A study of Fermi hole for some atomic systems

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Abstract

The electron correlation effect for inter-shell can be described by evaluating the Fermi hole $\Delta f(r_{12})$ and partial Fermi hole $\Delta g(r_{12}, r_1)$ for Li atom comparing with Be^+ and B^{2+} ions (Li-Like ions) using the approximation of Hartree-Fock wavefunction. Each plot of the physical properties in this work is normalized to unity. All results are obtained numerically by using computer programs.

WAVEFUNCTION APPROXIMATION

The Hartree-Fock (HF) atomic wavefunctions are independent particle-model approximations to non-relativistic Schrodinger equation for stationary states. The single determinant can be written as the antisymmetrized product of all occupied HF spin-orbital for atoms .

$$\Phi_{HF}(1\,2\,3\ldots N) = A\,\Pi(1\,2\,3\ldots N) \quad \ldots(1)$$

Where A is the antisymmetrized operator given by [1]:

$$A = \frac{1}{\sqrt{N!}} \sum_{P} (-1)^{P}\, P \quad \ldots (2)$$

$(-1)^P$ takes the values +1 and −1 for even and odd permutation, P is any permutation of the electron, and the factor $\frac{1}{\sqrt{N!}}$ introduced to ensure that the wavefunction is normalized.

The product $\Pi(123\ldots N)$ in equation (1) can be defined as[2]:

$$\Pi(1\,2\,3\cdots N) = \phi_1(1)\,\phi_2(2)\,\phi_3(3)\cdots\phi_N(N) \quad \ldots\ldots(3)$$

The Hartree-Fock spin-orbital ϕ are designated by the numerals 1,2,3…N starting with the lowest orbital with spin. Consequently all odd integers for α spin and all even ones for β spin[3,4].

For our purpose the wavefunction can be written as

$$\Phi_{HF}(1\,2\,3\ldots N) = \sum_{i<j}^{N} A_{ij}^{mn} (-1)^{P}\, A\Pi_{ij} \quad \ldots\ldots\ldots(4)$$

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Where the pair function A_{ij}^{mn} can be defined as [2]:

$$A_{ij}^{mn} = \phi_i(m)\phi_j(n) - \phi_j(m)\phi_i(n) \quad \text{.....(5)}$$

And Π_{ij} represents the product of all occupied HF-spin orbital except $\phi_i(m)$ and $\phi_j(n)$. i and j represent spin orbital labels, also m and n referred to electron labels.

Equation (1) can be expressed in the term of Slater determinant as follows[5]:

$$\Phi_{HF}(123\cdots N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(1)\phi_1(2) & \cdots & \cdots & \phi_1(N) \\ \phi_2(1)\phi_2(2) & \cdots & \cdots & \phi_2(N) \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \phi_N(1)\phi_N(2) & \cdots & \cdots & \phi_N(N) \end{vmatrix}$$

...(6)

The HF or analytic self-consistent field atomic wavefunction provided the uncorrelated description of each atom.

For any atom or ion, the Hartree-fock spatial orbital may be written as [6]:

$$\Phi = \sum_{i=1}^{j} c_i \chi_i$$

...(7)

Where c_i represents the constant coefficient yield from the SCF method to minimized the total energy.

And the basis function χ_i is the standard normalized Slater-type orbital (STO's) which given by:

$$\chi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_{\ell m}(\theta,\phi) \quad \text{.....(8)}$$

Where $R_{n\ell}(r)$ represented the radial part of the wavefunction and is given as:

$$R_{n\ell}(r) = N_{n\ell m}S_{n\ell}(r) \quad \text{.....(9)}$$

$N_{n\ell m}$ is The normalization constant and given as:

$$N_{n\ell m} = \frac{(2\zeta)^{n+\frac{1}{2}}}{[(2n)!]^{\frac{1}{2}}}$$

...(10)

and

$$S_{n\ell}(r) = r^{n-1}e^{-(\zeta r)}$$

...(11)

where $S_{n\ell}(r)$ is called Slater type orbital (STO's).

and $Y_{\ell m}(\theta,\phi)$ represented the angular part of the wavefunction.

Fermi hole calculations

In this work we will calculate the Fermi hole $\Delta f(r_{12})$ and the partial Fermi hole $\Delta g(r_{12}, r_1)$ for Li-like ion

The two-density function $\Gamma_{ij}(r_1, r_2)$ for Li-like ions can be expressed for the singlet state inter-shell $KL(^1S)$ after integrated over all spins and angular functions as:

$$\Gamma_{KL(^1S)}(r_1, r_2) = \frac{1}{2}\left[R_{1s}^2(r_1)R_{2s}^2(r_2) + R_{2s}^2(r_1)R_{1s}^2(r_2)\right]$$

...(12)