Energies of the exponential cosine screened Coulomb potential

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The energy eigenvalues of the exponential cosine screened Coulomb potential for various eigenstates are accurately determined within the framework of the hypervirial Padé scheme.

The exponential cosine screened Coulomb (ECSC) potential

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

is of importance in solid-state physics. It is used in describing the potential between an ionized impurity and an electron in a metal[1,2] or a semiconductor,[3] and the electron-positron interaction in a positronium atom in a solid.[4] The bound-state energies of the ECSC potential were first calculated for the $1s$ state by a numerical method,[1] and for the s states by a variational method.[5] Recently, the energy eigenvalues of the ECSC potential[6,7] have been recalculated for the $1s$ state with the use of the ground-state logarithmic perturbation theory[8,9] and the Padé approximant method. The problem of determining the critical screening parameter λ_c for the s states is also studied.[10]

It has recently been shown that the problem of screened Coulomb potentials can be solved to a very high accuracy[11] by using the hypervirial relations[12–14] and the Padé approximant method. In this paper, we would like to report that the bound-state energies of the ECSC potential for all eigenstates can be accurately determined within the framework of the same hypervirial Padé scheme.

The ECSC potential can be expanded in power series of the screening parameter λ as

$$V(r) = -\frac{1}{r} e^{-\lambda r} \cos \lambda r = -\frac{1}{r} \sum_{k=0}^{\infty} V_k (\lambda r)^k \ , \tag{2}$$

where the potential coefficients V_k are given by

$$V_1 = -1 \ , \quad V_2 = 0 \ , \quad V_3 = \tfrac{1}{3} \ , \quad V_4 = -\tfrac{1}{6} \ , \quad V_5 = \tfrac{1}{30} \ , \ \ldots \ . \tag{3}$$

Here, we use atomic units so that the distances are measured in $a_0 = \kappa h^2 / m^* e^2$, and energies in $m^* e^4 / \kappa^2 h^2$, where m^* is the effective mass and κ is the dielectric constant. The hypervirial relations for screened Coulomb potentials have been derived in a previous paper[14] as

$$(E + V_1 \lambda) \langle r^j \rangle = -\frac{1}{2} \left[\frac{2j+1}{j+1} \langle r^{j-1} \rangle + \left(-\frac{jl(l+1)}{j+1} + \frac{1}{4} j(j-1) \right) \langle r^{j-2} \rangle + \sum_{k=2}^{\infty} \frac{2j+k+1}{j+1} V_k \lambda^k \langle r^{j+k+1} \rangle \right] , \tag{4}$$

$$j \geq 0 \ ,$$

where l is the orbital angular momentum quantum number. Assuming that the energy E_n and the expectation

TABLE. I. Energy eigenvalues as a function of screening parameter λ for the $1s$ state in atomic units.

λ	$E[10, 10]$	$E[10, 11]$	Perturbation	Variational
0.70	−0.000 168	−0.000 043	+0.050 624	−0.000 614
0.60	−0.028 244	−0.028 232	−0.004 987	−0.028 031
0.50	−0.077 680	−0.077 679	−0.068 047	−0.077 606
0.40	−0.142 439	−0.142 439	−0.139 153	−0.142 418
0.30	−0.219 416	−0.219 416	−0.218 619	−0.219 411
0.20	−0.306 335	−0.306 335	−0.306 235	−0.306 334
0.10	−0.400 885	−0.400 885	−0.400 883	−0.400 885
0.08	−0.420 464	−0.420 464	−0.420 464	−0.420 464
0.06	−0.440 201	−0.440 201	−0.440 201	−0.440 201

TABLE II. Energy eigenvalues as a function of screening parameter λ for the $2s$ and $2p$ states in atomic units.

λ		$E[10,10]$	$E[10,11]$	Perturbation	Variational
0.15	$2s$	−0.005 250	−0.005 260		
0.10	$2s$	−0.034 941	−0.034 941	−0.034 425	−0.034 935
	$2p$	−0.032 469	−0.032 469	−0.032 042	
0.08	$2s$	−0.050 387	−0.050 387	−0.050 222	−0.050 384
	$2p$	−0.048 997	−0.048 997		
0.06	$2s$	−0.067 421	−0.067 421	−0.067 385	−0.067 421
	$2p$	−0.066 778	−0.066 778		
0.04	$2s$	−0.085 769	−0.085 769	−0.085 767	−0.085 769
	$2p$	−0.085 591	−0.085 591		
0.02	$2s$	−0.105 104	−0.105 104	−0.105 104	−0.105 104
	$2p$	−0.105 075	−0.105 075	−0.105 075	

values $\langle r^j \rangle$ can be expanded as

$$E_n = \sum_{k=0}^{\infty} E_n^{(k)} \lambda^k , \quad \langle r^j \rangle = \sum_{k=0}^{\infty} C_j^{(k)} \lambda^k , \tag{5}$$

we obtain the following recurrence relations for the ECSC potential[11]:

$$C_j^{(k)} = n^2 \left[\frac{2j+1}{j+1} C_{j-1}^{(k)} + \left(\frac{jl(l+1)}{j+1} + \frac{1}{4} j(j-1) \right) C_{j-2}^{(k)} + \frac{2j+3}{j+1} V_2 C_{j+1}^{(k-2)} + \cdots + \frac{2j+k+1}{j+1} V_k C_{j+k-1}^{(0)} \right]$$
$$+ 2n^2 (E_n^{(k)} C_j^{(0)} + E_n^{(k-1)} C_j^{(1)} + \cdots + E_n^{(2)} C_j^{(k-2)}) , \quad j \geq 0 \tag{6}$$

and

$$E_n^{(k)} = -\frac{1}{k} \sum_{m=0}^{k} m V_m C_{m-1}^{(k-m)} , \tag{7}$$

where n is the principal quantum number. The recurrence relations (6) and (7) can be used to calculate the energy coefficients $E_n^{(k)}$ from a knowledge of $C_j^{(m)}$ and $E_n^{(m)}$ with $m \leq k-2$ in a hierarchial manner.

The energy perturbation series E_n in (5) appears divergent for large λ. However, it is found that one can still calculate the bound-state energies of the

TABLE III. Energy eigenvalues as a function of screening parameter λ for the $3s$, $3p$ and $3d$ states in atomic units.

λ		$E[10,10]$	$E[10,11]$	Perturbation	Variational
0.07	$3s$	−0.000 740	−0.000 750		
0.06	$3s$	−0.005 461	−0.005 462	−0.004 538	−0.005 454
	$3p$	−0.004 471	−0.004 472		
	$3d$	−0.002 308	−0.002 309		
0.05	$3s$	−0.011 576	−0.011 576		
	$3p$	−0.010 929	−0.010 929	−0.010 538	
	$3d$	−0.009 555	−0.009 555	−0.009 292	
0.04	$3s$	−0.018 823	−0.018 823	−0.018 707	−0.018 822
	$3p$	−0.018 453	−0.018 453		
	$3d$	−0.017 682	−0.017 682		
0.02	$3s$	−0.036 025	−0.036 025	−0.036 022	−0.036 025
	$3p$	−0.035 968	−0.035 968	−0.035 965	
	$3d$	−0.035 851	−0.035 851	−0.035 849	

TABLE IV. Energy eigenvalues as a function of screening parameter λ for the $4s$, $4p$, $4d$, and $4f$ states in atomic units.

λ		$E[10,10]$	$E[10,11]$	Perturbation	Variational
0.04	$4s$	−0.000 119	−0.000 125	+0.001 079	−0.000 118
0.03	$4s$	−0.005 270	−0.005 270		
	$4p$	−0.005 033	−0.005 033		
	$4d$	−0.004 539	−0.004 539		
	$4f$	−0.003 748	−0.003 748		
0.02	$4s$	−0.012 572	−0.012 572	−0.012 539	−0.012 572
	$4p$	−0.012 486	−0.012 486	−0.012 454	
	$4d$	−0.012 310	−0.012 310	−0.012 283	
	$4f$	−0.012 038	−0.012 038	−0.012 019	
0.01	$4s$	−0.021 438	−0.021 438	−0.021 436	−0.021 437
	$4p$	−0.021 424	−0.021 424	−0.021 424	
	$4d$	−0.021 398	−0.021 398	−0.021 397	
	$4f$	−0.021 358	−0.021 358	−0.021 357	

ECSC potential to a high accuracy by forming the Padé approximants[15] to the energy series. The $[N,M+1]$ Padé approximant to the energy series is given by

$$E[N,M+1] = E^{(0)} + \lambda E^{(1)} \frac{1+\lambda p_1+\lambda^2 p_2+\cdots+\lambda^M p_M}{1+\lambda q_1+\lambda^2 q_2+\cdots+\lambda^N q_N}$$

$$= E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots + \lambda^{N+M+1} E^{(N+M+1)} . \quad (8)$$

In this paper, we confine ourselves to the calculation of the Padé approximants $E[10,10]$ and $E[10,11]$.

In Tables I–IV, we present the calculated energy eigenvalues of $E[10,10]$ and $E[10,11]$ as a function of screening parameter λ for the $1s$, $2s$-$2p$, $3s$-$3d$, and $4s$-$4f$ states, respectively. Our calculated values of the energy eigenvalues are compared with those of the perturbation and variational calculations by Lam and Varshni.[5] As can be seen from Tables I–IV, the calculated values of $E[10,10]$ and $E[10,11]$ for various values of λ totally coincide, except for a few values of screening parameter λ very close to the critical screening parameter λ_c. It is therefore evident that the present scheme of calculation is more accurate than the s-state variational scheme of Lam and Varshni[5] for large values of λ. To appreciate the merit of the Padé approximant method, we list, in Table V, the coefficients p_i and q_i in the [10,11] Padé approximant for the $1s$ and $2s$ states. It is evident that the coefficients p_i and q_i are functions of the principal quantum number n and the orbital angular momentum quantum number l. Though the coefficients p_i and q_i may become large, the resultant Padé approximants yield almost exact energy eigenvalues.

Our calculated value of the critical screened parameter λ_c for the $1s$ state is $\lambda_c = 0.701$ as compared with that of $\lambda_c = 0.72$ by Bonch-Bruevich and Glasko[1] and

TABLE V. The coefficients p_i and q_i in the [10,11] Padé approximant for the $1s$ and $2s$ states.

p_i	$n=1$	$n=2$	q_i	$n=1$	$n=2$
p_1	2.2051(1)	5.3175(1)	q_1	2.2052(1)	5.3175(1)
p_2	2.2472(2)	1.3066(3)	q_2	2.2572(2)	1.3206(3)
p_3	1.2927(3)	1.7014(4)	q_3	1.3135(3)	1.7703(4)
p_4	4.3599(3)	1.0557(5)	q_4	4.5588(3)	1.2123(5)
p_5	7.6958(3)	−5.7237(4)	q_5	8.7473(3)	1.2472(5)
p_6	2.9384(3)	−4.6880(6)	q_6	6.0873(3)	−3.7721(6)
p_7	−1.1688(4)	−1.8709(7)	q_7	−7.1713(3)	−2.0795(7)
p_8	−1.2969(4)	3.9930(7)	q_8	−1.2616(4)	−6.9031(5)
p_9	2.9543(3)	2.3820(8)	q_9	−2.8605(3)	1.5003(8)
p_{10}	2.9318(3)	−3.3108(8)	q_{10}	7.7612(2)	1.6938(7)

of $\lambda_c = 0.7115$ by Lam and Varshni.[5] We remark here that it is rather difficult to determine very accurately the values of λ_c for the ECSC potential either by using the Padé approximants $E[10, 11]$ or by some other methods.[5,10] In order to determine the values of λ_c accurate to several decimals in the present scheme, it seems that some higher Padé approximants and quadruple precision are needed.

In conclusion, we have shown that the bound-state energies of the exponential cosine screened Coulomb potential for all eigenstates can be accurately determined within the framework of the hypervirial Padé scheme, even though the energy series for the ECSC potential may not be a Stieltjes series.[15] The present scheme of calculating the energy eigenvalues for the ECSC potential is quite simple and straightforward, and its advantage over the s-state variational scheme of Lam and Varshni[5] and the ground-state logarithmic perturbation theory of Eletsky *et al.* is obvious. Finally, we remark that the present method of calculation can also be extended to a more general ECSC potential $V(r) = -(1/r)e^{-\lambda r}\cos(b\lambda r)$ with different scale factors in the exponential and cosine functions.

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