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Hypervirial solution for the generalized exponential cosine-screened Coulomb potential

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The bound-state energy spectrum of the generalized exponential cosine-screened Coulomb potential is obtained by employing the hypervirial equations with the Hellman-Feynman theorem applied to the screening parameters λ and μ independently. The energy eigenvalues are obtained up to the fourth order of the screening parameters.

I. INTRODUCTION

The generalized exponential cosine-screened Coulomb potential[1] (GECSCP), given by

$$V(r) = -\frac{a}{r}\exp(-\lambda r)\cos(\mu r) , \tag{1}$$

involves a wide class of model potentials that finds applications in various fields of physics such as plasma physics,[2,3] nuclear physics,[4,5] and solid-state physics.[6-9]

Because of the importance of this potential in atomic phenomena, it has been extensively studied by using numerical and analytical methods, both perturbative[10-16] and nonperturbative.[17-30] Recently this potential for the $\mu=\epsilon\lambda$ case has also been solved by Chatterjee[29] by following the method of Grant and Lai.

In the present work, we employ the same method by taking the screening parameters freely. It is shown that the results obtained by us are reduced to the ones obtained by Chatterjee.

II. THE METHOD AND CALCULATIONS

The radial part of Schrödinger equation (with $m=\hbar=1$) for a particle in a spherically symmetric potential can be written as

$$Hu(r) = Eu(r) , \tag{2}$$

where the Hamiltonian H is given by

$$H = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r) , \tag{3}$$

and the boundary conditions are $u=0$ at $r=0$, and $u\to 0$ as $r\to\infty$. Now we use the hypervirial theorem

$$\left\langle u(r) \left| \left[r^j\frac{d}{dr}, H\right] \right| u(r)\right\rangle = 0 \tag{4}$$

to obtain

$$E\langle r^j\rangle = \langle r^j V(r)\rangle + \tfrac{1}{2}(j+1)^{-1}\left\langle r^{j+1}\frac{dV(r)}{dr}\right\rangle - \tfrac{1}{8}j(j+1)^{-1}[j^2-4l(l+1)-1]\langle r^{j-2}\rangle . \tag{5}$$

Substituting the expansions

$$V(r) = \sum_{n,m=0}^{\infty} V_{nm}\lambda^n\mu^{2m}r^{n+2m-1} , \tag{6}$$

$$V_{nm} = -a\frac{(-1)^{n+m}}{n!(2m)!} , \tag{7}$$

$$\langle r^j\rangle = \sum_{n'',m''=0}^{\infty} C_j^{(n'',m'')}\mu^{n''}\lambda^{m''} , \tag{8}$$

and

$$E_n = \sum_{n',m'=0}^{\infty} E_n^{(n',m')}\mu^{n'}\lambda^{m'} \tag{9}$$

into Eq. (5), we obtain

$$\sum_{n',m',n'',m''=0}^{\infty} E_n^{(n',m')}C_j^{(n'',m'')}\lambda^{m'+m''}\mu^{n'+n''} = \sum_{n,m,n'',m''=0}^{\infty}\frac{n+2j+2m+1}{2(j+1)}V_{nm}C_{n+j+2m-1}^{(n'',m'')}\lambda^{n+m''}\mu^{2m+m''} - \tfrac{1}{8}j(j+1)^{-1}[j^2-4l(l+1)-1] \times \sum_{n'',m''=0}^{\infty} C_{j-2}^{(n'',m'')}\lambda^{m''}\mu^{n''} \tag{10}$$

TABLE I. Comparison of the energy eigenvalues for $0 \leq \beta_1, \beta_2 < 0.1$ as calculated from the dynamical approach (Ref. 32) with those to fourth order of the screening parameters.

State	β_1	β_2	E_{nl}/a^2	State	β_1	β_2	E_{nl}/a^2
1*s*	0.02	0.05	−0.480 072 8	1*s*	0.02	0.02	−0.480 007 8 (−0.480 007 8)
2*s*	0.02	0.05	−0.106 072 4	2*s*	0.02	0.02	−0.105 103 2 (−0.105 103 6)
2*p*	0.02	0.05	−0.105 927	2*p*	0.02	0.02	−0.105 088 (−0.105 074 6)
3*s*	0.02	0.05	−0.041 272	3*s*	0.02	0.02	−0.036 016 (−0.036 025 6)
3*p*	0.02	0.05	−0.040 94	3*p*	0.02	0.02	−0.035 98 (−0.035 596 77)
3*d*	0.02	0.05	−0.040 60	3*d*	0.02	0.02	−0.035 95 (−0.035 850 3)
4*s*	0.02	0.05	−0.031 03	4*s*	0.02	0.02	−0.012 48 (−0.012 581 1)
4*p*	0.02	0.05	−0.030 43	4*p*	0.02	0.02	−0.012 43 (−0.012 491 5)
4*d*	0.02	0.05	−0.029 82	4*d*	0.02	0.02	−0.012 38 (−0.012 310 5)
4*f*	0.02	0.05	−0.0292	4*f*	0.02	0.02	−0.0123 (−0.012 034 7)
1*s*	0.02	0.08	−0.480 209 6	1*s*	0.02	0.10	−0.480 354 4
2*s*	0.02	0.08	−0.108 580 2	2*s*	0.02	0.10	−0.111 711 8
2*p*	0.02	0.08	−0.108 124	2*p*	0.02	0.10	−0.110 810
3*s*	0.02	0.08	−0.058 419	3*s*	0.02	0.10	−0.082 767
3*p*	0.02	0.08	−0.057 21	3*p*	0.02	0.10	−0.080 38
3*d*	0.02	0.08	−0.055 95	3*d*	0.02	0.10	−0.077 86
4*s*	0.02	0.08	−0.105 65	4*s*	0.02	0.10	−0.220 85
4*f*	0.02	0.08	−0.103 04	4*f*	0.02	0.10	−0.215 27
4*d*	0.02	0.08	−0.100 34	4*d*	0.02	0.10	−0.209 45
4*f*	0.02	0.08	−0.0976	4*f*	0.02	0.10	−0.2034
1*s*	0.05	0.02	−0.449 969 3	1*s*	0.05	0.05	−0.450 117 2 (−0.450 117 4)
2*s*	0.05	0.02	−0.074 62	2*s*	0.05	0.05	−0.076 41 (−0.076 449 7)
2*p*	0.05	0.02	−0.0747	2*p*	0.05	0.05	−0.0762 (−0.076 056 1)
3*s*	0.05	0.02	−0.0041	3*s*	0.05	0.05	−0.0106 (−0.011 662 7)
3*p*	0.05	0.02	−0.0041	3*p*	0.05	0.05	−0.0102 (−0.010 947 4)
3*d*	0.05	0.02	−0.0041	3*d*	0.05	0.05	−0.010 (−0.009 495 4)
1*s*	0.05	0.08	−0.4504080	1*s*	0.05	0.10	−0.450 695
2*s*	0.05	0.08	−0.08043	2*s*	0.05	0.10	−0.084 95
2*p*	0.05	0.08	−0.0797	2*p*	0.05	0.10	−0.0836
3*s*	0.05	0.08	−0.0210	3*s*	0.05	0.10	−0.0564
3*p*	0.05	0.08	−0.0286	3*p*	0.05	0.10	−0.0537
3*d*	0.05	0.08	−0.027	3*d*	0.05	0.10	−0.0519
4*s*	0.05	0.08	−0.048	4*s*	0.05	0.10	−0.148
4*p*	0.05	0.08	−0.046	4*p*	0.05	0.10	−0.144
4*d*	0.05	0.08	−0.044	4*d*	0.05	0.10	−0.140
4*f*	0.05	0.08	−0.042	4*f*	0.05	0.10	−0.134 967
1*s*	0.08	0.02	−0.4198	1*s*	0.08	0.08	−0.420 461 (−0.420 463 6)
2*s*	0.08	0.02	−0.0430	2*s*	0.08	0.08	−0.0499 (−0.050 392 2)

TABLE I. (*Continued*).

State	β_1	β_2	E_{nl}/a^2	State	β_1	β_2	E_{nl}/a^2
2p	0.08	0.02	−0.0432	2p	0.08	0.08	−0.0491 (−0.048 961 0)
1s	0.08	0.05	−0.420035	1s	0.08	0.10	−0.420 87
2p	0.08	0.05	−0.0452	2s	0.08	0.10	−0.0551
2d	0.08	0.05	−0.0451				
				2p	0.08	0.10	−0.0537
				3s	0.08	0.10	−0.0081
				3p	0.08	0.10	−0.0060
				3d	0.08	0.10	−0.0040
1s	0.10	0.08	−0.400 389	1s	0.10	0.02	−0.399 618
2s	0.10	0.08	−0.0283	2s	0.10	0.02	−0.02165
2p	0.10	0.08	−0.0276	1s	0.10	0.05	−0.399 882
1s	0.10	0.10	−0.400 875 (−0.400 883 9)	2s	0.10	0.05	−0.023 578
2s	0.10	0.10	−0.033 50 (−0.03 496 77)	2p	0.10	0.05	−0.0235
2p	0.10	0.10	−0.0321 (−0.032 349 8)				

From the normalization condition that $\langle r^0 \rangle = 1$, we use

$$C_0^{(n,m)} = \delta_{0n}\delta_{0m} , \tag{11}$$

and the energy of the unperturbed nth S states are given by

$$E_n^{(0,0)} = -\frac{a^2}{2n^2}, \quad n = 1,2,3,\ldots . \tag{12}$$

From Eq. (10), we deduced a series of 15 recurrence relations and solved them to get the perturbed energy terms up to the fourth order of the screening parameters λ and μ. For example, the first three recurrence relations obtained by equating the coefficients of $\lambda^0\mu^0$, $\lambda\mu^0$, and $\lambda^0\mu$ are

$$E_n^{(0,0)}C_j^{(0,0)} = \frac{2j+1}{2(j+1)} V_{00} C_j^{(0,0)} - \tfrac{1}{8} j(j+1)^{-1}[j^2 - 4l(l+1) - 1] C_{j-2}^{(0,0)} , \tag{13a}$$

$$E_n^{(0,1)}C_j^{(0,0)} + E_n^{(0,0)}C_j^{(0,1)} = \frac{2j+1}{2(j+1)} V_{00} C_{j-1}^{(0,1)} + V_{10} C_j^{(0,0)} - \tfrac{1}{8} j(j+1)^{-1}[j^2 - 4l(l+1) - 1] C_{j-2}^{(0,1)} , \tag{13b}$$

and

$$E_n^{(1,0)}C_j^{(0,0)} + E_n^{(0,0)}C_j^{(0,1)} = \frac{2j+1}{2(j+1)} V_{00} C_{j-1}^{(1,0)} - \tfrac{1}{8} j(j+1)^{-1}[j^2 - 4l(l+1) - 1] C_{j-2}^{(1,0)} . \tag{13c}$$

By defining $L = l(l+1)$, the expansion coefficients used in the calculation of the energy eigenvalues are as follows:

$$C_1^{(0,0)} = (3n^2 - L)/2a , \tag{14a}$$

$$C_2^{(0,0)} = n^2(5n^2 - 3L + 1)/2a^2 , \tag{14b}$$

$$C_3^{(0,0)} = n^2[35n^4 + 5n^2(-6L + 5) + 3L(L-2)]/8a^2 , \tag{14c}$$

$$C_0^{(0,2)} = 0 , \tag{14d}$$

$$C_1^{(0,2)} = n^2(7n^4 + 5n^2 - 3L^2)/8a^3 , \tag{14e}$$

$$C_1^{(2,0)} = n^2(-7n^4 - 5n^2 + 3L^2)/8a^3 , \tag{14f}$$

$$C_2^{(2,0)} = n^4[-45n^4 + n^2(14L - 63) + 5L(3L+2)]/8a^4 , \tag{14g}$$

$$C_1^{(1,2)} = 0 , \tag{14h}$$

$$C_1^{(2,1)} = n^4[73n^4 + n^2(-14L + 83) - L(27L + 10)]/16a^4 . \tag{14i}$$

Here we used the Hellman-Feynman theorem for the screening parameters λ and μ to define perturbed energies in terms of expansion coefficients of the potentials

$$\left\langle \frac{\partial H}{\partial \lambda} \right\rangle = \frac{\partial E}{\partial \lambda} \tag{15a}$$

and

$$\left\langle \frac{\partial H}{\partial \mu} \right\rangle = \frac{\partial E}{\partial \mu} , \tag{15b}$$

to get

$$m'E_n^{(n',m')}=\sum_{\substack{n=1\\m=0}} nV_{nm}C_{n+2m-1}^{(n'-2m,m'-n)} \tag{16a}$$

and

$$n'E_n^{(n',m')}=\sum_{\substack{n=0\\m=1}} 2mV_{nm}C_{n+2m-1}^{(n'-2m,m'-n)} . \tag{16b}$$

Therefore calling $\beta_1=\lambda/a$ and $\beta_2=\mu/a$, we write the bound-state energy spectrum in the powers of the screening parameters λ and μ as

$$E_{nl}/a^2=-\frac{1}{2n^2}+\beta_1+\tfrac{1}{4}(-3n^2+L)(\beta_1^2-\beta_2^2)+\frac{n^2}{12}(5n^2-3L+1)(\beta_1^3-3\beta_1\beta_2^2)$$
$$+\frac{n^2}{192}[-77n^4+5n^2(6L-11)+3L(5L+2)](\beta_1^4+\beta_2^4)+\frac{n^2}{32}[49n^4+5n^2(-6L+7)-3L(L+2)]\beta_1^2\beta_2^2 . \tag{17}$$

III. RESULTS AND CALCULATIONS

We have derived the entire bound-state energy spectrum of the potential (GECSP) in the powers of the screening parameters λ and μ. In the solution, we employed the hypervirial equation with the Hellman-Feynman theorem applied to the screening parameters separately. This procedure provides a solution for the energy eigenvalues, which are a function of two free parameters having different physical properties; therefore the solution covers the special forms of the potential. One can easily interpret the variation of each parameter and truncate the expansion by arranging the terms especially in the higher-order contributions. One can also easily extend the solution in parallel with the truncation procedure by considering only one of the parameters.

Our results are consistent with previous works.[12,16,31,32] Some numerical values of energies of the first four states for different values of β_1 and β_2 are also compared with those obtained recently by applying the dynamical-group technique.[32]

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