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Study of the atomic form factor in ion – atom collisions process

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Abstract:-

The function $|F_{lm}(K)|^2/K^3$ has been studied theoretically in the collisions process of 95 MeV/u $Ar^{18+}$with Li atom in ground state 2s and exited states 3s and 4s for emission energies of electrons(10,30,100 eV.). The results show that the function $|F_{lm}(K)|^2/K^3$ has many peaks in different ranges of momentum transfer K but strong peak at $K \to 0$ and reaches to minimum at $K \approx k$ (momentum of emitted electron) for ground state 2s but reaches to minimum at $K < k$ for exited states 3s and 4s. The function $|F_{lm}(K)|^2/K^3$ decreased with increasing of energy of electrons emission. Computer program in Fortran language has been built to solve the numerical formulas in this work.

1.Introduction:-

The atomic form factor $F_{lm}(K)$ as a function to momentum transfer K is an important parameter to be evaluated in the most theoretical studies and in calculation of inelastic collision cross section for electrons emission in charge particles-atom collisions[1]. Scattering or collision of the charge particles and atoms can be classified into two types elastic scattering and inelastic scattering. The internal state of the atoms or the system are not be change in elastic scattering but change in inelastic scattering[2]. Theoretical treatment of inelastic collision of charge particles with atom can be classified into two types those dealing with fast collisions and those dealing with slow ones. The velocity of the incident particle used in this classification is that the particle velocity is fast or slow relative to a mean orbital velocity of atomic electrons in the shell or subshell[3]. When the charge particles is in cident, significant momenta can be transfer in this collision to the atomic electrons as a virtual photons. This momenta or energy change the internal state of atom, as ionized this atom[4,5]. The emission of electrons in the ionization of atoms process by fast ions are emitted from bound state to continuum state along the ion beam direction. This electrons move slowly in the projectile-centered reference system, their behavior is mainly studied by study of their differential cross section[6-8].

To study the differential cross section the electrons emission; must be study the atomic form factor which is a function of the momentum transfer and the velocity of the charge particles. The final state and initial state of emitted electron describes the atomic form factor, Therefore atomic form factor is very important in theoretical treatment in inelastic collisions[9].

This work was carried out to study the atomic form factor in ion-atom collision process has been represented by the function $|F_{lm}(K)|^2 / K^3$. Atomic units ($\hbar = e = m_e = 1$) are used in this work.

2.Theory

In general case the differential cross section for electrons emission with energy E is given by [10]

$$\frac{d\sigma}{dEd\Omega} = 4Z_p^2 M^2 \frac{K_f}{K_i} k \int_{K_{min}}^{K_{max}} \frac{|F_{if}(K)|^2}{K^4} d\Omega_f \qquad ...(1)$$

Where Z_p and M are projectile charge and reduced mass, respectively,

$$\vec{K} = \vec{K}_f - \vec{K}_i \qquad ...(2)$$

is the momentum transfer, so K_f and K_i is the final and initial momentum of projectile, and

$$k = \sqrt{2E} \qquad ...(3)$$

is the momentum of ejected electron, $d\Omega_f$ is solid angle of the scattered projectile, K_{max} and K_{min} is the maximum and minimum momentum transfer and the $F_{if}(K)$ is the atomic form factor ;it is given by

$$F_{if}(K) = \int \psi_f^*(r,\theta,\phi) e^{-i\vec{K}.\vec{r}} \psi_i(r,\theta,\phi) d^3r \qquad ...(4)$$

Where ψ_f and ψ_i are the final and initial wave functions for ejected electrons.

The atomic form factor is useful to expand it over the final angular momentum state; that allow for use of numerical wave functions ψ_f and ψ_i [11,12]. The expansion is given by

$$F_{if}(K) = \sum_{lm} F_{lm}(K) Y_{lm}(\Omega) \qquad ...(5)$$

Where Y_{lm} are the spherical harmonics for the angular momentum l and the magnetic quantum number m of the final state.

By using equation (5) into equation (1) one obtain

$$\frac{d\sigma}{dEd\Omega} = 4Z_p^2 M^2 \frac{K_f}{K_i} k \int_{K_{min}}^{K_{max}} \left| \sum_{lm} \frac{F_{lm}(K)}{K^2} Y_{lm}(K) \right|^2 d\Omega_f \qquad ...(6)$$

So

$$d\Omega_f = \sin\theta_f \, d\theta_f \, d\phi_f \qquad ...(7)$$

The integral over azimuthal angle $d\phi_f$ gives 2π, equation (7) become

$$d\Omega_f = 2\pi \sin\theta_f \, d\theta_f \qquad ...(8)$$

From equation (2), one obtains

$$d\theta_f = \frac{K}{K_i K_f \sin\theta_f} dK \qquad ...(9)$$

By using equation (9) into equation (8), one obtains

$$d\Omega_f = 2\pi \frac{K}{K_i K_f} dK \qquad ...(10)$$

By using equation (10) into equation (6), one obtains

$$\frac{d\sigma}{dEd\Omega} = 8\pi Z_p^2 M^2 \frac{1}{K_i^2} k \int_{K_{min}}^{K_{max}} \sum_{lm} \frac{|F_{lm}(K)|^2}{K^3} |Y_{lm}(K)|^2 dK \qquad ...(11)$$

The function $|F_{lm}(K)|^2 / K^3$ in equation (11) is the key parameter to calculate the differential cross section for electron emission, therefore it is very important to study this function.

3.Atomic form factor calculation

The atomic form factor $F_{lm}(K)$ is given by [10]

$$F_{lm}(K) = \sqrt{4\pi} e^{i\delta_l} Y_{lm}(\Omega_K) f_{E\ln} \qquad ...(12)$$

Where

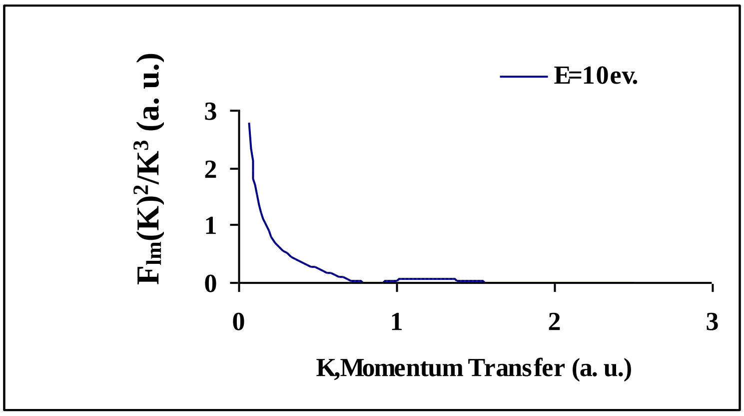
$$f_{Enl} = \int R_{El}(r) j_l(Kr) R_{ns} 9r) r^2 dr \qquad ...(13)$$

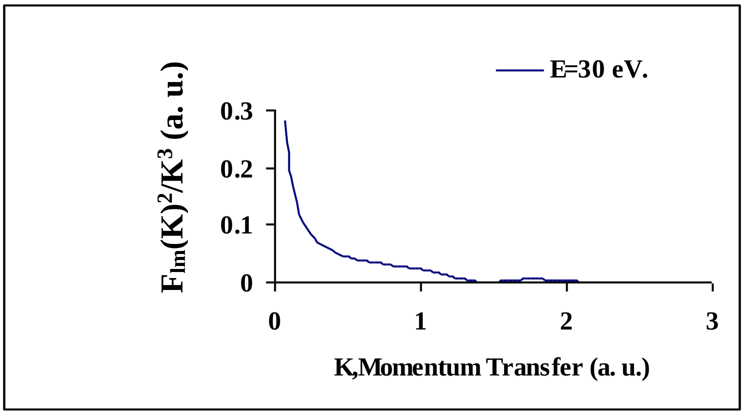
is the redial matrix element which contain a Bessel function $j_l(Kr)$ and the redial wave functions R_{ns} and R_{El} associated with ψ_i and ψ_f, respectively, the solid angle Ω_K specifics the direction of the momentum transfer and δ_l is the phase shift which calculated by partial wave method [13].

4. Result and Discussion :-

Redial wave functions R_{ns} have been estimated by Clementi et al[14] and it is normalize over the position of electron r because the electron is bounded and it is in negative energy . In this study ; redial wave functions R_{ns} represented the redial wave function of electron in 2s-orbital of Li atom. But can not normalize redial wave functions R_{Es} over the position of electron r because the electron is not bounded and it is in positive energy. Redial wave functions R_{Es} represented the redial wave function of emitted electron and this emitted electron transition to continuum spectra (positive energy). The final redial wave function of ejected electron normalize over its energy because of the electron ejected can be in an orbital Es,Ep,Ed,Ef,Eg,etc., final continuum states[12].

The function $|F_{lm}(K)|^2 / K^3$ has been studied for electrons emission from Li atom in ground state (2s) and exited states (3s and 4s) in the collisions process of 95 MeV/u $Ar^{18+}$with Li atom. The function $|F_{lm}(K)|^2 / K^3$ has been calculated for dipole transitions $(l = 1)$after regrouping the diagonal $(l = l')$ and nondiagonal$(l \neq l')$ terms in equation (11). The result illustrated in figure (1) that the function $|F_{lm}(K)|^2 / K^3$ for the ground state 2s of Li for E=10,30 and 100eV has many peaks but strong peak at $K \to 0$ and it is reaches to its minimum value at momentum transfer $K \approx k$ momentum of emitted electron. Also figure (1) shows that the function $|F_{lm}(K)|^2 / K^3$ decreases with increases of energy of emitted electrons. Figure (2) shows the function $|F_{lm}(K)|^2 / K^3$ for the exited state 3s for E=10,30 and 100eV. The results show that the function $|F_{lm}(K)|^2 / K^3$ reaches to its minimum value at momentum transfer $K < k$. Figure (3)shows the function $|F_{lm}(K)|^2 / K^3$ for the exited state 4s for E=10,30 and 100eV.





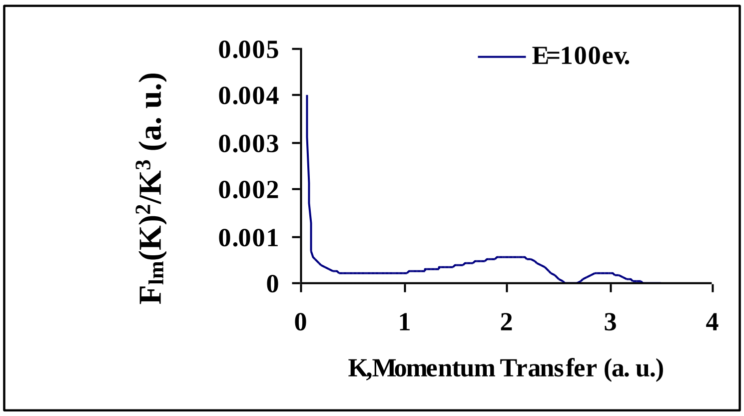


Fig. (1) : The function $|F_{lm}(K)|^2/K^3$ for the ground state 2s for E=10,30 and 100eV

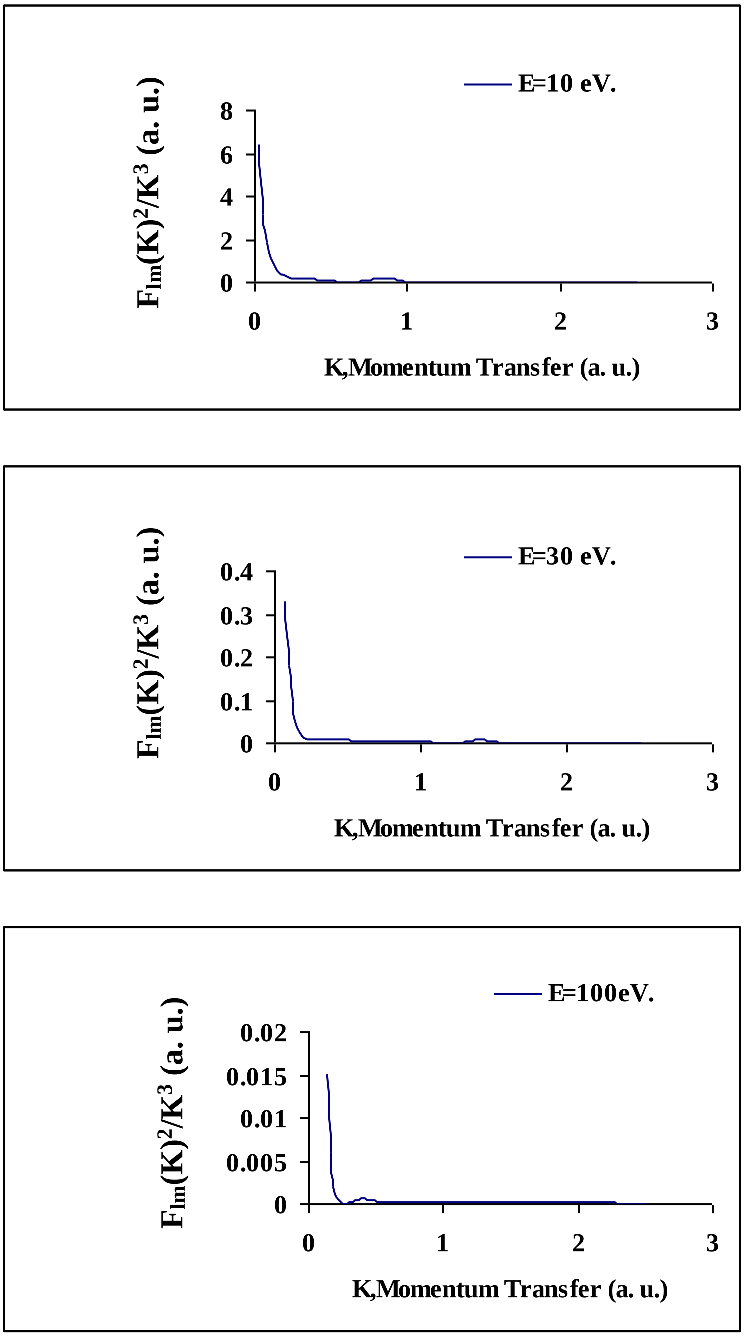


Fig. (2): The function $|F_{lm}(K)|^2/K^3$ for the exited state 3s for E=10,30 and 100eV

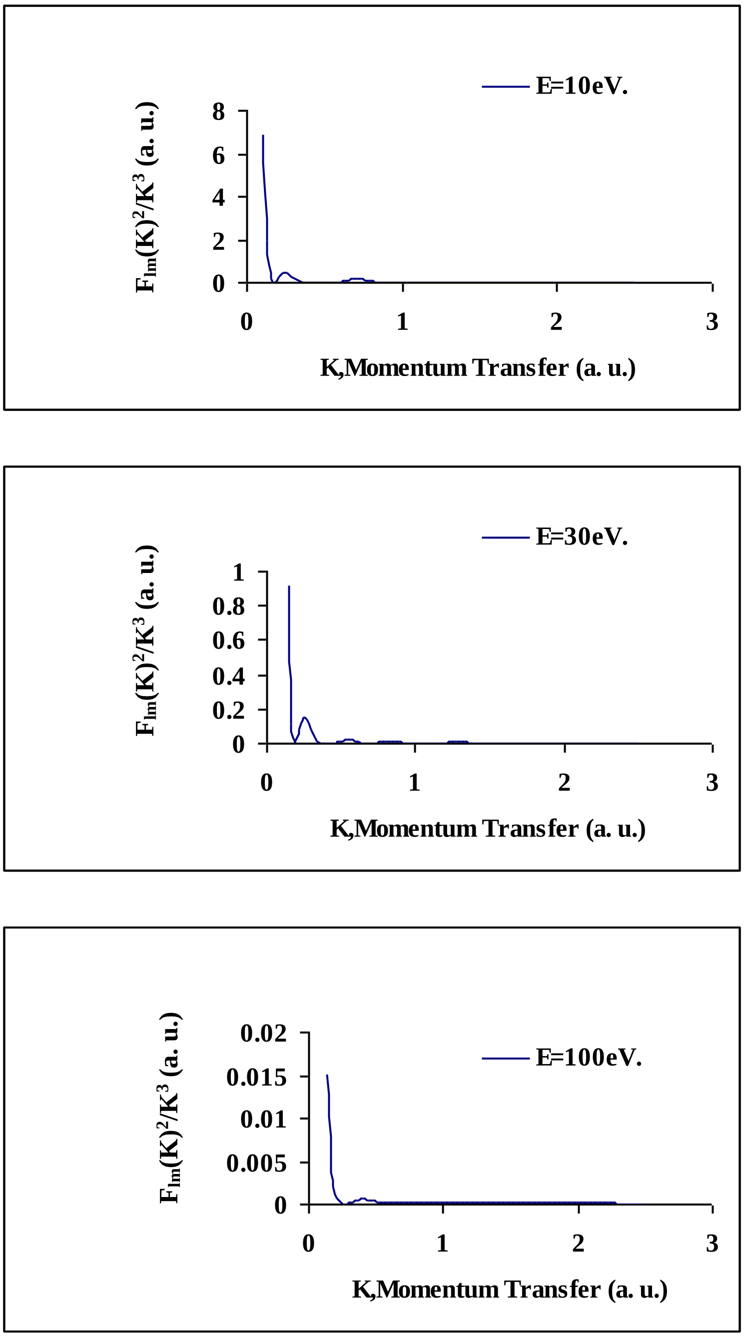


Fig. (2): The function $|F_{lm}(K)|^2/K^3$ for the exited state 4s for E=10,30 and 100eV

5-Conclusions

1- The function $\left|F_{lm}(K)\right|^2/K^3$ has many peaks but strong peak at $K \to 0$ and it reaches to its minimum value at $K \approx k$ (momentum of emitted electron) for ground state 2s.

2- The function $\left|F_{lm}(K)\right|^2/K^3$ reaches to its minimum value at $K < k$ for exited states 3s and 4s.

3- The value of the function $\left|F_{lm}(K)\right|^2/K^3$ decreases with increases of energy of emitted electron.

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دراسة عامل الشكل الذري في عملية تصادم ايون-ذرة

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الخلاصة:-

درســـت الدالة $\left|F_{lm}(K)\right|^2/K^3$ نظريا بعملية تصـــادم ايون الآركون Ar^{18+} وبطاقة 95 MeV/u مع ذرة الليثيوم بالحالة الأرضية 2s والحالتين المثارتين 3s و4s للالكترونات المنبعثة بطـــــــــاقات (10,30, 100 eV.). أظهرت النتائج بان لهذه الدالة $\left|F_{lm}(K)\right|^2/K^3$ عدة قمم للدالة ولكن هناك قمة حادة عند $K \to 0$ وتصل إلى القيمة الدنيا تقريبا عندما يكون الزخم المنتقل K يساوي تقريبا قيمة زخم الإلكترون المنبعث($K \approx k$) من الحالة الأرضــية 2s.ولكن وتصــل إلى القيمة الدنيا تقريبا عندما $K < k$ للحلتين المثارتين 3s و 4s. وان قيمة الدالة $\left|F_{lm}(K)\right|^2/K^3$ تتناقص بزيادة طاقة الإلكترون المنبعث.كتب برنامج في الحاســوب بلغة فورتران لحل الصيغ العددية في البحث.