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Relativity of Pseudo-Spherical Concept and Hartree-Fock Concept for Condensed Matter

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Abstract: ***The function $F_{n,l}$ (r) ;the radial part of of the pseudo-wave function Φ_k (r, θ , Φ) is expressed in terms of ion-core electron density, $\rho_{n,l}$ (r) and its relation with the radial part $P_{n,l}$ (r) of Hartree- Fock wave function. A new mathematical function ps_l (x) called as pseudo-spherical function has been developed which is similar to other mathematical functions, and helpful in determining many types of electron densities. The physical and mathematical developments on various aspects such as functional densities have been described. It is further emphasized that $F_{n,l}$ (r) and $P_{n,l}$ (r) functions and core electron density at different electronic states of the atom that both the functions posses strong correlationship. Study concludes that the present development resulted into an innovative simpler path in the orientation of condensed matter as well as Mathematical Physics.***

Keywords: ***radial part, pseudo wave function, electron density, condensed matter, mathematical physics***

I. INTRODUCTION

In recent years, Hartree and Hartree-Fock (HF) methodology and pseudo potential (PS) formalism[1,2] have given new orientations to the free electron concept of solids. In both cases the potential used 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. On introducing these repulsive potentials, the corresponding single particle Hamiltonian of both cases are given by

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

$$H_{PS} = -\left(\frac{h^2}{2m} \nabla^2 - \frac{Ze^2}{r} + V(r) \right) = -\left(\frac{h^2}{2m} \nabla^2 + V_{PS}(r) \right)$$

This describes the corresponding Schrödinger quantum mechanical equations as given by

$$H_{HF} \mid \Psi_k > = [\, T + V_{HF}] \mid \Psi_k > = E_k \mid \Psi_k > \tag{1}$$

$$H_{PS} \mid \Phi_K > = [\, T + V_{PS}] \mid \Phi_K > = E_k \mid \Phi_K > \tag{2}$$

The single particle Hartree-Fock Wave function Ψ_k (r) oscillates due to deep core potential where as single particle pseudo-wave function is smooth over the core region[3,4]. The objective of the present paper is to differentiate above analogy on the basis of wave functions and potentials used. For the first time pseudo-wave radial functions $F_{n,l}$ (r) with respect to Hartree- Fock radial functions $P_{n,l}$ (r) have been investigated .Here n and *l* are total quantum and orbital quantum number, respectively.

The pseudo-spherical concept introduced through this paper has given birth to a new pseudo- spherical function ps_l (x).

In present paper the physical and mathematical developments of newly introduced pseudo-spherical function ps_l (x) have been discussed. Different functional densities have been discussed on the basis of core electron density, $\rho_{n,l}$ (r) in our pseudo-spherical functional approach while a parallel description for Hartree-Fock methodology has been discussed elsewhere.

II. ANALYSIS

A. Physical Developments

In spherical co-ordinate (r,θ,ϕ)system the Hartree-Fock wave function is expressed by[5,6]

$$\Psi_K(r, \theta, \phi) = 1/r \; P_{n,l}(r) \; y,l, m\, (\theta, \phi) \; X_{ms}. \tag{3}$$

Where $y_{l,m}$ (θ,ϕ) is a spherical harmonic and X_{ms} a spin magnetic quantum number respectively of the electron states. Their radial wave equation is described by,

$[d^2/dr^2+2Z/r-l(l+1)/r^2-1/n^2]\, P_{n,l,}(r)=0$ (4)

Similarly, we are making an effort in expressing pseudo-wave function[5] $\Phi_K(r, \theta, \phi)$ of equation (2) as follows:

$\Phi_K(r, \theta, \phi) = r^{1-2}\, F_{n,l}\,(r)\, L\,(\theta, \phi)$ (5)

Where $F_{n,l}$ (r) is radial part, $L(\theta, \phi)$ is spherical harmonic part as well as the corresponding radial part of our methodology ;is given by

$$y''+\frac{2(l-1)}{r}y'+\left[\frac{-l(l+1)+(l-1)(l-2)}{r^2}+\frac{2m}{\hbar^2}\{\mathrm{E}-Vp(r)\}\right]y=0 \qquad (6)$$

Where y= $F_{n,l}$ (r) and the substitutions $r = x / \alpha$ and $\alpha = [(2m / \hbar^2)\ \{ E–V_P\ (r) \}\ ]^{1/2}$ have been useful in developing core concepts. To construct[7] the solution of Eq.(6) inside the core region where the potential is having spherical symmetry it is necessary to adjust the amplitude of $F_{n,l}$ (r) function. After some mathematical exercise

Eq. (6) transforms to

$$\frac{d^2y}{dx^2}+\frac{2(l-1)}{x}\frac{dy}{dx}+\left[1+\frac{-l(l+1)+(l-1)(l-2)}{x^2}\right]y=0 \qquad (7)$$

Where $y = ps_l\,(x)$. $ps_l\,(x)$ is called pseudo-spherical function.

Eq.(7) has a series solution given by

$$y=\sum_{r=0}^{\infty}\frac{(-1)^r a_0 x^{2r+2}}{2^{2r}r!\left(l+\frac{3}{2}\right)_r} \qquad (8)$$

The function $F_{n.l}$ (r) related to the core electron density ρ_R (r) as

$$F_{n.l}\,(r) = (4\pi\, r/cq_B{}^2Z)\ \sum_{n'=l}\ \sum_{l'=0}^{nl}\ \rho_{n'l,'}\,(r) = (4\pi\, r/cq_B{}^2Z)\ \rho_R\,(r) \qquad (9)$$

$$\rho_{n'l,'}\,(r) = \sum_m\ \sum_l\ \Phi_{n,,l,,m}\,(r-r_j)\, f_{n,l}\,(r)\, \Phi_{n,l,m}\,(r-r_j) \qquad (10)$$

Here, c is constant, q_B is a screening parameter, ρ_R (r) the repulsive density, $f_{n,l}$ (r) the probability of occupying state and j the ion position.

B. Functional Densities

All types of densities of real space (r-space) and momentum space (q-space) corresponds to functional densities. The valence charge density ρ_A is given by

$\rho_A = Z / \Omega = -(4\pi e^2/q^2)^{-1}V_A\,(q)$; where $V_A(q)$ is the attractive part of pseudo-potential Vps (q), also the core electron density $\rho_{n.l}$ (q) is expressed by[5]

$\Sigma\rho_{n.l}\,(q) = \rho_R\,(q) = (4\pi e^2 / q^2)^{-1}\, V_R\,(q)$ (11) where V_R (q) is the repulsive part of pseudo- potential $V_{ps}(q)$, in this way

$$V_{ps}(q) = \{- (4\pi e^2 / q^2)\, \rho_A - \rho_R\,(q)\ \}$$
$$= - (4\pi e^2 / q^2)\, \rho_{ps}\,(q) \qquad (12)$$

where we define the pseudo-electron density ρ_{ps} (q) in Fourier transformed q-space we express

$$\rho_R\,(q) = \sum_{n,l}\ \rho_{n.l}\,(q) = (Z/\Omega)\, \Sigma\, ps_l\,(qr_n) \qquad (13)$$

$$\rho_R\,(0) = \sum_{n,l}\ \rho_{n.l}\,(0) = (Z/\Omega)\, '\sum_l 2\,(2l+1) \qquad (14)$$

The Fourier transform of repulsive potential finally gives a relation between $F_{n,1}$ (r) and ps_l (x) functions, as

$$\int \sum_{n,l}\ F_{n,l}\,(r)\, \sin\,(qr) = \Sigma\, ps_l\,(qr_n) \qquad (15)$$

Eq. (13) provides the r-space functional form of core electron density as

$$\rho_R(r) = \int \rho_R(q)\, e^{iq,r}\, dr = \sum_{n,l} \rho_{n.l}(r)$$

$$= (Z/2\pi^2 r) \int \sum_{n,l} ps_l(qr_n)\, q \sin(qr) dq \qquad (16)$$

finally the relationship[1] between radial functions $F_{n,l}(r)$ [pseudospherical approximation], $P_{n,l}(r)$ [Hartree or Hartree-Fock approximation] and core electron density $\rho_{n,l}(r)$ is expressed as

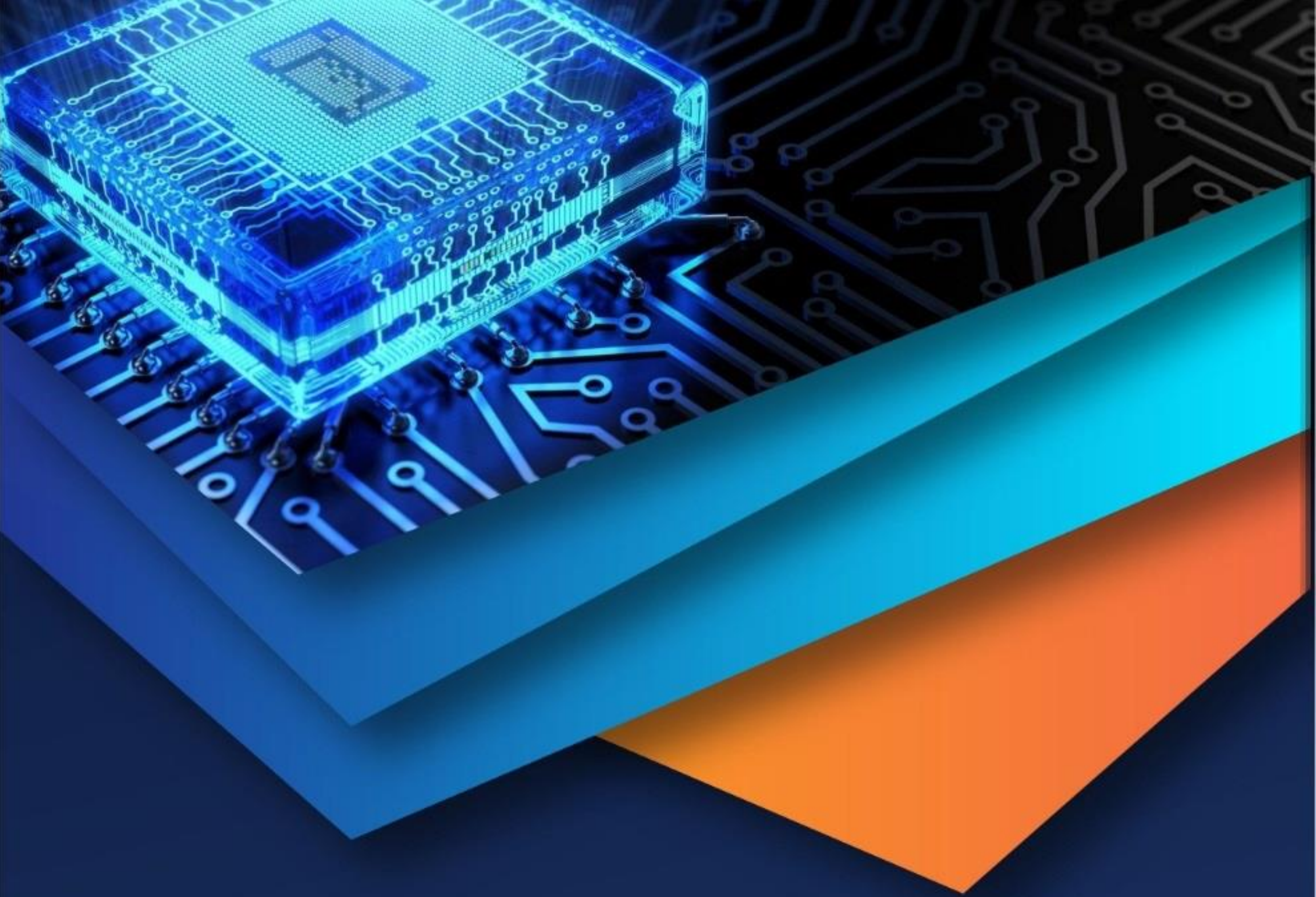
$$\sum_{n,l} 2(2l+1) P^2_{n.l}(r) = \sum_{n,l} \rho_{n.l}(r)\, 4\pi r = \sum_{n,l} c\, q_B{}^2 Z\, r\, F_{n,l}(r) \qquad (17)$$

III. CONCLUSIONS

1) The given relationship is a strong evidence which relates the Pseudo spherical concept and Hartree Fock concept. The present pseudo –wave functional description follows fully the frame work of pseudo-potential theory, which gives orientation to the physical problems of Condensed matter Physics.
2) The wave function $F_{n,l}(r)$ may describe directly the dynamics of pseudo-atom in a simple way as compared to Hartree or Hartree-Fock approaches. $F_{n,l}(r)$ function is also more suitable and open an easy way for finding core electron density $\rho_{n,l}(r)$ of metals.

REFERENCES

[1] B.J.Austin V.Heine and I.J.Sham,Phys. Rev. 127,276 (1962)
[2] W.A.Harrison, Phys.Rev.,131,2433(1963),Pseudopotential Theory of Metals Benjamin.,Inc.,New York,(1966)
[3] D.R. Hartree, The calculations of Atomic structure ,John Wiley and Sons,Inc., Newyork 1957.p.58
[4] G.N.Watson,Theory of Bessel functions,2nd Ed. Macmillan NewYork,1945
[5] W.W.Piper,Phys.Rev.123,12 81(1961)
[6] C.F.Fischer,The Hartree-Fock method for atoms, John Wiley and Sons Inc.Newyork,1957 p.58.
[7] R.W.Shaw and W.A. Harrision,Phys.Rev. **163** ,604 (1967)



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