Bound-state energies for the superposed screened Coulomb potential

L. K. Sharma[a*], Pranav Saxena[b] and Ashok K. Nagawat[b]
[a]*Department of Physics, University of Botswana, Gaborone*
[b]*Department of Physics, University of Rajasthan, Jaipur*

(Received 22 May 2008)

The bound-state eigen energies for all angular momenta for the superposition of two static screened Coulomb potentials (SSCP), having different coupling constants and screening parameters, have been evaluated by approximating it to the Eckart potential. The eigen-energy values for the single SSCP are found to have been enhanced considerably due to this superposition.

I. INTRODUCTION

During the last few years considerable effort [1-10] has gone in evaluating the energy levels of atoms related to static screened Coulomb potential (SSCP). Since the Schrödinger equation for such potentials does not admit exact analytic solutions, approximate methods have to be used. One such method is Ecker-Weizel approximation (EWA) [1]. Solving Schrödinger equation, Faridfathi *et al.* [11] obtained supersymmetric solutions of a PT-symmetric and Hermitian/non-Hermitian forms of quantum systems for the exponential cosine screened Coulomb (ECSC) potential. Using Hamiltonian hierarchy inspired variational method they obtained approximate eigenvalues and corresponding wavefunctions. The problem of spinless particle subject to a general mixing of vector and scalar Coulomb potentials in a two-dimensional world was discussed by de Castro [12] for the Klien-Gordon equation. Filho *et al.* [13] analysed screened Coulomb potential, using the formalism that a super symmetric quantum mechanics supplies a trial wavefunction to be used in variational method. Portnoi [14] applied variable-phase method to obtain bound states for an attractive Coulomb potential, statically screened by a two-dimensional electron gas. They observed that as the screening is increased, sets of bound state with differing quantum numbers appear degenerately.

In the present paper we investigate the problem of superposed screened Coulomb potential which exhibits a modified screening effect compared to a Yukawa potential.

The potential considered by us has the form:

$$V(r) = -(g_1 e^{-\delta r} + g_2 e^{-\lambda \delta r})/r \qquad (1)$$

where g_1 and g_2 are coupling constants, δ the screening parameter and λ the strength of screening.

It may be of interest to note that for $g_1 = e^2$ and $g_2 = 0$ potential (1) is transformed to the well-known Debye potential which finds application in plasma physics describing effectively the interaction of plasma-sea on a localized two particle system. The strength of screening is affected by temperature and density of plasma-sea. At a given temperature and density the average radius would exceed one- half of the average inter-nuclear separation. In this region the approximation that electron is bound to single proton no longer remains valid. One must, therefore, take into account systems in which the electron is bound in screened Coulomb potential having a more general form and potential (1) actually depicts such a situation.

Following Eckart [15], the no-zero angular momentum states can be treated by replacing the superposed screened Coulomb potential

$$V_{eff}(r) = V(r) + \frac{l(l+1)}{2r^2} \qquad (2)$$

by a suitable Eckart potential V_E. From this it is possible to derive exact analytic solutions for different values of the screening parameter δ.

The energy values E_{nl} calculated (in *au*) for potential (1) for different values of n and l have been shown in Tables I-IV. To observe the effect of superposition of a SSCP with a modified screened Coulomb potential $(-g_2 e^{-\lambda \delta r})/r$, corresponding energy values have also been shown in these tables. Finally, a brief discussion on the work done in this paper has been given.

**The first author (LKS) is at present spending his sabbatical leave at the University of Rajasthan, Jaipur, India where this work was completed. The author thanks the department of Physics for the facilities provided to him.*

II. GENERAL SOLUTION

The radial Schrödinger equation for potential (2) can be written as

$$\frac{d^2u}{dr^2} + 2[E - V_{eff}(r)]u(r) = 0 \tag{3}$$

where system of units used is $m = c = \hbar = 1$. $V_{eff}(r)$ can be approximated by the following Eckart potential [15]

$$V_E(r) = -\frac{V_0\delta e^{-\delta r}}{1-e^{-\delta r}} + \frac{\beta(\beta+1)\delta^2 e^{-\delta r}}{2(1-e^{-\delta r})^2} \tag{4}$$

with

$$V_0 = g_1 \frac{(1-e^{-\delta \bar{r}})}{\delta \bar{r}}\left[1 + \frac{g_2}{g_1}e^{-(\lambda-1)\delta \bar{r}}\right], \quad g_1 \neq 0 \tag{5}$$

and

$$\beta(\beta+1) = \frac{l(l+1)e^{\delta \bar{r}}{V_0}^2}{{g_1}^2\left[1 + \frac{g_2}{g_1}e^{-(\lambda-1)\delta \bar{r}}\right]^2}. \tag{6}$$

In Eqs. (5) and (6), $\bar{r}$ represents some mean distance of the electron in the nl state [1]. On replacing $V_{eff}(r)$ by V_E in Eq. (3), one gets

$$\left[\frac{d^2}{dr^2} + 2E + \frac{2V_0\delta e^{-\delta r}}{(1-e^{-\delta r})} - \frac{\beta(\beta+1)\delta^2 e^{-\delta r}}{2(1-e^{-\delta r})^2}\right]u(r) = 0. \tag{7}$$

Setting

$$y = e^{-\delta r}, \quad E = -\frac{\alpha^2}{2} \text{ and } u(r) = y^{\frac{\alpha}{\delta}}(1-y)^{\beta+1}\phi(y) \tag{8}$$

in Eq. (7), the hyper-geometric equation so obtained has the form

$$\begin{aligned} &y(y-1)\frac{d^2\phi}{dy^2} + \left[1 + \frac{2\alpha}{\delta} - \left(\frac{2\alpha}{\delta} + \beta + 3\right)y\right]\frac{d\phi}{dy} \\ &+ \left[\frac{2V_0}{\delta} - \beta(\beta+1)\frac{2\alpha}{\delta} - (\beta+1)^2\right]\phi(y) = 0. \end{aligned} \tag{9}$$

The solution of Eq. (9) can be written as

$$\phi(y) = P\,{}_2F_1(a,b,c;y) + Qy^{-\frac{2\alpha}{\delta}}\,{}_2F_2(a-c+1, b-c+1, 2-c; y) \tag{10}$$

where

$$a = 1 + \beta + \frac{2\alpha}{\delta} + \frac{V_0}{\alpha}$$

$$b = 1 + \beta - \frac{V_0}{\alpha} \tag{11}$$

$$c = 1 + \frac{2\alpha}{\delta}.$$

The boundary condition $u(r) = 0$ at $r = \infty (y = 0)$ demands $Q = 0$. For obtaining the solution from the other boundary condition $u(r) = 0$ at $r = 0\,(y = 1)$, the function ${}_2F_1(a,b,c;y)$ will have to be reduced to a polynomial. For this

$$a = -n_r, \quad n_r = 0,1,2,\ldots. \tag{12}$$

Eq. (12) gives

$$\alpha = \left[\frac{V_0}{(n-l+\beta)} - \frac{\delta}{2}(n-l+\beta)\right]^2 > 0. \tag{13}$$

Eqs. (8) and (13) finally yield the following for the binding energy

$$E_{nl} = -\frac{1}{2}\left[\frac{V_0}{(n-l+\beta)} - \frac{\delta}{2}(n-l+\beta)\right]^2 \tag{14}$$

where $n = n_r + l + 1$. The solution of Eq. (6) gives

$$\beta = -\frac{1}{2} + \left[0.25 + \frac{l(l+1){V_0}^2 e^{\delta \bar{r}}}{{g_1}^2\left\{1 + \frac{g_2}{g_1}e^{-(\lambda-1)\delta \bar{r}}\right\}^2}\right] \tag{15}$$

It can be seen from Eq. (15) that $\beta > l$ for any finite value of δ. Further, β vanishes when l is zero. It may also be noted that for $g_1 = \cos\delta r$, $g_2 = 0$ and $l = 0$, one gets directly from Eq. (14) the expression for E_{ns} of ECSC potential with Eckner-Weizel approximation [9]. The expression (14) is valid for all angular momentum states. Further, for the choice $V_0 = 1$ and $\beta = l$, it yields $E_{nl} = -\frac{1}{8n^2}(2 - n^2\delta)^2$, which are independent of l. The l degeneracy of the eigenvalues was eliminated by Greene *et al.* [16] using a variational parameter. In our case we have introduced energy dependent strength parameters V_0 and β to remove the l degeneracy of the energy eigenvalues.

To determine the discrete energy levels one needs to specify $\bar{r}$. Even studies done on Yukawa potential [17,18] have failed to specify $\bar{r}$. However, considering $\bar{r}$ as a function of *n* and δ, several expressions for $\bar{r}$ have been tried and it is observed that the following choice for $\bar{r}$:

$$\bar{r} = n^2(1+2\delta) - n^3(\delta + 2\delta^2) + n^4\left(\frac{\delta^2}{2} + \delta^3\right) - n^5\left(\frac{\delta^3}{6} + \frac{\delta^4}{3}\right) + O(\delta^5). \quad (16)$$

works better for *s*-states. This expression for $\bar{r}$ may be regarded as an arbitrary one which is obtained by trial and error. In fact it is difficult to give theoretically a precise assessment of the veracity of the approximation made in calculating E_{nl}. We have therefore, transformed our potential (1) to SSCP by setting $g_2 = 0$, and have calculated E_{ns}, using the above expression of $\bar{r}$. Our results for *s*-states have been compared with those obtained by variational technique [4] in Table I. These two results agree to within 1.6% up to 4*s*-states throughout the range of δ as shown in the table. Further for the same choice of $\bar{r}$ the results for $l \neq 0$ are calculated ranging between 0.0001 and 0.12. Using this choice of $\bar{r}$, values of E_{nl} have been obtained for potential (1) for $2p-4d$ states. These values are shown in Tables II and III. To observe the effect of superposition considered, energy values for a single SSCP potential [10] are also shown in Tables II and III.

v. The dependence of E_{nl} on parameters g_2 and λ has been shown in Table IV.

III. CONCLUSIONS

We conclude our work with the following remarks:

i. The superimposed effective screened coulomb potential can be approximated to Eckart potential for treating the non-zero angular momentum bound states of the class of potential (1). For $g_2 = 0$ and $l = 0$ the expression for the values of E_{ns} is in complete agreement with that of Lam *et al.* [4].

ii. For the single SSCP potential considered in this paper, the numerical energy eigenvalues increase considerably on account of superposition of two potentials.

iii. For the lower range of screening parameter δ, the energy eigenvalues in different states $3p-3d$, $4p-4d$, etc. remain almost the same, but the change becomes appreciable when δ approaches the critical screening parameter δ_c above which the bound state does not exist.

iv. The effect of gradual variation in the strength of screening λ does not change the energy values considerably. It is seen that for a very large value of λ, a variation of 4% in λ gives a variation of about 1.3% in energy. However, as expected, the variation in g_2 brings about an appreciable change in the energy eigenvalues.

TABEL I. Energy eigenvalues (- E_{ns}) in au as a function of the screening parameter δ for $2s-4s$ states of the potential (1) with $g_1 = 1$, $g_2 = 0$ are shown and compared with those by the variational technique given in another column B.

δ	E_{2s}		E_{3s}		E_{4s}	
	A	B*	A	B*	A	B*
0.001	0.1241	0.1240	0.05456	0.05456	0.03026	0.03026
0.01	0.11526	0.11529	0.04618	0.04620	0.02241	0.02236
0.02	0.1057	0.1061	0.03798	0.03802	0.01535	0.01538
0.03	0.09733	0.09753	0.03083	0.03089	0.09968	0.00999
0.04	0.0891	0.0894	0.02462	0.02469	0.00593	0.00596
0.1	0.04912	0.04993	--	--	---	---

*See Reference [4].

TABEL II. Energy eigenvalues (- E_{nl}) in au as a function of the screening parameter δ for $2p$ to $3d$ states for the potential (1) with $\lambda = 2$, $g_1 = 1$ and $g_2 = 1$ are shown in Col. A and compared with those of Dutt *et al.* [10] for the SSCP in Col. B.

δ	E_{2p}		E_{3p}		E_{3d}	
	A	B**	A	B**	A	B**
0.001	0.4950	0.1240	0.2250	0.05456	0.2250	0.05456
0.002	0.4901	---	0.2141	----	0.2141	----
0.01	0.4523	0.1152	0.1771	0.04612	0.1771	0.04611
0.02	0.4085	0.1059	0.1401	0.03777	0.1401	0.03772
0.025	0.3882	0.1015	0.1258	0.03397	0.1258	0.03391
0.05	0.2095	0.0810	0.0691	0.01845	0.0686	0.01826
0.1	0.1735	0.0479	0.0156	---	0.0141	---
0.11	0.1547	---	0.0104	---	0.00969	----
0.12	0.1375	---	0.00648	----	0.00580	----
0.3	0.00449	---	---	----	----	----

**See Reference [10].

TABEL III. Energy eigenvalues (- E_{nl}) in au as a function of the screening parameter δ for $4p - 4f$ states of potential (1) with $\lambda = 2$, $g_1 = 1$ and $g_2 = 1$ are shown in Col. A and compared with that of Dutt *et al.* [10] in Col. B.

δ	E_{4p}		E_{4d}		E_{4f}	
	A	B***	A	B***	A	B***
0.0001	0.1245	---	0.1245	---	0.1245	----
0.001	0.1201	0.03026	0.1201	0.03026	0.1201	0.03026
0.005	0.1022	0.02650	0.1022	0.02649	0.1022	0.02649
0.01	0.0836	0.02224	0.0836	0.02223	0.0836	0.0222
0.02	0.0552	0.01506	0.0551	0.01501	0.0551	0.0149
0.025	0.0448	0.01208	0.0446	0.01201	0.0444	----
0.03	0.0359	-----	0.0357	--	0.0355	----
0.05	0.0131	-----	0.0128	---	0.0125	-----

***See Reference [10].

TABLE IV. Variation of s-states eigenenergies with strength of screening λ and coupling parameter g_2 .

State	Energy	g_1	g_2	A	δ
	0.49001	1	0	2	0.01
	1.0987	1	0.5	2	0.01
	3.0440	1	1.5	2	0.01
1*s*	4.3952	1	2.0	2	0.01
	0.9193	1	1.0	100	0.01
	0.9095	1	1.0	102	0.01
	0.9066	1	1.0	104	0.01

REFERENCES

[1] G. Ecker *et al*., Ann. Der. Phys. (Liepzig), **17**, 126 (1956).
[2] G. J. Iafrate *et al*., Phys. Rev., **182**, 244 (1969).
[3] F. J. Rogers *et al*., Phys. Rev. A, **1**, 1577 (1970).
[4] C. S. Lam *et al*., Phys. Rev. A, **4**, 1875 **(1971**); Phys. Rev. Lett., **59A**, 363 (1976).
[5] H. J. W. Müller-Kirsten *et al*., J. Math. Phys., **14**, 1291 (1973).
[6] M. Bednar, Ann. Phys., **75**, 805 (1973).
[7] J. McEnnan *et al*., Phys. Rev. A, **13**, 532 (1976).
[8] C. H. Mehta *et al*., Phys. Rev. A, **17**, 84 (1978).
[9] R. Dutt, Phys. Lett. **73 A**, 310 (1979).
[10] R. Dutt *et al*., Phys. Lett., **83A**, 65 (1981).
[11] G. Faridfathi et al., J. Math. Chem., **42**, 289 (2007).
[12] A. S. De Castro, Int. J. Mod. Phys., **21A**, 5141 (2006).
[13] E. D. Filho *et al*., Mod. Phys. Lett. A, **15**, 1253 (2000).
[14] M. E. Portnoi *et al*., Solid State Comm., **103**, 325 (1997).
[15] C. Eckart, Phys. Rev., **35**, 1303 (1930).
[16] R. L. Greene *et al*., Phys. Rev. A, **14**, 2363 (1976).
[17] B. Talukdar *et al*., J. Math. Phys., **19**, 1654 (1978).
[18] U. Das *et al*., J. Math. Phys., 20, 887 (1979).