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# Improved condition for the absence of bound states and converging analytic bounds to critical screening parameter

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**Abstract.** Converging lower bound to the critical screening parameter $D_c$ associated with the ground state of a two-particle system interacting through a cut-off Coulomb potential is obtained analytically using an improved condition for the absence of bound states. The predicted numerical result for the lower bound is found to be within $10^{-3}$% of the exact result. On the other hand, a multi-parameter variational approach yields a tight upper bound, within 0·54% of the exact result. It is shown that the critical screening parameter for the excited $s$-states can also be determined in an approximate way. We obtain $D_c^{ns} \approx [0{\cdot}764435\, n^{-2} + 0{\cdot}617737\, n^{-3}]^{-1}$ where $n$ is the principal quantum number. The predicted $D_c$ for various quantum states ($n$ = 1 to 8) are in good agreement with the values obtained numerically by Singh and Varshni.

**Keywords.** Improved condition; absence of bound states; critical screening parameter.

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## 1. Introduction

In recent times, various attempts have been made and reported in the literature to obtain analytic bounds on the number of bound states for a given potential with or without spherical symmetry (Jost and Pais 1951; Bargmann 1952; Schwinger 1961; Calogero 1965; Chadan 1968; Glaser *et al* 1976; Chadan and Martin 1977; Chadan and Mol 1980; Chadan and Grosse 1982; Sidharth 1983). Glaser *et al* (1976) obtained an optimal condition

$$\frac{(p-1)^{p-1}\,\Gamma(2p)}{p^p\Gamma^2(p)} \int_0^\infty r^{2p-1} \left|\frac{2m}{\hbar^2} V(r)\right|^p \mathrm{d}r < 1 \tag{1}$$

for the absence of bound states and in case of spherically symmetric potentials, the optimizing parameter $p$ is constrained to be in the range $1 \leqslant p \leqslant \frac{3}{2}$. Using this bound, the minimum strength ($V$) of an attractive potential necessary to produce a zero energy bound state was computed for several potentials. It has been observed that although the discrepancy of the predicted $V$ in comparison to the exact numerical results is less than 1% for the smooth potentials such as the Gaussian, exponential and Yukawa, it is about 4% for the step potential (square well). Similar results were obtained by Sidharth (1983) who employed different inequality theorems to the Schwinger's variational formula for the phase shift.

Recently Dutt *et al* (1985) showed that stringent lower bound to the minimum strength of a potential to support at least one bound state can be obtained following the

iterative method of Hemmer (1973) as applied to an integral equation. It emerges that the method works nicely for the square well and it is observed that the accuracy of the bounds can be improved to any arbitrary degree because of the convergence property of the iterative procedure. The purpose of the present work is to show that nonrigorous analytic techniques are adequate to predict both-side bounds quite accurately for certain parameters such as the critical screening coefficient in the scattering theory. For the sake of illustration, we prefer to handle a discontinuous potential for which the optimal bound (1) of Glaser *et al* predicts comparatively a poor result. We consider the cut-off Coulomb potential (COCP)

$$V(r) = \begin{matrix} -e^2/r \\ 0 \end{matrix} \begin{cases} r < D \\ r > D, \end{cases} \tag{2}$$

which occurs in several areas of physics (Cohen *et al* 1950; Rostokin 1966, Tanenbaum 1967; Mitchner and Kruger 1973; Mihajlov *et al* 1981). The problem of the hydrogen atom within spherical boxes with penetrable walls (Ley-Koo and Rubinstein 1979) involves this potential. The potential (2) has also been used to study the elastic electron-atom scattering (Majumdar *et al* 1982). There are special interests in studying this particular problem analytically: Singh and Varshni (1984) have recently studied the bound state energies of the COCP by numerical method. Their study reveals that the ordering of the binding energies with respect to the angular momentum quantum number $l$ is quite distinct from that observed in case of the static screened Coulomb potential (SSCP), $V(r) = -e^2e^{-\lambda r}/r$. The binding becomes weaker as $l$ increases for the SSCP, while the reverse is the case for the COCP. Furthermore, it has been shown by Taylor and his co-workers (Semon and Taylor 1977; Goodmansion and Taylor 1980) that although the differential scattering cross-section for the SSCP goes to the Coulomb (Rutherford) value in the limit of vanishing screening coefficient, the same limiting cross-section for the COCP is higher than the Coulomb cross-section due to the additional contribution coming from the scattering of particles off the discontinuity in the potential at $r = D$. It is of interest to investigate the COCP analytically because, although the SSCP has been studied in great detail by analytic methods, scant attention has been given to the COCP. A parameter of special interest is the critical screening parameter $D_c$ for the ground state which is the smallest value of $D$ below which no state will be bound by the potential.

In this paper, we present two different analytic approaches to obtain both the lower and the upper bounds to the critical screening parameter of the ground state of the COCP. The analytic expression for the lower bound is obtained by the use of Mercer's theorem (Smirnov 1964) which relates the eigenvalues of an integral equation to the iterated traces of the kernel. For the upper bound calculation, we employ a multi-parameter variational procedure. We observe that a non-Coulombic trial function gives better results than a hydrogen-like trial function indicating that the COCP departs from the pure Coulomb potential significantly near the critical screening region. The details of the lower and upper bound calculations are presented in §§2 and 3 where, we also discuss the accuracy of our predicted lower and upper bounds to $D_c^{1s}$ in comparison to the exact result obtained numerically.

In the concluding section, we discuss the possibility of determining the critical screening parameters, $D_c^{ns}$ for the higher excited $s$-states. It turns out that an empirical form describing the dependence of $D_c^{ns}$ on the principal quantum number $n$ can be obtained. The expression thus obtained predicts reasonably good results for $n = 1$ to 8.

## 2. Determination of the lower bound

The COCP can be mathematically represented as

$$V(r) = -\theta(D-r)/r, \tag{3}$$

where $\theta(x)$ is the Heaviside step function, which is zero for $x$ negative, but is unity for $x$ positive. Then the radial Schrödinger equation for the $s$-wave bound states of the COCP can be written in atomic units as

$$\mathrm{d}^2\chi/\mathrm{d}r^2 + 2[E + \theta(D-r)/r]\chi(r) = 0, \tag{4}$$

where the radial function $\chi(r) = rR(r)$ satisfies the boundary conditions

$$\chi(0) = \chi(\infty) = 0. \tag{5}$$

Changing the variable

$$x = r/D, \tag{6}$$

(4) becomes

$$\beta\mathrm{d}^2\chi/\mathrm{d}x^2 + [E + \theta(1-x)/x]\chi(x) = 0, \tag{7}$$

in which $\beta = 1/2D.$ (8)

For determining the critical screening parameters, we require to set $E = 0$ in (7) to simulate the situation for just disappearance of the bound states. The eigenfunctions are not square integrable since zero energy is the threshold of the continuous spectrum. However, it is known that bounded solutions of (7) with $E = 0$ exist only for a discrete set of values $\beta_1, \beta_2, \ldots$ which correspond to the critical screening parameters of various $ns$-states

$$\beta_n = 1/2D_c^{ns} \qquad (n = 1, 2, 3, \ldots), \tag{8a}$$

where $n$ is the principal quantum number. We now convert (7) into a Fredholm integral equation with a symmetric kernel. Incorporating the boundary conditions (5), we recast (7) into an integral equation

$$\beta\chi(x) = \int_0^x \theta(1-y)\chi(y)\,\mathrm{d}y + \int_x^\infty (x/y)\theta(1-y)\chi(y)\,\mathrm{d}y. \tag{9}$$

Defining

$$\chi(x) = [x/\theta(1-x)]^{1/2}\psi(x) \tag{10}$$

(9) is transformed to a homogeneous Fredholm integral equation

$$\beta\psi(x) = \int_0^\infty K(x, y)\psi(y)\,\mathrm{d}y, \tag{11}$$

where the kernel

$$\begin{aligned} K(x, y) &= [(x/y)\theta(1-x)\theta(1-y)]^{1/2} \qquad y > x \\ &= [(y/x)\theta(1-x)\theta(1-y)]^{1/2} \qquad y < x, \end{aligned} \tag{12}$$

is real, symmetric and continuous. Using the iterated kernels defined as (Tricomi 1957)

$$K_{j+1}(x, y) = \int_0^\infty K_j(x, t)\, K(t, y)\, \mathrm{d}t, \tag{13}$$

one can evaluate the iterated traces

$$T_j = \int_0^\infty K_j(x, x)\, \mathrm{d}x \tag{14}$$

in closed form in a sequential manner. According to the Mercer's theorem (Smirnov 1964), one gets the identity

$$T_j = \sum_{n=1}^{\infty} (\beta_n)^j \qquad (j = 1, 2, 3, \ldots). \tag{15}$$

Using (8) in (15) one obtains

$$\sum_{n=1}^{\infty} (1/2D_c^{ns})^j = T_j. \tag{16}$$

Since each term in the sum is positive definite, we obtain the bound on the smallest screening parameter

$$D_c^{1s} \geqslant \tfrac{1}{2} T_j^{-(1/j)}. \tag{17}$$

Since the value of the critical screening parameter increases rapidly as one goes to the higher excited states, the contribution of the excited states to the sum in (16) decreases faster as one considers higher order trace relations. Consequently, the accuracy of the lower bound to $D_c^{1s}$ as given in (17) will be better if one evaluates traces of higher order. The trace calculations are, however, tedious and lengthy and hence we present here only the first six traces:

$$T_1 = 1, \quad T_2 = 1/2, \quad T_3 = 1/3, \quad T_4 = 11/48, \quad T_5 = 19/120,$$
$$T_6 = 473/4320. \tag{18}$$

One may easily check that the first order trace gives the Bargmann bound $D_c^{1s} \geqslant 0{\cdot}5$. To see how the lower bound improves as one goes from lower to higher trace relations, we cite here the numerical results obtained by the fifth and sixth traces:

$$\text{From } T_5, \qquad D_c^{1s} \geqslant \tfrac{1}{2} \cdot T_5^{-1/5} = 0{\cdot}7228622.$$
$$\text{From } T_6, \qquad D_c^{1s} \geqslant \tfrac{1}{2} \cdot T_6^{-1/6} = 0{\cdot}7228926, \tag{19}$$

which may be compared with the exact result, $D_c^{1s} = 0{\cdot}7228982$ (Singh and Varshni 1984). Our analytic result for the ground state critical screening parameter computed from the sixth order trace is thus accurate to $8 \times 10^{-4}\%$ as compared to its actual value.

## 3. Variational calculation for the upper bound

For this part, we follow a multi-parameter variational scheme first suggested by Hulthén and Laurikainen (1951) for the SSCP. We begin with (7) in which $E$ vanishes

identically when $\beta = \beta_c = 1/2D_c$. The requirement of just appearance of a bound state then leads us to the condition

$$D_c^{1s} \leqslant \tfrac{1}{2}(J/N)_{\min}, \tag{20}$$

where

$$J = \int_0^\infty \chi'^2 \, dx, \tag{21}$$

and

$$N = \int_0^\infty \chi^2 [\theta(1-x)/x] \, dx. \tag{22}$$

To compute the least extremum of the ratio $J/N$, we use the variational principle. First a hydrogen-like trial function was tried:

$$\chi(x) = \sum_{\nu=1}^{3} h_\nu x \exp(-\nu x), \tag{23}$$

where $h_\nu$'s are the variational parameters. This function yielded $D_c^{1s} \leqslant 0{\cdot}84146$, which is rather poor. Next, the following trial fu ıction was used:

$$\chi(x) = [1 - \exp(-\alpha x)] \sum_{\nu=1}^{n} h_\nu \exp(-\nu x). \tag{24}$$

Using (24) in (21) and (22), we get

$$J = \sum_{\mu=0} \sum_{\nu=0} h_\mu h_\nu \left[ \frac{(\alpha+\mu)(\alpha+\nu)}{(\mu+\nu+2\alpha)} - \frac{\alpha\mu + \alpha\nu + 2\mu\nu}{(\mu+\nu+\alpha)} + \frac{\mu\nu}{(\mu+\nu)} \right] \tag{25}$$

$$\begin{aligned} N = {} & h_0^2 [\gamma + \log(\alpha/2) + 2E_1(\alpha) - E_1(2\alpha)] \\ & + 2h_0 \sum_{\nu=1} h_\nu \left[ \left\{ \frac{(\nu+\alpha)^2}{\nu(\nu+2\alpha)} \right\} - E_1(\nu) + 2E_1(\nu+\alpha) - E_1(\nu+2\alpha) \right] \\ & + \sum_{\mu=1} \sum_{\nu=1} h_\mu h_\nu \left[ \log \left\{ \frac{(\mu+\nu+\alpha)^2}{(\mu+\nu)(\mu+\nu+2\alpha)} \right\} - E_1(\mu+\nu) \right. \\ & \left. + 2E_1(\mu+\nu+\alpha) - E_1(\mu+\nu+2\alpha) \right] \end{aligned} \tag{26}$$

in which $\gamma$ is the Euler's constant and $E_1$'s are the elliptic integrals,

$$E_1(z) = \int_1^\infty (e^{-zt}/t) \, dt \qquad (\mathrm{Re}\ z > 0). \tag{27}$$

Two calculations were carried out. In the first one, only two parameters, $h_0$ and $h_1$ were included in (24). The condition (20) yields

$$D_c^{1s} \leqslant 0{\cdot}73035,$$

which differs from the exact result by only 1 %. In the second calculation, $h_0$, $h_1$ and $h_2$ were retained in (24). The upper bound in this case is found to be

$$D_c^{1s} \leqslant 0{\cdot}726782,$$

which is within 0·54 % of the exact result. Thus the error is reduced by a factor of 2 as compared to the two-parameter calculation. We also notice that the results obtained

from the trial function (24) are much better than the result obtained from (23) which indicates that the COCP departs from the pure Coulomb potential significantly near the critical screening region.

## 4. Critical screening parameters for the excited levels

The critical screening parameters for the excited $s$-states of the COCP system can be computed in an approximate way if one assumes an empirical form

$$1/D_c^{ns} = \alpha_1/n^2 + \alpha_2/n^3, \tag{28}$$

in which $\alpha_1$ and $\alpha_2$ are unknown parameters. Using (28) in (16), we get

$$\sum_{n=1}^{\infty} (\alpha_1/n^2 + \alpha_2/n^3)^j = 2^j T_j. \tag{29}$$

Using the tabulated values of the zeta functions (Abramowitz and Stegun 1970)

$$\zeta(n) = \sum_{n=1}^{\infty} n^{-k}, \qquad (k = 2, 3, 4, \ldots,), \tag{30}$$

we obtain the first two relations from (16),

$$1{\cdot}64493407\alpha_1 + 1{\cdot}20205690\alpha_2 = 2T_1 = 2, \tag{31a}$$

$$1{\cdot}08232323\alpha_1^2 + 2{\cdot}07385552\alpha_1\alpha_2 + 1{\cdot}01734306\,\alpha_2^2 = 4T_2 = 2. \tag{31b}$$

Solving $\alpha_1$ and $\alpha_2$ from (31) we finally get for the COCP

$$1/D_c^{ns} = 0{\cdot}7644347\,n^{-2} + 0{\cdot}6177373\,n^{-3}. \tag{32}$$

From (32), we compute the critical screening parameters for the 1$s$ to 8$s$ states. In table 1 the predicted results are compared with the numerical results of Singh and Varshni (1984). It may be noticed that the agreement is quite satisfactory considering the simplicity of the calculation. It may be mentioned here that Patil (1984) obtained similar but more accurate analytic expression for the critical screening coefficient for

**Table 1.** Critical screening parameters for the $ns$-states of the cut-off Coulomb potential.

| | $D_c^{ns}$ | | |
|---|---|---|---|
| $n$ | Present results (equation (32)) | Numerical (Singh and Varshni 1984) | Percent difference |
| 1 | 0·72349 | 0·7228982 | 0·08 |
| 2 | 3·7268 | 3·8089078 | 2·16 |
| 3 | 9.2750 | 9·3608758 | 0·92 |
| 4 | 17·413 | 17·380036 | 0·19 |
| 5 | 28·154 | 27·866538 | 1·03 |
| 6 | 41·504 | 40·820419 | 1·67 |
| 7 | 57·466 | 56·241691 | 2·18 |
| 8 | 76·041 | 74·130359 | 2·58 |

arbitrary *nl*-state for the screened Coulomb potentials using an elaborate technique.

It emerges from our calculations that the lower (upper) bound results converge nicely from below (above) to its exact value. For the lower bound calculation, one can in principle achieve a numerical result to any desired accuracy by computing still higher order traces. The upper bound result can also be refined by considering more free parameters in the variational framework. In this respect, our approach has distinct advantage over the optimal formalism of Glaser *et al* (1976) in which the scope of improving the numerical predictions is limited due to the restriction on the free parameter $p$. Quite naturally, we expect that our present bound calculations can be extended to deal with higher angular momentum states although it is clear that the mathematical steps would be more complicated due to the fact that the kernel becomes singular for $l \neq 0$. Works in this direction is in progress at present.

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