Group Theoretic Approach to the Exponential Cosine Screened Coulomb Potential

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Z. Naturforsch. **40 a,** 453–455 (1985); received December 17, 1984

Perturbation method, using the properties of SO (2, 1) algebra is applied to get a simple analytical formula for energy eigenvalues of the exponential cosine screened Coulomb potential.

Recently, a great deal of interest has been focussed on the exponential cosine screened Coulomb potential (ECSC)

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

Its importance lies in the fact that it is used in describing the interaction between an electron and an ionized impurity in both metals and semiconductors [1–3]. Also, in Ref. [4] it has been used to describe the electron positron interaction in a positronium atom in a solid. The bound state energies of the ECSC potential were first calculated for the 1 s state by a numerical method [1] and for the s states by a variational, perturbation [5] and by the Ecker Weizel [6] approximation. Lai [7] has calculated the energy eigenvalues for all the states by Pade approximation. Hitherto, all the works on the ECSC potential except the perturbation method of [5] needed fairly extensive numerical calculations to evaluate the bound state energies. However, though simpler, the perturbation technique of [5] gives results for large λ which are in wide disagreement with results of Pade approximation estimate. (It is well known that the results obtained by Pade approximation are fairly accurate.) In this paper we shall use a group theoretic technique based on the application of the algebra of SO (2, 1) group to find a simple formula for the energy eigenvalues of all the states. Details of the method will be published elsewhere.

Before going into Schrödinger's equation we discuss some of the basic properties of SO (2, 1) group. The generators T_1, T_2, T_3 of SO (2, 1) group obey the following commutation relations

$$[T_1, T_2] = -i T_3 , \quad [T_2, T_3] = i T_1 , \quad [T_3, T_1] = i T_2 , \tag{2}$$

and the Casimir invariant is

$$Q = T_3^2 - T_1^2 - T_2^2 . \tag{3}$$

Now choosing T_1, T_2, T_3 in the following way [8]:

$$T_1 = -\tfrac{1}{2}(r \Delta + r) , \quad T_2 = -i \left(1 + r \frac{\partial}{\partial r}\right), \tag{4}$$

$$T_3 = -\tfrac{1}{2}(r \Delta - r) , \quad \text{where}$$

$$\Delta = \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_j} , \quad r = (x_j x_j)^{1/2} , \tag{5}$$

it is easily seen that T_1, T_2, T_3 satisfy the commutation relations (2).

Introducing the operators $T_\pm = T_1 \pm i T_2$ we obtain from (2) and (3)

$$[T_3, T_+] = T_+ ; \quad [T_3, T_-] = -T_- ; \quad [T_-, T_+] = 2 T_3 \tag{6}$$

$$\text{and} \quad Q = T_3^2 - \tfrac{1}{2}(T_+ T - + T_- T_+) . \tag{7}$$

The Hermitean representation of the algebra of SO (2, 1) generated by T_3, $T_\pm$ is given by

$$\begin{aligned} &T_3 \mid l, m, n\rangle = n \mid l, m, n\rangle , \\ &T_\pm \mid l, m, n\rangle = \sqrt{l + 1 \pm n)\,(\pm n - l)} \mid l, m, n \pm 1\rangle , \\ &(T_3^2 - T_1^2 - T_2^2) \mid l, m, n\rangle = l\,(l+1) \mid l, m, n\rangle , \end{aligned} \tag{8}$$

where $n = n_r + l + 1$, n_r being the radial quantum number and l being the orbital angular momentum.

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

$$V(r) = -\frac{1}{r} \sum_{k=0}^{\infty} V_k (\lambda r)^k , \tag{9}$$

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where the potential coefficients V_k are given by

$$V_1 = -1\,; \quad V_2 = 0\,; \quad V_3 = \frac{1}{3}\,;$$
$$V_4 = -\frac{1}{6}\,; \quad V_5 = \frac{1}{30}\,. \tag{10}$$

Here, we use atomic units so that the distances are measured in $a_0 = k\,\hbar^2/m^*\,e^2$ and energies in $m^*\,e^4/k^2\,\hbar^2$, where m^* is the effective mass and k the dielectric constant.

The Schrödinger equation with potential (1) reads

$$\left\{-\frac{1}{2}\,\Delta - \frac{1}{r}\,e^{-\lambda r}\cos\lambda\,r\right\}\Psi(r) = E\,\Psi(r)\,. \tag{11}$$

Substituting (10) in (11) we get

$$\left\{-r\,\Delta - 2 + 2\,\lambda\,r - 2\,E\,r - \frac{2}{3}\,\lambda^3\,r^3 + \frac{1}{3}\,\lambda^4\,r^4 - \frac{1}{15}\,\lambda^5\,r^5\right\}\Psi(r) = 0\,. \tag{12}$$

In terms of the generators T_3, $T_\pm$, (12) reads

$$\begin{aligned}&\left\{T_3 + \frac{T_+}{2} + \frac{T_-}{2} - 2 + (2\,\lambda - 2\,E)\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)\right.\\&\quad - \frac{2}{3}\,\lambda^3\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^3 + \frac{1}{3}\,\lambda^4\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^4\\&\quad\left. - \frac{1}{15}\,\lambda^5\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^5\right\}\Psi = 0\,.\end{aligned} \tag{13}$$

We now give the 'tilt' transformation [9] to each of the operators as

$$\begin{aligned}e^{-i\,T_2\theta}\,T_3\,e^{i\,T_2\theta} &= T_3\cosh\theta + \left(\frac{T_+}{2} + \frac{T_-}{2}\right)\text{Sinh}\,\theta\,,\\ e^{-i\,T_2\theta}\,T_+\,e^{i\,T_2\theta} &= T_+\cosh\theta + T_3\sinh\theta\,,\\ e^{-i\,T_2\theta}\,T_-\,e^{i\,T_2\theta} &= T_-\cosh\theta + T_3\sinh\theta\,.\end{aligned} \tag{14}$$

Using (14) in (13) we get

$$\begin{aligned}&\left\{T_3\,e^{\theta} + \frac{T_+}{2}\,e^{\theta} + \frac{T_-}{2}\,e^{\theta} - 2 + (2\,\lambda - 2\,E)\,e^{-\theta}\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)\right.\\&\quad\left. - \frac{2}{3}\,\lambda^3\,e^{-3\theta}\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^3 + \frac{1}{3}\,\lambda^4\,e^{-4\theta}\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^4 - \frac{1}{15}\,\lambda^5\,e^{-5\theta}\left(T_3 - \frac{T_+}{2} - \frac{T_-}{2}\right)^5\right\}\Psi' = 0\,,\end{aligned} \tag{15}$$

where $\Psi' = e^{i\,T_2\theta}\,\Psi\,.$ (16)

We take the zeroth-order energy as

$$E^{(0)}_{n,l}(\theta) = \langle n, l\,|\,(\tilde{H} - E)\,|\,n, l\rangle\,, \tag{17}$$

where $\tilde{H} - E$ is given by the bracketed portion of (15) divided by $2\,n\exp(-\theta)$ and then added by E.

Expanding the last three terms of (15) and collecting only the diagonal terms we get after some straightforward algebra

$$\begin{aligned}E^{(0)}_{n,l}(\theta) &= \frac{e^{2\theta}}{2} - \frac{e^{\theta}}{x} + \lambda - \frac{1}{6}\,\lambda^3\,e^{-2\theta}\,(5\,x^2 - 3\,y + 1)\\&\quad + \frac{1}{48}\,\lambda^4\,e^{-3\theta}\,(35\,x^4 + 25\,x^2 - 30\,x^2\,y + 3\,y^2 - 6\,y)\\&\quad - \frac{1}{240}\,\lambda^5\,e^{-4\theta}\,(63\,x^4 + 87\,x^2 + 6\\&\qquad - 70\,x^2\,y - 38\,y + 15\,y^2)\,,\end{aligned} \tag{18}$$

where

$$x = n_r + l + 1\,, \quad y = l\,(l + 1)\,. \tag{19}$$

Now, we demand that θ will be such that E will be minimum,

$$\text{i.e.}\,\frac{\mathrm{d}E^{(0)}_{n,l}(\theta)}{\mathrm{d}\theta} = 0 \tag{20}$$

and

$$\frac{\mathrm{d}^2E^{(0)}_{n,l}(\theta)}{\mathrm{d}\theta^2} > 0\,. \tag{20a}$$

Substituting $E^{(0)}_{n,l}(\theta)$ from (18) in (20) we get

$$\begin{aligned}&e^{6\theta} - \frac{e^{5\theta}}{x} + e^{2\theta}\,\frac{\lambda^3}{3}\,(5\,x^2 - 3\,y + 1)\\&\quad - \frac{1}{16\,x}\,e^{\theta}\,\lambda^4\,(35\,x^4 + 25\,x^2 - 30\,x^2\,y + 3\,y^2 - 6\,y)\\&\quad + \frac{\lambda^5}{60}(63\,x^4 + 87\,x^2 + 6 - 70\,x^2\,y - 38\,y + 15\,y^2) = 0.\end{aligned} \tag{21}$$

Equations (18) and (21) together give $E^{(0)}_{n,l}$ for various values of λ.

In Tables 1–4, we list the energy eigenvalues of various states for values of λ not greater than 0.5.

As can be seen from Tables 1–4, our results even in the lowest order agree to within 2% for the entire range of values of λ upto 0.4. In order to compare

Table 1. Energy eigenvalues for the 1 s state in atomic units.

λ	E (Present)	E (Pade)	E (Perturbation)	E (Variational)
0.06	−0.440200	−0.440201	−0.440201	−0.440201
0.08	−0.420463	−0.420464	−0.420464	−0.420464
0.10	−0.400883	−0.400885	−0.400883	−0.440885
0.20	−0.306268	−0.306335	−0.306235	−0.306334
0.30	−0.218939	−0.219416	−0.218619	−0.219411
0.40	−0.140662	−0.142439	−0.139153	−0.142418
0.50	−0.073523	−0.077679	−0.068047	−0.077606

Table 2. Energy eigenvalues for the 2 S and 2 p states in atomic units.

λ		E (Present)	E (Pade)	E (Perturbation)	E (Variational)
0.02	2 S	−0.105104	−0.105104	−0.105104	−0.105104
	2 p	−0.105075	−0.105075	−0.105075	
0.04	2 S	−0.085769	−0.085769	−0.085767	−0.085769
	2 p	−0.085580	−0.085591		
0.06	2 S	−0.067419	−0.067421	−0.067385	−0.067421
	2 p	−0.066767	−0.066778		
0.08	2 S	−0.050382	−0.050387	−0.050222	−0.050384
	2 p	−0.048953	−0.048997		
0.10	2 S	−0.034951	−0.034941	−0.034425	−0.034935
	2 p	−0.032330	−0.032469	−0.032042	

Table 3. Energy eigenvalues for the 3 S, 3 p and 3 d states in atomic units.

λ		E (Present)	E (Pade)	E (Perturbation)	E (Variational)
0.02	3 S	−0.036025	−0.036025	−0.036022	−0.036025
	3 p	−0.0.35968	−0.035968	−0.035965	
	3 d	−0.035850	−0.035851	−0.035849	
0.04	3 S	−0.018847	−0.018823	−0.018707	−0.018822
	3 p	−0.018457	−0.018453		
	3 d	−0.017663	−0.017682		
0.05	3 S	−0.011677	−0.011576		
	3 p	−0.010954	−0.010929	−0.010538	
	3 d	−0.009493	−0.009555	−0.009292	
0.06	3 S	−0.005875	−0.005462	−0.004538	−0.005454
	3 p	−0.004606	−0.004472		
	3 d	−0.002140	−0.002309		

Table 4. Energy eigenvalues for the 4 S, 4 p, 4 d and 4 f states.

λ		E (Present)	E (Pade)	E (Perturbation)	E (Variational)
0.01	4 S	−0.021438	−0.021438	−0.021436	−0.021437
	4 p	−0.021424	−0.021424	−0.021424	
	4 d	−0.021398	−0.021398	−0.021397	
	4 f	−0.021358	−0.021358	−0.021357	
0.02	4 S	−0.012581	−0.012572	−0.012539	−0.012572
	4 p	−0.012492	−0.012486	−0.012454	
	4 d	−0.012310	−0.012310	−0.012283	
	4 f	−0.012034	−0.012038	−0.012019	
0.03	4 S	−0.005382	−0.005270		
	4 p	−0.005105	−0.005033		
	4 d	−0.004550	−0.004539		
	4 f	−0.003715	−0.003748		

our perturbation method with that of [5] and [6] we have calculated the energy eigenvalues for $\lambda = 0.5$ for 1 s state and for $\lambda = 0.06$ for 3 S, 3 p, 3 d states and we have got much better agreement than both the References. We remark here that to get the results we had to retain terms of the order of λ^5 only, whereas terms of the order of λ^{21} were needed in [7] to get the results which are within 98 per cent agreement with the results of the present paper. To obtain the energy eigenvalues for larger values of λ as well as to calculate the critical screening parameter λ_c one needs to make tedious but straightforward higher order (in λ) calculations.

We thank R. Kundu of I.S.I. for helping us in computer calculations.

[1] V. L. Bonch-Bruevich and V. B. Glasko, Sov. Phys. Dokl. Acad. Sci. **4,** 147 (1959).

[2] N. Takimoto, J. Phys. Soc. Japan **14,** 1142 (1959).

[3] V. L. Bonch-Bruevich and Sh. M. Kogan, Sov. Phys. Solid State **1,** 1118 (1960).

[4] E. P. Prokopev, Sov. Phys. Solid State **9,** 993 (1967).

[5] C. S. Lam and Y. P. Varshni, Phys. Rev. **A6,** 1391 (1972).

[6] P. P. Ray and A. Ray, Phys. Letts. **78A,** 443 (1980).

[7] C. S. Lai, Phys. Rev. **A26,** 2245 (1982).

[8] M. Bednar, Ann. Physics **75,** 305 (1973).

[9] A. O. Barut, Dynamical Groups and Generalized Symmetries in Quantum Theory, Univ. of Canterbury Press, Christ Church, New Zealand 1971.