−0.143 455	−0.142 439
0.5	−0.080 546	−0.077 680
0.6	−0.036 561	−0.028 244
0.7	−0.026 375 0	−0.000 168

TABLE II. Energy eigenvalues for the $2s$ and $2p$ states in atomic units.

λ		E (Present)	E (Padé)
0.02	$2s$	−0.105 103	−0.105 104
0.02	$2p$	−0.105 074	−0.105 075
0.04	$2s$	−0.085 762	−0.085 769
0.04	$2p$	−0.085 560	−0.085 591
0.06	$2s$	−0.067 388	−0.067 421
0.06	$2p$	−0.066 783	−0.066 778
0.08	$2s$	−0.050 288	−0.050 387
0.08	$2p$	−0.049 014	−0.048 997
0.10	$2s$	−0.034 721	−0.034 941
0.10	$2p$	−0.032 509	−0.032 469
0.15	$2s$	−0.004 561	−0.005 250

TABLE III. Energy eigenvalues for the $3s$, $3p$, and $3d$ states in atomic units.

λ		E (Present)	E (Padé)
0.02	$3s$	−0.036 016	−0.036 025
0.02	$3p$	−0.035 966	−0.035 968
0.02	$3d$	−0.035 850	−0.035 851
0.04	$3s$	−0.018 702	−0.018 823
0.04	$3p$	−0.018 430	−0.018 453
0.04	$3d$	−0.017 685	−0.017 682
0.05	$3s$	−0.011 316	−0.011 576
0.05	$3p$	−0.010 879	−0.010 929
0.05	$3d$	−0.009 563	−0.009 555
0.06	$3s$	−0.005 013	−0.005 461
0.06	$3p$	−0.004 387	−0.004 471
0.06	$3d$	−0.002 324	−0.002 308
0.07	$3s$	−0.000 086	−0.000 740

TABLE IV. Energy eigenvalues for the $4s$, $4p$, $4d$, and $4f$ states in atomic units.

λ		E (Present)	E (Padé)
0.01	$4s$	−0.021 433	−0.021 438
0.01	$4p$	−0.021 422	−0.021 424
0.01	$4d$	−0.021 397	−0.021 398
0.01	$4f$	−0.021 357	−0.021 358
0.02	$4s$	−0.012 517	−0.012 572
0.02	$4p$	−0.012 465	−0.012 486
0.02	$4d$	−0.012 306	−0.012 310
0.02	$4f$	−0.012 038	−0.012 038
0.03	$4s$	−0.005 052	−0.005 270
0.03	$4p$	−0.004 947	−0.004 033
0.03	$4d$	−0.004 523	−0.004 539
0.03	$4f$	−0.003 750	−0.003 748
0.04	$4s$	−0.000 342	−0.000 119

$$\delta_2=\frac{3(1-a)(3-a)\hbar^2}{8m}, \tag{21}$$

$$\delta_3=\frac{(2-a)\hbar^2}{m}, \tag{22}$$

$$\delta_4=-\frac{5(2-a)\hbar^2}{4m}, \tag{23}$$

$$\delta_5=-\frac{3\hbar^2}{4m}+\frac{r_0^7V^{(v)}(r_0)}{120Q}, \tag{24}$$

$$\delta_6=\frac{7\hbar^2}{8m}+\frac{r_0^8V^{(vi)}(r_0)}{720Q}. \tag{25}$$

III. RESULTS

For any given choice of n and l, Eq. (6) becomes a transcendental equation which can be solved numerically to obtain r_0. Substitution of r_0 into Eqs. (5) and (11)–(25) immediately gives the energy eigenvalues. In all our calculations, we have used atomic units so that $\hbar=m=1$.

We list our energy values for various states in Tables I–IV and compare them with the Padé-approximation calculations.[6] The variation of the ground state ($1s$) energy with the screening parameter λ is shown in Fig. 1. Also, to see how closely our results agree with the Padé-approximation calculation we have plotted the percent error of our results (for the $1s$ state) in the region $\lambda\leq 0.5$. It is clear from Fig. 2, that for $\lambda\geq 0.4$, the successive contributions from the perturbation series are substantial and one needs to consider higher-order terms in $1/\bar{k}$ expansion to get better accuracy. In this context it has to be kept in mind that the shift a is chosen in such a way so as to reproduce the exact analytic results for the Coulomb potential.[1] Consequently, the energy values we have obtained are especially accurate for small λ. However, as is evident from Table I, the shifted $1/N$ expansion, to the order considered here, still predicts that the $1s$ state for λ as large as 0.7 is a bound state, which the ordinary perturbation theory does not.[7]

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