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Study of Radial Part of Pseudo wave Function using Pseudo-spherical Methodology in Condenser Matter

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***Abstract:** The radial part of $F_l(r)$ of the pseudo Schrödinger equation has been developed in pseudo potential approach. Also the pseudo spherical function $F_l(r)$, the radial part of pseudo wave function $\phi_k(r, \theta, \phi)$ is expressed in terms of ion-core electron density, $P_l(r)$ of Hartree or Hartree-Fock one electron wave function $\psi_k(r, \theta, \phi)$*

To develop the present equation, a new pseudo spherical function $Y_l(r)$ has been investigated which is helpful in determining many types of electron densities.

The present study orients the study related to condenser matter as well as mathematical physics.

***Keywords:** radial part, pseudo potential, wave function, Hartree-Fock, electron densities*

I. INTRODUCTION

In the free electron concepts of solids, Hartree and Hartree-Fock (HF) methodology and pseudo potential (PS) formalism have given new orientations. The potential usedin both cases is of central field type. In both cases the self-consistent field approximation is used where the effect of the interaction of a given electron with all others is replaced by some repulsive potential. Using these repulsive potentials the corresponding single particle Hamiltonian of HF methodology and PS methodology are given by –

$$H_{HF} = \left[\frac{-\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r} + V(r)\right] = \left[\frac{-\hbar^2}{2m}\nabla^2 + V_{HF}(r)\right]$$

$$H_{PS} = \left[\frac{-\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r} + V(r)\right] = \left[\frac{-\hbar^2}{2m}\nabla^2 + V_{PS}(r)\right] \qquad \text{….. (1)}$$

Here, Hartree-Fock potential $V_{HF}(r)$ consists of self consistent core potential and valance electron potential $-Ze^2/r$, while pseudo potential $V_{PS}(r)$ is the sum of same valance electron potential $-Ze^2/r$ and electron-ionic model interaction potential $V_R(r)$.

The corresponding Schrödinger quantum mechanical equations are given by

$$H_{HF}\left|\psi_k\right\rangle = [T + H_{HF}]\left|\psi_k\right\rangle = E_k\left|\psi_k\right\rangle$$

$$H_{PS}\left|\phi_k\right\rangle = [T + H_{PS}]\left|\phi_k\right\rangle = E_k\left|\phi_k\right\rangle \qquad \text{….. (2)}$$

Where T is kinetic energy and E_k is energy Eigen value.

A. Physical Developments

In spherical co-ordinate system, (r, θ, ϕ), the pseudo Schrödinger equation is given by

$$\left[\frac{-\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r} + V_{PS}(r)\right]\phi_k = E_k\phi_k \qquad \text{….. (3)}$$

$$\therefore \left[\frac{-\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\beta}{r^2}\right\} - \frac{Ze^2}{r} + V_{PS}(r)\right]\phi_k = E_k\phi_k$$

Here, $\left[\beta = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$

$$\therefore \left[\frac{-\hbar^2}{2m}\left\{\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{\beta}{r^2}\right\} - \frac{Ze^2}{r} + V_{PS}(r)\right]\phi_k = E_k\phi_k$$

Put $\beta = l(l+1)$

$$\therefore \left[\frac{-\hbar^2}{2m}\left\{\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right\} - (E_k - V)\right]\phi_k = 0$$

Where, V = $\left[\frac{-Ze^2}{r} + V_{PS}(r)\right]$

$$\therefore \left[\left(\frac{-\hbar^2}{2m}\left\{\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right\}\right) - (E_k - V)\right]\phi_k = 0$$

$$\therefore \left[\left\{r^2\frac{\partial}{\partial r^2} + 2r\frac{\partial}{\partial r} - l(l+1)\right\} + r^2\frac{2m}{\hbar^2}(E_k - V)\right]\phi_k = 0$$

$$\therefore r^2y'' + 2ry' + \{\alpha r^2 - l(l+1)\}y = 0 \qquad \text{...... (4)}$$

Where $\alpha = \frac{2m}{\hbar^2}(E_k - V)$ & y= ϕ_k

Suppose, $\alpha r^2 = \sum_{m=0}^{\infty} a_m r^m$ and solution y is of the form

$$y = \sum_{k=0}^{\infty} b_k r^{k+\rho} \qquad \text{...... (5)}$$

thus by some mathematical exercise, A solution of equation (4) is given by

$$Y_l(r) = b_o r^{\rho}\left[1 - \sum_{k=1}^{\infty}\frac{|Ck|}{k!(2\rho+2)_k}r^k\right] \qquad \text{...... (6)}$$

Where, $\rho = \frac{1}{2}\left(-1 \pm \sqrt{(2l+1)^2 - 4a_0}\right)$ ...... (7)

and

$$|Ck| = \begin{vmatrix} 2\rho+2 & 0...... & 0..... & 0..... & a_1 \\ a_1 & 2(2\rho+3).... & 0..... & 0...... & a_2 \\ a_2 & a_1 & 3(2\rho+4).... & 0.... & a_3 \\ \cdots & \cdots & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \\ a_{n-2} & a_{n-3} & ... & a_{1(n-1)}(2\rho+n)... & a_{n-1} \\ a_{n-1} & a_{n-2} & .... & a_1 & a_n \end{vmatrix} \quad ...\ (8)$$

Note: Solution (6) for $\rho = \rho_1 = \frac{1}{2}\left(-1+\sqrt{(2l+1)^2-4a_0}\right)$ and

$\rho = \rho_2 = \frac{1}{2}\left(-1-\sqrt{(2l+1)^2-4a_0}\right)$Are independent, if $\rho_1 \neq \rho_2$ and $\rho_1 - \rho_2$ is not an integer. We have,

$$Y_l(r) = b_o r^{\rho}\left[1-\sum_{k=1}^{\infty}\frac{|Ck|}{k!(2\rho+2)k}r^k\right] \quad ....\ (9)$$

In spherical co-ordinate (r,θ,ϕ) system the Hartree-Fock wave function is expressed as

$$\psi_{\ k}(r,\theta,\phi) = \frac{1}{r}P_{n,l}(r)y,l\,m(\theta,\phi)\,\chi_{ms} \quad ....\ (10)$$

Whose radial function is given by

$$Y_{n,l}(r) = \frac{1}{r}P_{n.l}(r) \quad .....\ (11)$$

Multiply and divide equation (9) by r

$$\therefore Y_l(r) = b_o\frac{r^{\rho+1}}{r}\left[1-\sum_{k=1}^{\infty}\frac{|Ck|}{k!(2\rho+2)k}r^k\right]$$

$\therefore$ from equation (11)

$$P_l(r) = b_o\, r^{\rho+1}\left[1-\sum_{k=1}^{\infty}\frac{|Ck|}{k!(2\rho+2)k}r^k\right] \quad ....\ (12)$$

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Now we express the pseudo Schrödinger equation in spherical co-ordinate system (r,θ,ϕ) similar to Hartree-Fock wave function as

$$\phi_k(r,\theta,\phi) = r^{l-2} F_{n.l}(r)\, L((\theta,\phi) \qquad \text{.... (13)}$$

$\therefore$ pseudo spherical radial function is given by

$$Y_\ell(r) = r^{l-2} F_\ell(r) \qquad \text{.... (14)}$$

Now multiply and divide equation (9) by r^{l-2}

$$= \qquad b_o \frac{r^{\rho+l-2}}{r^{l-2}} \left[1 - \sum_{k=0}^{\infty} \frac{|C_k|}{k!(2\rho+2)_k} r^k \right]$$

$$\therefore F_l(r) = b_o \frac{r^{\rho}}{r^{l-2}} \left[1 - \sum_{k=0}^{\infty} \frac{|C_k|}{k!(2\rho+2)k} r^k \right] \qquad \text{.... (15)}$$

B. Special Case

If $a = 0$, then $\rho = l$ therefore equation (12) becomes

$$P_l(r) = b_o r^{l+1} \left[1 - \sum_{k=1}^{\infty} \frac{|C_k|}{k!(2\rho+2)_k} r^k \right] \qquad \text{..... (16)}$$

Similarly,

$$F_l(r) = b_o r^2 \left[1 - \sum_{k=0}^{\infty} \frac{|C_k|}{k!(2\rho+2)_k} r^k \right] \qquad \text{.... (17)}$$

II. NUMERICAL COMPUTATION AND RESULTS

In order to see the study between pseudo spherical methodology and Hartree and Hartree-Fock methodology, we have computed: $\mathbf{F_l(r)}$using equation (15) for different values of l= 0,1 and 2 .We have taken the values of a_0=1,a_1=1.Computation results are shown in fig.(1) a,b,c,d,e & f.

1) Fig.(1d) ,Variation of $F_0(r)$ for l=0 , as r increases then $F_0(r)$ varies from zero ,initially it is -ve then varies from –ve to 9.8×10^7Å up to r = 8 Å and then varies exponentially.
2) Fig.(1e) $F_1(r)$ for l=1 as r increases from zero $F_1(r)$ varies from -2.46×10^2Å to -7.1×10^8Å up to r = 8 Å. The behavior shows that upto r= 4Å , $F_1(r)$ has variation almost constant and for higher values of r it shows exponential behavior.
3) Fig.(1f), Variation of $F_2(r)$ for l=2 as r increases then $F_2(r)$ varies from -6.5×10^1Å to -4×10^{10}Å up to r = 8 ÅThe behavior shows that up to r= 4Å , $F_2(r)$ has variation almost constant and for higher values of r it shows exponential behavior .

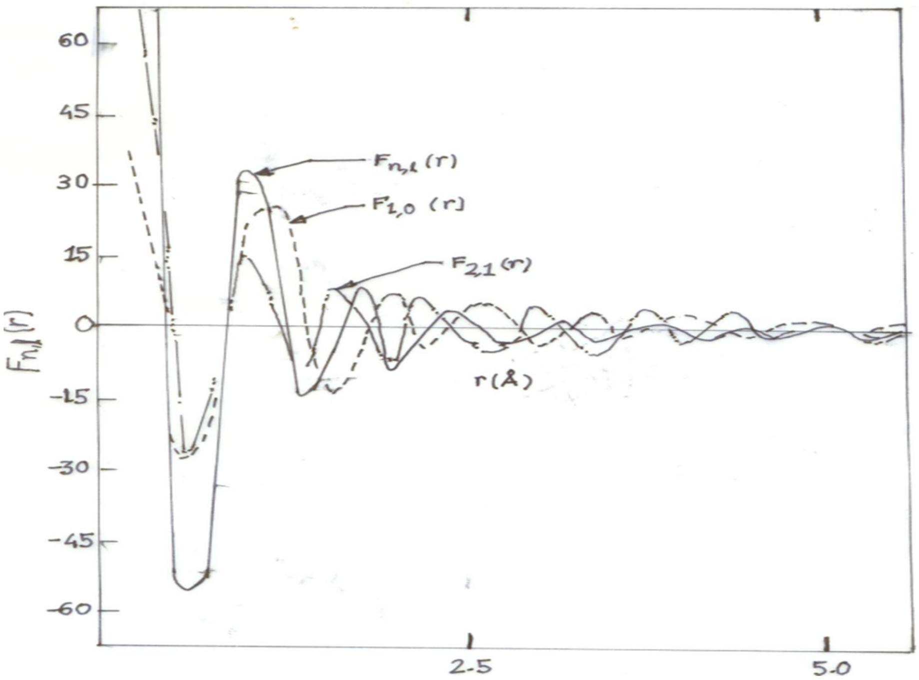

Fig.1 $F_{n,l}(r)$ Versus 'r'

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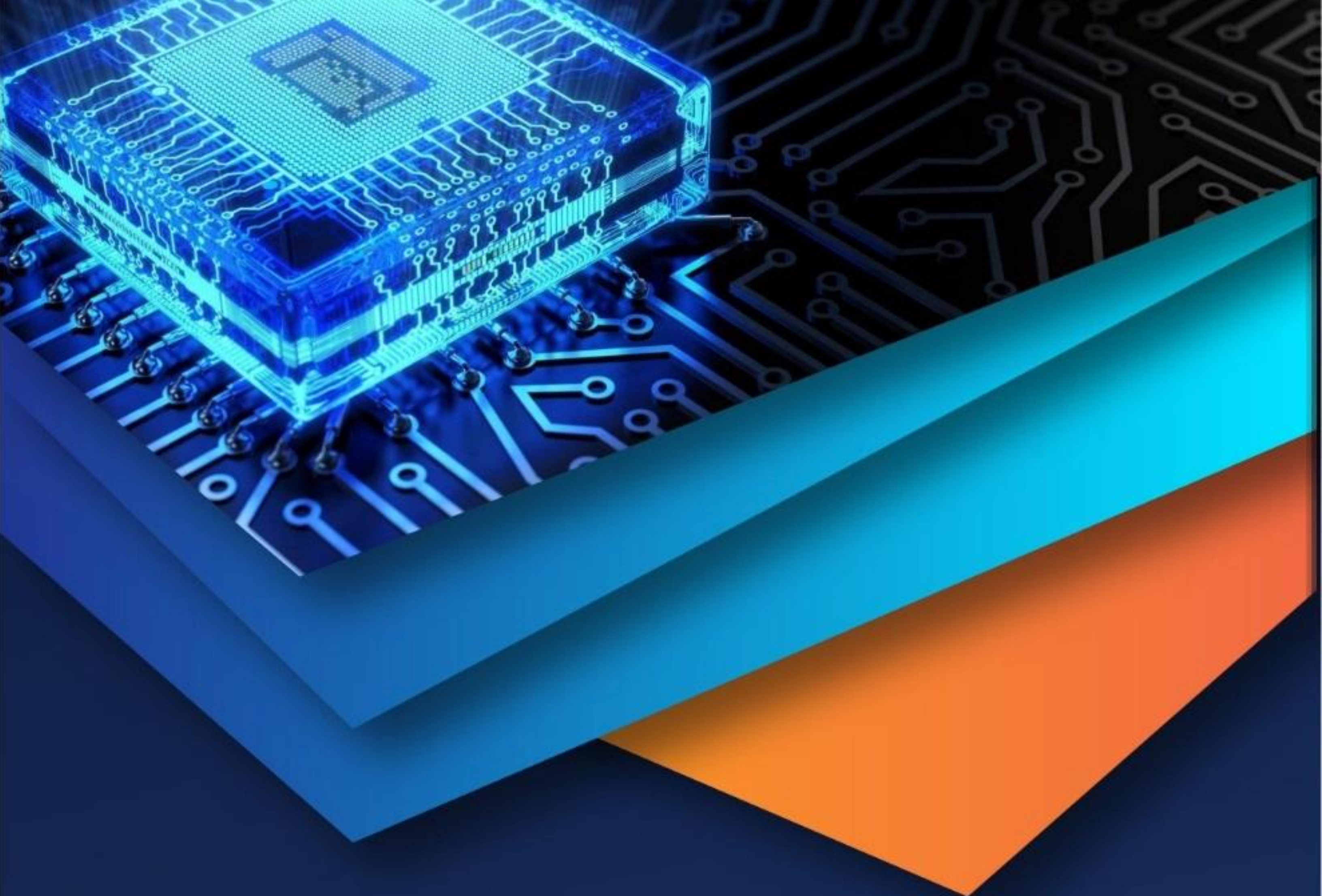

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