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General Screened Coulomb Potential : Nonperturbative Solutions

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جهد كولوم بالمسح العام : حلول دقيقة غير تقريبية

لالت كومار شارما ، فيليب موني وصامويل شيميدزا

خلاصة: أوجدت طاقات الربط لعدة ذرات متفاعلة عن طريق جهد كولومب بالمسح باستخدام حلول دقيقة غير تقريبية. كما تم دراسة تغير الدالة الموجية مع تغير المسافة (r) وقد توافقت نتائج الدراسة توافقا تاما مع حسابات سابقة.

ABSTRACT: Using nonperturbative solutions, the binding energies for different atoms have been evaluated for the screened Coulomb potentials. The variation of the wavefunction with distance r has also been studied. The results obtained are in excellent agreement with earlier calculations.

KEYWORDS: Nonperturbative solutions, screened Coulomb potentials and binding energies.

1. Introduction

It is well- known that there are some processes which although occurring outside the nucleus are dominated by distances which are small on the atomic scale (Compton wavelength distances). In atomic photo-effect for example, Pratt and Tseng (1972) have argued that for a wide range of photo energies, electron Compton wavelength distances are of primary importance. In such a case, the knowledge of screened wavefunction is desirable for including the effects of screening, at least for small distances r . Furthermore, internal conversion (see e.g. Singh and Varshni, 1984), threshold pair production (see e.g. Tseng and Pratt, 1971) and single quantum annihilation (see e.g. Tseng and Pratt, 1973) phenomena are also characterized by small distances on the atomic scale. The normalization screening theory has been applied successfully to explain the anomalously large photo-defect cross-section in molecular hydrogen (see e.g. Cooper, 1974). There are many atomic and nuclear processes which are characterized by the behaviour of an electron wavefunction at the origin. One such phenomenon is the orbital electron capture, because in this process only the region of overlap between electron and nuclear wavefunction is involved.

The screened Coulomb potential also finds importance in atomic phenomena involving electronic transitions. It has been treated numerically and analytically by various workers using different methods, such as WKBJ method (see e.g. Schiff, 1968), the quantum defect method (see e.g. Faridfathi and Sever, 2007) and different types of perturbation methods. Realizing the utility of the screened Coulomb potential, several

variational calculations (see e.g. Greene and Aldrich, 1976, Lam and Varshni, 1971, Roussel and O' Connel, 1974, Harris, 1962) have been done and tables of energy as a function of screening parameters have been compiled. McEnnan *et al.* (1976) used analytic perturbation theory for non-relativistic cases, while Green and Aldrich (1976) applied a non-perturbative approach to the problem. Later Mehta and Patil (1978[a]), using an approximate and non-perturbative approach, considered a potential of the form: $V(r) = \dfrac{-Ze^2}{(r+\beta)}$ and found that S-wave energy level $E(\beta)$, as a function of parameter β, has a singularity at the origin. These authors have studied the behaviour of the bound-state energy for this potential (a modified Coulomb potential), as a function of the parameter β. It may be of interest that this potential may also serve as an approximation to the potential due to a smeared charge rather than a point charge, and may be pertinent potential for the description of mesonic atoms.

When a classical charged two-particle system is influenced by a plasma sea, the Coulomb potential is replaced by a static screened Coulomb potential, the so-called Debye potential (see e.g. Lam and Varshni, 1976), to explain the interaction. Ray and Ray (1980) obtained s-matrix, discrete energies and wavefunctions for the s- states of an exponential cosine screened Coulomb (ECSC) potential in Ecker-Weizel (EW) approximation. Dutt (1979) and Dutt *et al.* (1981) obtained bound s-state energies of an electron in ECSC potential by analytical method, using EW approximation. They further proposed an extension of EW approximation to treat the non-zero angular momentum bound-states of a class of screened Coulomb potentials and obtained discrete energies for the Yukawa potential. It may be of interest to note (see e.g. Alhaidri *et al*, 2008) that screened Coulomb potential also describes the shielding effect of ions embedded in plasmas.

Motivated by the growing importance of the screened Coulomb potential, we have considered in this paper a general potential of the form

$$V(r) = -\frac{Ze^2}{r\left(1+\delta_0 r^n\right)}, \tag{1}$$

where δ_0 is a screening parameter.

The energy eigenvalues and wavefunctions for different values of n for the potential (1) have been obtained by an approximate and a non-perturbative approach.

2. Calculation of Eigenenergies

The radial Schrödinger equation with potential (1) can be written as

$$\left[-\frac{1}{2r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{Z}{r\left(1+\delta r^n\right)} + \frac{l(l+1)}{2r^2}\right]R(r) = E\,R(r). \tag{2}$$

In equation (2), we have used atomic units (unit of length $\alpha_0 = \dfrac{\hbar^2}{me^2}$ and unit of energy $= -\dfrac{me^4}{\hbar^2}$) and $\delta = (\alpha_0)^n \delta_0$.

Setting $\psi(r) = \dfrac{R(r)}{r}$, equation (2) is transformed to

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + V_1^{eff}(r)\right]\psi(r) = E\psi(r). \tag{3}$$

In equation (3),

$$V_1^{\,eff}(r) = \frac{-Z}{r\left(1+\delta r^n\right)} + \frac{l(l+1)}{2r^2}\ . \tag{4}$$

$V_1^{\,eff}(r)$ may also be written in the form

$$V_2^{\,eff}(r) = \frac{-Z\delta r^{n-1}}{\left(1+\delta r^n\right)\ln\left(1+\delta r^n\right)} + \frac{\delta^2 l(l+1) r^{2n-2}}{2\ln\left(1+\delta r^n\right)\left[\left(1+\delta r^n\right)^{\frac{1}{2}} - \left(1+\delta r^n\right)^{-\frac{1}{2}}\right]}\ . \tag{5}$$

As $V_2^{\,eff}(r)$ tends to $V_1^{\,eff}(r)$ for $\delta r^n < 1$, i.e. $\left(\delta r^n\right)^2 << 1$, and hence we can neglect terms of order $\left(\delta r^n\right)^2$ or higher in the expansions of expressions involving $\left(1+\delta r^n\right)$. Thus, equation (3) with the help of equation (5) takes the form

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{Z\delta r^{n-1}}{\left(1+\delta r^n\right)\ln\left(1+\delta r^n\right)} + \frac{\delta^2 l(l+1) r^{2n-2}}{2\ln\left(1+\delta r^n\right)\left[\left(1+\delta r^n\right)^{\frac{1}{2}} - \left(1+\delta r^n\right)^{-\frac{1}{2}}\right]}\right]\psi(r) = E\psi(r)\ . \tag{6}$$

Further, setting

$$\begin{aligned} E &= -\frac{1}{2}a^2\delta^2, \\ \psi(r) &= \phi(r)e^{-a\delta r^n}\ , \end{aligned} \tag{7}$$

equation (6) becomes

$$\begin{aligned} &-\frac{1}{2}\frac{d^2\phi}{dr^2} + an\delta r^{n-1}\frac{d\phi}{dr} - \frac{Z\delta\phi(r)r^{n-1}}{\left(1+\delta r^n\right)\ln\left(1+\delta r^n\right)} \\ &+ \frac{\delta^2 l(l+1)\phi(r)r^{2n-2}}{2\ln\left(1+\delta r^n\right)\left[\left(1+\delta r^n\right)^{\frac{1}{2}} - \left(1+\delta r^n\right)^{-\frac{1}{2}}\right]} \\ &-\frac{n^2a^2\delta^2}{2}r^{2n-2}\phi(r) + \frac{n}{2}(n-1)a\delta r^{n-2}\phi(r) = E\phi(r). \end{aligned} \tag{8}$$

Now, a change of variable $y = \ln\left(1+\delta r^n\right)$ along with the approximations

$$\phi'(r) = n\delta e^{-y}\left(\frac{y}{\delta}\right)^{\frac{n-1}{n}}\phi'(y),$$

and

$$\phi''(r)=\left[n\delta\left(\frac{y}{\delta}\right)^{\frac{n-1}{n}}\right]^2\frac{e^{-y}}{ny}(1-y)\left[ny\phi''(y)+(n-1-n\,y)\phi'(y)\right],$$

for $n=1,\ l=0$ (for the s states), transforms equation (8) to

$$y(1-y)\phi''(y)-y(1+2a)\phi'(y)+y^2\phi'(y)+\frac{2Z}{\delta}\phi(y)=0\,. \tag{9}$$

In equation (9), terms involving δ^2 (for the region $\delta^2<<1$) have been neglected. Further, to observe the usefulness of the results with $n\neq 1$ in potential (1), the study is restricted to those processes which occur in the region $r\cong 1$. Thus from equation (8),

$$\begin{aligned}&y\,(1-y\,)\phi''(y\,)-y\,(3-2y\,)\phi'(y\,)+\frac{1}{2}\phi'(y\,)-2a\,y\,\phi'(y\,)+\frac{Z}{2\delta}\phi(y\,)\\&-\frac{a}{2}\left(1+y\,+y^{\,2}\right)\phi(y\,)=0,\end{aligned} \tag{10}$$

for $n=2$, and

$$\begin{aligned}&y\,(1-y\,)\phi''(y\,)+y^{\,2}\phi'(y\,)-y\,(3+2a)\phi'(y\,)+2\phi'(y\,)+\left(\frac{2Z}{\delta}-2a\right)\phi(y\,)\\&-2ay\,(1+y\,)\phi(y\,)=0,\end{aligned} \tag{11}$$

for $n=-1$

2.1 Solutions for the case $n=1$

Assuming $\phi(y)$ to be of the form

$$\phi(y)=\sum_{i=0}^{\infty}C_i\,y^{i+\sigma}\ , \tag{12}$$

and substituting it in equation (9), one finds on equating the coefficients of like powers of y that $\sigma=1$ for s-states and the C_i's satisfy the following recursion relation

$$C_{i+1}=\frac{\left[(i+1)(i+2a+1)-\dfrac{2Z}{\delta}\right]C_i}{(i+1)(i+2)}. \tag{13}$$

If the series (13) is to terminate after a certain finite number of terms (i.e. $C_{M+1}=0$), then

$$(M+1)(M+2a_M+1)-\frac{2Z}{\delta}=0\,. \tag{14}$$

This expression is identical with the similar expression obtained by Greene and Aldrich (1976) for $Z=1$. Equation (14) now determines the quantity a_M and hence the energy. The wavefunction $\psi_{Ml}(r)$ may now be written as

$$\psi_{Ml}(r) = e^{-a_M \mu r} \sum_{M=0}^{M} C_M \left[\ln(1+\mu r)\right]^{M+\sigma} , \tag{15}$$

where δ is replaced by a variational parameter μ as trial function. Thus

$$\psi_{Ml}(r) = k\mu r e^{-a_M \mu r} .$$

The condition of normalization finally yields, $k^2 = 4{a_M}^2 \delta$, where μ has been set such that

$$\mu + \frac{\delta}{a_M} = 0 .$$

Now the expression (see e.g. Greene and Aldrich, 1976)

$$E = \int_0^\infty \psi_{M\,l}(r) \left[-\frac{1}{2}\frac{d^2}{d\,r^2} - \frac{Z}{r\left(1+\delta\, r^n\right)} + \frac{l(l+1)}{2\,r^2} \right] \psi_{Ml}(r)\, dr , \tag{16}$$

yields the following for the binding energy

$$E = \int_0^\infty \psi_{1s}\, D_l[\psi_{1s}]\, dr = -\left[\frac{Z\delta}{2} - \frac{\delta^2}{4} \right] , \tag{17}$$

where in the above relations the notations have the following meaning

$$D_l = -\frac{1}{2}\frac{d^2}{d\,r^2} - \frac{Z}{r\left(1+\delta\, r^n\right)} + \frac{l(l+1)}{2r^2},$$

$$\psi_{1s} = N^{-1} e^{-a_{1s}\delta r} \ln(1+\delta r) \text{ and } a_{1s} = \left[\frac{Z}{\delta} - \frac{1}{2} \right].$$

2.2 Solutions for the Case $n = 2$

Again for $n = 2$ in potential (1), C_i 's satisfy the relation

$$C_{i+1} = \frac{\left[(i+1)\left(i + 2a + \frac{1}{2} \right) - \left(\frac{Z}{2\delta} \right) + \left(\frac{a}{2} \right) \right] 2C_i}{i\,(2i+1)}, \quad \text{with } \sigma = 0. \tag{18}$$

This yields for s -states and for

$$M = 0,\ a_0 = \frac{Z}{\delta} ,$$

$$M = 1,\ a_1 = \left(\frac{Z}{5\delta} - \frac{3}{5} \right). \tag{19}$$

2.3 Solutions for the Case $n = -1$

Similarly for s -states and for $n = -1$ and $\sigma = 0$, the recursion relation is

$$C_{i+1} = \frac{\left[i(i+2a+2) - 2\left(\frac{Z}{\delta} \right) + 2a \right] C_i}{(i+1)(i+2)} . \tag{20}$$

Equation (20) yields

$$a_0 = \frac{Z}{\delta},$$

and

$$a_1 = \left(\frac{Z}{2\delta} - \frac{3}{4}\right). \tag{21}$$

The above values of a_M finally give the expression for the wavefunctions

$$\psi_{Ml}(r) = e^{-a_M \delta r^n} \sum_{M=0}^{M} C_M \left[\ln\left(1+\delta r^n\right)\right]^{M+\sigma}. \tag{22}$$

The wavefunctions given by equation (22) are only approximate and their resemblance to the exact wavefunctions depends on the extent to which $V_2^{eff}(r)$ approximates $V_1^{eff}(r)$ in the approximation $\left(\delta r^n\right) << 1.$

3. Results and Discussions

(A) Using equation (17) in Table 1 the binding energy values (in keV) for $n=1$ and for different atoms with Z ranging between 34 and 84 have been given. The values of the screening parameters chosen and the corresponding experimental values have also been depicted in the same table, while Table 2 shows the binding energy values calculated for $n=-1.$

Table 1. Bound state energies E (keV) with $n=1$ as a function of Z and δ

Z	δ	E	
		Present study with $n=1$ in potential (1)	Experimental (Reference Mehta and Patil, 1978[b])
34	0.09	-1.52	-1.27
39	0.095	-1.84	-1.70
44	0.100	-2.19	-2.21
49	0.120	-2.93	-2.79
54	0.130	-3.50	-3.46
59	0.135	-4.12	-4.20
64	0.16	-5.11	-5.02
69	0.18	-6.20	-5.94
74	0.20	-7.39	-6.95
84	0.22	-9.22	-9.31

Table 2. Bound state energies E (keV) with $n=-1$ as a function of Z and δ

Z	δ	E		
		Present study with $n=1$ in potential (1)	By dispersion relation (Reference Mehta & Patil, 1978[b])	By perturbative approach (Reference Iyer, 1980)
34	0.09	-1.52	-1.30	-1.36
39	0.095	-1.84	-1.74	-1.55
44	0.100	-2.19	-2.25	-2.12
49	0.120	-2.92	-2.82	-2.80
54	0.130	-3.49	-3.45	-3.53
59	0.135	-4.11	-4.15	-4.44
64	0.160	-5.10	-4.92	-5.22
69	0.180	-5.81	-5.76	-----
74	0.200	-7.37	-6.66	-----
84	0.220	-9.20	-8.66	-----

(B) It should be noted here that the method of investigation used by us involves a minimum number of parameters and is quite straightforward as compared to the methods used by previous authors (see e.g. Greene and Aldrich, 1976, Rogers *et al*., 1970 and Roussel and O' Connel, 1974).

4. Conclusions

(A) From Table 1 it is seen that that the agreement between the calculated and the observed values is poor for lower values of Z but it improves for higher values of Z .

(B) From Table 2, the results on the binding energy values for $n=-1$ show a reasonably good agreement with the energy values obtained by Iyer (1980). It may also be mentioned here that the screened Coulomb potential (1) changes to a form considered by Mehta and Patil (1978[a]) for this value of n. The energy values obtained by us are comparable to those obtained in their study.

(C) The potential considered in this paper is of general form, and the comparison of shapes obtained for the wavefunction $\psi_{Ml}(r)$ for $n=1$ (Figures 1 and 2) reveals that within the interior of the atom, i.e. $\delta r<1$, shapes of all the screened Coulomb potentials are similar and correspond primarily to the Coulombic form. This enhances the chances of possible use of $\psi_{Ml}(r)$ as the trial wavefunctions**.**

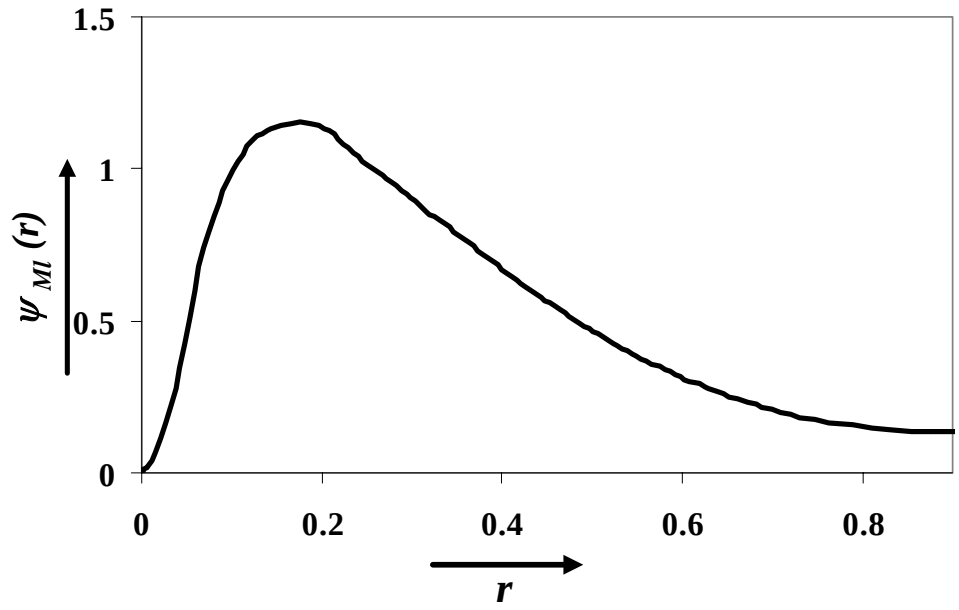

Figure 1. Unnormalised radial wave function $\psi_{M1}(r)$ for 1s state and for n = 1 of Aluminium (Z = 13). Distances are in electron Compton wavelengths.

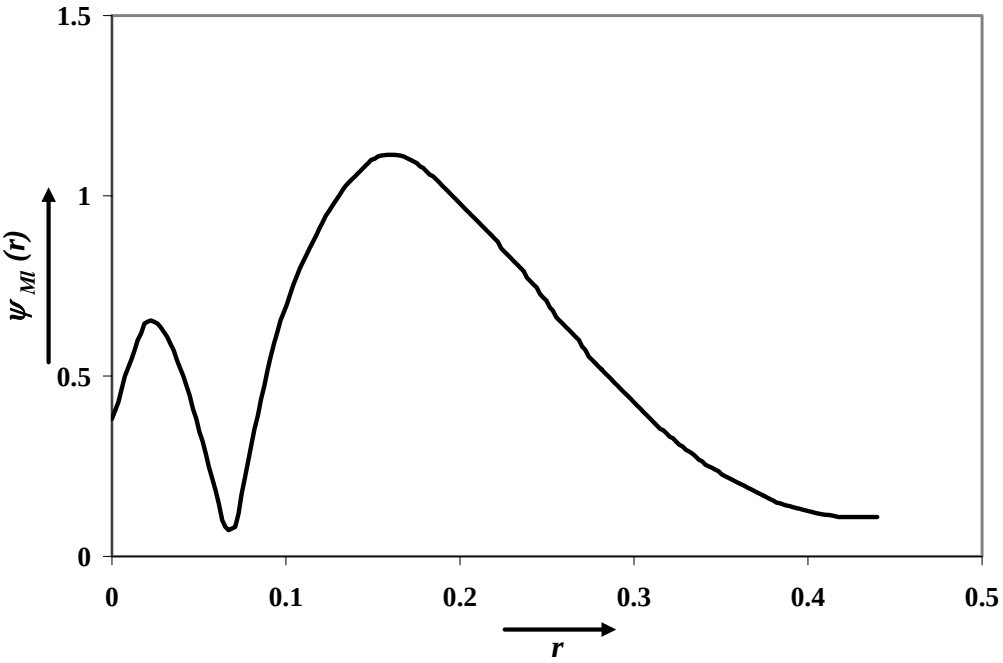

Figure 2. Unnormalised radial wave function $\psi_{M1}(r)$ for 1s state and for n = 1 of Gold (Z = 79). Distances are in electron Compton wavelengths.

(D) Further, it is observed that there is a shift of maxima for $n = 2$ towards origin for increasing values of Z (Figure 3). For the same value of n, however, magnitude of the wavefunction is found to fall-off rapidly with increase in r for higher values of Z.

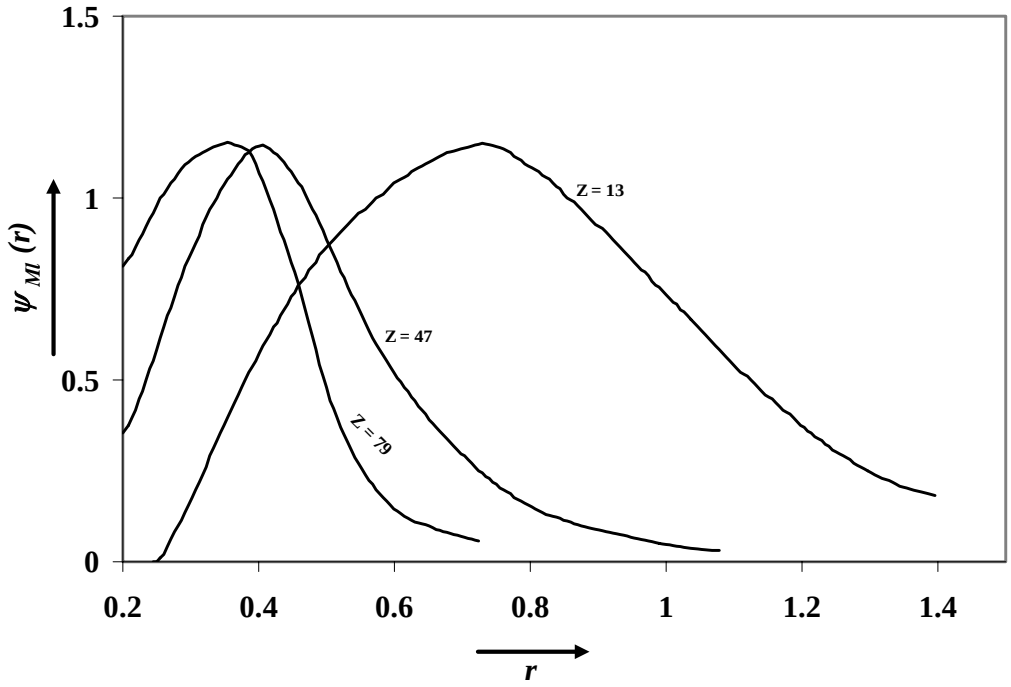

Figure 3. Unnormalised radial wave function $\psi_{M\,l}(r)$ for 2s state and for n = 2 of Aluminium (Z = 13), Silver (Z = 47) and Gold (Z = 79). Distances are in electron Compton wavelengths.

(E) Finally, we conclude with the remark that fairly satisfactory results of binding energies for the potential (1) can be obtained only for $n = 1$ and that the utility of the results for the case $n \neq 1$ is restricted to the processes occurring in the region $r \cong 1$.

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