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ELECTRON-POSITRON CORRELATION ENERGY DUE TO SCREENING IN METALS.

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ABSTRACT

A model is proposed for calculating electron–positron correlation energy due to screening in metals using the jellium model of solids. The model shows that the electron-positron correlation energy due to screening depends on the inverse of the screening length. It also show that the electron positron correlation energy due to screening varies with the electron gas parameter in the same manner as the electron –positron correlation energy calculated using the perturbed hypernetted chain approximation which shows the consistency of the model. The result further reveals that the higher the screening length of the electrons in the metal, the higher its correlation energy due to screening.
Key words: Metals, Screening, positron, correlation energy.

INTRODUCTION

Screening is the removal of electric field at large distances from the positive charge (Inkson, 1984) Screening arises from the Hartree self-consistent field and is a manifestation of the interaction between particles (Ashcroft and Mermin, 1976). When an impurity is introduced into an electron gas, the electrons form charge clouds about the impurity and screens out the impurity at large distances. In an electron gas, the positron acts as an impurity which destroys the homogeneity of the electron gas so that even at large distances from the positron, where the potential is screened out, the exact single wave function will be phase shifted away from the unperturbed plane wave state (Lowy, 1982). The correlation energy of a system of electrons is the energy calculated with proper allowance for the coulomb correlation minus the Hartree – Fock energy (Raimes, 1963).

Electron–positron correlation energy is the change in the energy of a system consisting of electrons after introducing a positron into the system (Boronski and Stachowiak, 1998). The change in the energy of a system due to screening between the positron and electrons is called electron positron correlation energy due to screening. The explanation of screening phenomenon involves the applications of dielectric function, which thus represents the solution of the screening problem (Harrison, 1979). The dielectric function is defined in terms of the electronic response to an external perturbation whose understanding gives an insight into the screening properties of metals and alloys including Friedel oscillation and renormalization of phonon frequencies (Harrison, 1979).

The screening of a positron in an electron gas has been the test of many body theories. Kahana (1963) proposed the Bethe–Goldstone approach that he used to explain positron annihilation rate in metals. The theory gave results that agreed with experimental values for metallic densities. Solander and Statt in Gondzik and Stachowiak (1985) explained screening of positrons in an electron gas in terms of non – linear two component plasma. The theory was used to explain electron–positron annihilation rate in metals which was found to be dependent upon the momentum of the electrons in the fermi surface. Aponen and Pajanne (1979) described screening in an electron gas by means of interacting bosons. They obtained good result for annihilation rate of positron in metals. Gondzik and Stachowiak (1985) used the theory of quantum liquids together with the theory of Hartree–Fock to explain the screening of particles in an electron gas. The electron–positron annihilation rate they calculated were in good agreement with experimental results espacially in the regions of low electron density.

In this work, we propose a model that can be used to calculate electron – positron correlation energy due to screening and test the model using simple metals.

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THEORY

If a positron is introduced into a solid, the potential established in the solid as a result of the presence of the positron is

$$\phi(r) = \frac{e}{r} \quad \text{.....(1)}$$

where e is electronic charge and r is the distance between the referenced electron and the positron.

As a result of the presence of the positron, there will be an electrostatic potential, V(r) that will be built up as a result of the motion of the electrons. Then the total potential is

But the induced electrostatic potential is

$$U(r) = \phi(r) + V(r) \quad \text{.....(2)}$$

$$E = -\nabla\phi(r)$$

and

$$\nabla^2\phi = -4\pi\rho(r)$$

where ρ(r) is the charge density. But by Sommerfeld model (Inkson, 1984)

$$r(r) = eu(r)N(E_f)$$

$$\nabla^2\phi = 4\pi eu(r)N(E_f)$$

$$\nabla^2 u(r) - \nabla^2 v(r) = 4\pi eu(r)N(E_f)$$

Neglecting the negative sign, we have

But $\lambda^2 = 4\pi eN(E_f)$ (Inskon,1984 and Kittel,1996) where $1/\lambda$ is the Thomas Fermi

$$\phi(r) = u(r) - v(r)$$

$$\nabla^2[u(r) - v(r)] = 4\pi eu(r)N(E_f) \quad \text{.....(3)}$$

screening length and $N(E_F)$ is the density of states for a free electron gas.

$$\therefore \nabla^2 u(r) - 4\pi eu(r)N(E_f) = \nabla^2 v(r)$$

$$\therefore (\nabla^2 - \lambda^2)(r) = \nabla^2 v(r) \quad \text{.....(5)}$$

$$[\nabla^2 - 4\pi eN(E_f)]u(r) = \nabla^2 v(r) \quad \text{.....(4)}$$

In order to generate a self consistent equation, we assume that the positron cannot distinguish between the applied potential and the induced potential crested by the movement of the electrons so that it responds or feels the total potential u(r) (Inkson, 1984). So we set the right hand of equation (5)

$$\therefore (\nabla^2 - \lambda^2)u(r) = 0 \quad \text{.....(6)}$$

Table 1: Result obtained for electron – positron correlation energy due to screening, E_{sc} and electron positron correlation energy, E_c according to the perturbed hypernetted chain approximation for different metals used to test the model.

Metal	r_s	E_{sc}	E_c	Metal	r_s	E_{sc}	E_c
Li	3.25	-0.81	-0.82	Ti	1.92	-0.93	-1.06
Na	3.93	-0.56	-0.74	Va	1.64	-1.11	-1.15
K	4.86	-0.52	-0.67	Cr	1.86	-0.97	-1.08
Rb	5.20	-0.51	-0.65	Mn	2.14	-0.84	-1.01
Cs	5.63	-0.50	-0.62	Fe	1.85	-0.97	-1.08
B	1.88	-0.95	-1.08	Co	2.07	-0.86	-1.03
Mg	2.66	-0.70	-0.90	Ni	2.07	-0.86	-1.03
Ca	3.27	-0.61	-0.82	Cu	2.12	-0.85	-1.01
St	3.36	-5.58	-0.78	Zn	2.31	-0.78	-0.97
Ba	3.70	-0.57	-0.77	Yt	2.61	-0.71	-0.91
Al	2.07	-0.86	-1.02	Zr	2.11	-0.85	-1.02
Ga	2.19	-0.82	-1.00	Nb	2.13	-0.84	-1.01
In	2.41	-0.75	-0.95	Mo	1.84	-0.97	-1.09
Th	2.48	-0.74	-0.94	Te	1.79	-1.00	-1.10
Si	2.00	-0.89	-1.04	Ru	1.93	-0.92	-1.06
Ge	2.09	-0.86	-1.02	Rh	1.95	-0.92	-1.06
Sn	3.02	-0.64	-0.85	Pd	2.23	-0.79	-0.98
Pb	2.09	-0.66	-0.87	Ag	2.39	-0.76	-0.95
At	2.53	-0.73	-0.93	Au	2.39	-0.76	-0.90
Bi	2.67	-0.70	-0.90	Cd	2.59	-0.71	-0.92
Sc	2.32	-0.78	-0.97	Pt	2.00	-0.89	-1.04
Nb	2.13	-0.84	-1.01	Ir	2.25	-0.80	-0.98
Wa	2.04	-0.88	-1.03	Hg	2.66	-0.70	-0.90
Re	1.99	-0.90	-1.05				
Os	1.96	-0.92	-1.05				

to zero and consider only the homogeneous part.

In the spherical polar co-ordinate, the equation becomes

$$(r^2\frac{d^2}{dr^2}+2r\frac{d}{dr}-\lambda^2)u(r)=0 \quad \text{.....(7)}$$

Subject to the boundary conditions:

(i) $u(r) = e/r$ as $r \to 0$

(ii) $u(r) = 0$ as $r \to \infty$

The solution of equation (7) above is as follow (Inkson, 1984)

$$u(r)=\frac{e[\exp(-\lambda r)]}{r} \quad \text{. . . . . (8)}$$

But the correlation energy due to screening, E_{sc} is obtained from the induce

potential, V_{ind} as follows (Inkson,1984).

$$E_{sc} = \lim_{r\to 0}(\frac{-e}{2}V_{ind}) \quad \ldots(9)$$

$$V_{ind} = \frac{e[\exp(-\lambda r)]}{r} - \frac{e}{r} \quad \ldots(10)$$

Differentiating equation (11) and subsituting the limit, we have

But in atomic unit, energy is measured in Rydberg (Ry) and e=1

$$\therefore V_{ind} = \frac{e}{r}[\exp(-\lambda r) - 1]$$

$$E_{sc} = \lim_{r\to o}\left\{\frac{-e}{2}[\frac{e}{r}(\exp(-\lambda r) - 1)]\right\} \quad \ldots(11)$$

$$\therefore E_{sc} = \frac{\lambda}{2}$$

$$E_{sc} = \frac{\lambda e^2}{2} \quad \ldots(12)$$

But λ is the inverse of the Thomas Fermi screening length, which is a measure of the distance within which the screening is effectively completed and is of the order of the inter particle spacing. It is given by the expression (Ashcroft and Mermin, 1976).

$$\lambda = \frac{2.95}{r_s^{\frac{1}{2}}} \quad \ldots(13)$$

where r_s is the electron gas parameter defined as

$$r_s = \left(\frac{3}{4\pi vn}\right)^{\frac{1}{3}}\frac{1}{a_0} \quad \ldots(14)$$

where v is the valency, n is the electronic concentration of the metal and a_0 is the Bohr's radius.

$$\therefore E_{sc} = \frac{2.95}{2r_s^{\frac{1}{2}}} \quad \ldots(15)$$

In the perturbed hypernetted chain approximation, the electron – positron correlation energy is given by the expression (Boronski and Stachowiak, 1998):

$$E_c(r_s) = \frac{a}{(r_s - d)^2} + \frac{b}{(r_s - d)} + c \quad \ldots(16)$$

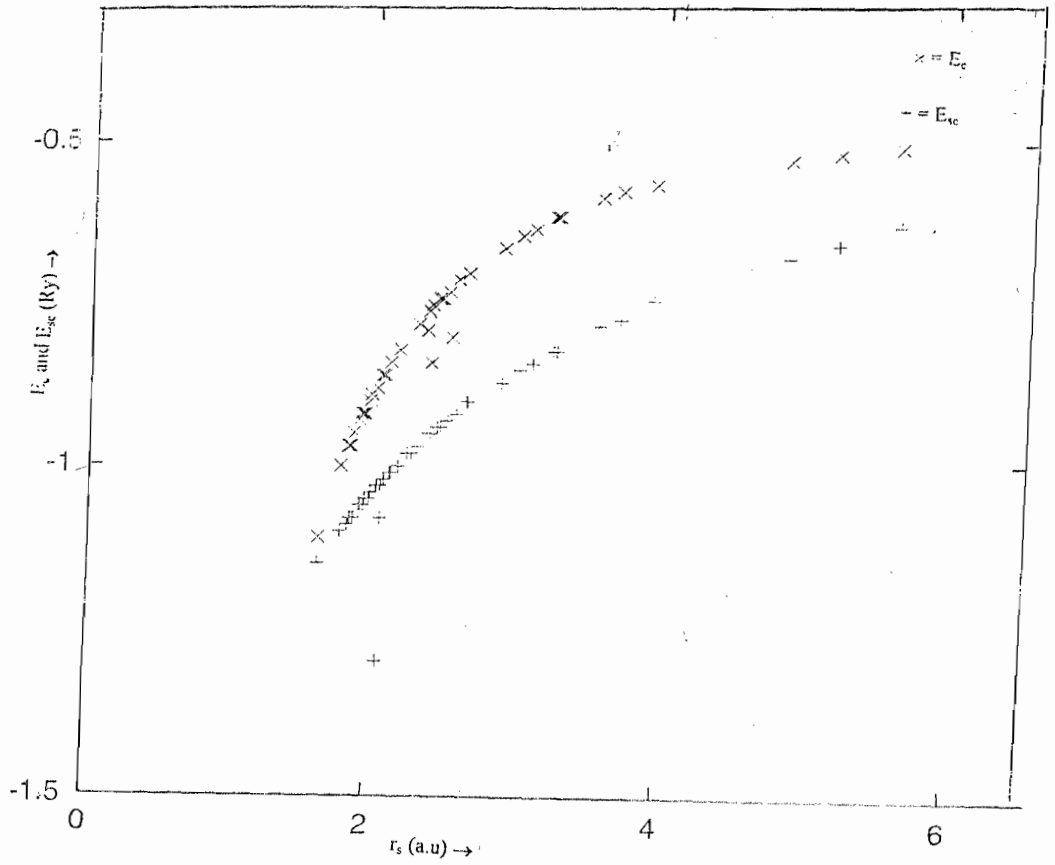

Fig 1: Variation of electron – positron correlation energy E_c and electron – positron correlation energy due to screening, E_{sc} with electron gas parameter, r_s.

'where a, b, c, and d are constants depending on the value of r_s . In the metallic range, the values of a, b, c and d are given by Boronski and Stachwoiak (1998) as a = -2.385415, b = -0.1732167, c = 0.4562613 and d = -1.0.

In this work, electron – positron correlation energy due to screening is calculated using equation (15) while the total electron positron correlation energy is calculated using equation (16) for alkaline, alkaline earth, group three, single semiconductors, transition and noble metals of the periodic table. Their variation with the electron gas parameter is studied.

RESULTS AND DICUSSION

The electron – positron correlation energy according to the perturbed hypernetted chain approximation and the electron–positron correlation energy due to screening were calculated for fifty elements consisting of: alkaline, alkaline earth, transition, noble metals and single semiconductors. Their variation with the electron gas parameter, r_s is as shown in table 1 and figure I.

The figure show that the electron–positron correlation energy calculated using the perturbed hypernetted chain approximation varies directly with r_s . The electron positron correlation energy due to screening also exhibit similar variation with r_s. This reveals that electron–positron correlation energy due to screening contributes to the total electron–positron correlation energy. As shown in the figure, the lower the value of r_s, the higher the contribution of screening to the total electron -positron correlation energy. This applies to the alkaline, alkaline earth metals, semiconductors like germanium, silicon and gallium, and the transition metals. For $r_s > 3$, the contribuction of correlation energy due to screening to the electron–positron correlation energy is smaller to that contributed for $r_s < 3$. The alkaline metals fall in this range of r_s and the properties of the alkaline metals can be explained easily with the jellium model of solids (Gondzik and Stachowiak, 1985). The obtained result shows that screening contributes to the electron - positron correlation energy in metals. For all the metals investigated, the value of the electron–positron correlation energy is higher than the electron–

positron correlation energy due to screening. This is because, electron–positron correlation energy depends not only on r_s but also on some constants and the electron–positron correlation energy due to screening contributes also to the correlation energy.

CONCLUSION

A model for calculating electron–positron correlation energy due to screening is developed. The model was tested using with the perturbed hypernetted chain approximation model for calculating electron–positron correlation energy for metals of different electron gas parameter r_s. The results obtained show that electron – positron oorrelation energy calculated using the perturbed hypernetted chain approximation is higher than the electron – positron correlation energy due to screening. The results further show that while the electron – positron correlation energy due to screening depends only on the electronic concentration of the metal through the electron gas parameter, r_s. But the electron -positron correlation energy according to the perturbed hypernetted chain approximation depends on r_s as well as some constants and the contribuction from the screening correlation energy.

Since the perturbed hypernetted chain approximation is the most recent and the best approximation for calculating electron – positron correlation energy, the proposed model follows the same trend as it does which shows that the proposed model is consistent with the approximation.

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