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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 used in 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 –

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

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

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

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

$$H_{PS} |\phi_k\rangle = [T + H_{PS}] |\phi_k\rangle = E_k |\phi_k\rangle \quad \dots (2)$$

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

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

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

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

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

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

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

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

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

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

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

$$y = \sum_{k=0}^{\infty} b_k r^{k+\rho} \quad \dots\dots (5)$$

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

$$Y_l(r) = b_0 r^\rho \left[1 - \sum_{k=1}^{\infty} \frac{|Ck|}{k!(2\rho+2)_k} r^k \right] \quad \dots\dots (6)$$

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

and

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

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

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

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

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

$$\psi_k(r, \theta, \phi) = \frac{1}{r} P_{n,l}(r) y_l m(\theta, \phi) \chi_{ms} \dots (10)$$

Whose radial function is given by

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

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)

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

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

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

∴ pseudo spherical radial function is given by

$$Y_\ell(r) = r^{l-2} F_\ell(r) \quad \dots (14)$$

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

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

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

B. Special Case

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

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

Similarly,

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

II. NUMERICAL COMPUTATION AND RESULTS

In order to see the study between pseudo spherical methodology and Hartree and Hartree-Fock methodology, we have computed: $F_l(\mathbf{r})$ 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 $9.8 \times 10^7 \text{ \AA}$ up to $r = 8 \text{ \AA}$ and then varies exponentially.
- 2) Fig.(1e) $F_1(r)$ for $l=1$ as r increases from zero $F_1(r)$ varies from $-2.46 \times 10^2 \text{ \AA}$ to $-7.1 \times 10^8 \text{ \AA}$ up to $r = 8 \text{ \AA}$. The behavior shows that upto $r = 4 \text{ \AA}$, $F_1(r)$ 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 $-6.5 \times 10^1 \text{ \AA}$ to $-4 \times 10^{10} \text{ \AA}$ up to $r = 8 \text{ \AA}$. The behavior shows that up to $r = 4 \text{ \AA}$, $F_2(r)$ has variation almost constant and for higher values of r it shows exponential behavior.

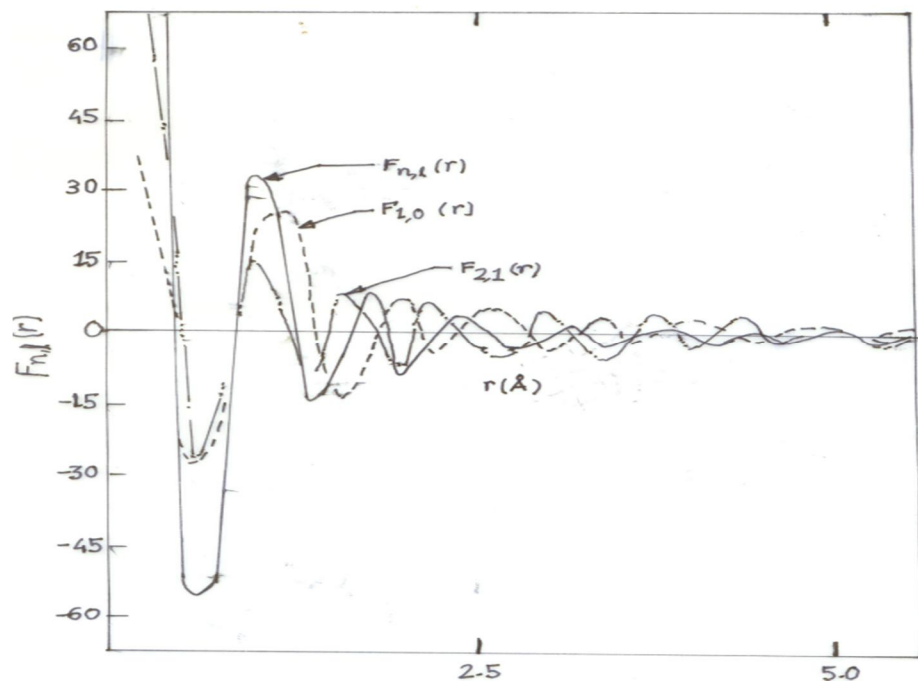


Fig.1 $F_{n,l}(r)$ Versus 'r'

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