The Angular Correlation of Positron Annihilation Radiation in Atoms

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Abstract

Positron annihilation techniques provide several ways to probe atomic-scale defects in materials. This is because positrons are trapped by open volume and also by negative charged defects. We study the importance of the non-local electron-positron pair interaction for positron annihilation characteristics in a certain number of atoms. This is accomplished by using Hartree-Fock approximation, giving rise to non-local electron-positron correlation function. We apply this formalism to study the momentum-dependent electron-positron momentum densities (or the *angular correlation)*. Our results of $P(\theta)$ in the present approach is compared to those obtained within a various approximations, where we get a good agreement for (Kr,Xe)-atoms and reasonable for other atoms.

الخلاصة

تستخدم تقنية فناء البوزترونات بعدة طرق من اجل معرفة العيوب في المواد. ان سبب ذلك هو ان البوزترونات ممكن ان تحصر في حجم مفتوح وكذلك بواسطة عيوب سالبة الشحنة. يتم دراسة أهمية تفاعل زوج الالكترون–بوزترون غير الموضعي لحالة فناء البوزترونات في عدد معين من الذرات. لقد تم إنجاز ذلك باستخدام تقريب هارتري–فوك، من استخلاص دالة ترابط غير موضعية لزوج الالكترون–بوزترون. لقد طبقنا هذه الصيغة من اجل دراسة كثافة الالكترون–بوزترون المعتمدة على الزخم أو ما يسمى (بالترابط الزاوي). تمت مقارنة نتائج الترابط الزاوي $(P(\theta))$ مع قيم نظرية مختلفة، وكانت النتائج جيدة لحالة ذرات الكربتون والزنون ومقبولة لذرات أخرى.

1. Introduction

When a positron and an electron annihilate each other resulting in two gamma rays, the $\gamma - rays$ travel in opposite directions in the center of mass frame of reference. This is simply a result of momentum conservation. However, from the frame of reference of the laboratory, the two gamma rays do not usually travel in exactly opposite directions. The difference between the angle of emission of the two photons allows the total momentum of the two photons system to be calculated. From conservation of momentum, the momentum of the annihilating electron can be deduced by measuring the *angular correlation* of the annihilating $\gamma - rays$, the electron momentum distribution (as seen by the positron) may be obtained [Fraser, 1995].

The positron annihilation in atoms so far provides a better mean for the investigations of the dynamic behaviors of annihilating pairs, since the *angular correlation* of two-photons annihilation radiation is related to the linear momentum distribution of them. If positrons are assumed to be thermalized before annihilation, and the annihilation probability is again assumed to be the same for electrons of all different momentum, then the *angular correlation* of two gamma rays will give the momentum distribution of electrons in atoms. The positron lifetime in the material depends on the local electron density at the site of the positron annihilation [Hakala *et al.,* 1998].

While testing with annihilation radiation a circuit selecting the coincident pulses from two annihilation counters, it was relized that the *angular correlation* between the two annihilation photons could may be measured with far greater accuracy. As a result, it was considered that precise measurement of the *angular* *correlation*, which would throw some light on the momentum distribution of the centers of mass of the annihilating pairs, and hence, on their mean momentum, was worth attempting. The measurement of the momentum distribution of annihilating electron-positron pairs is, together with the positron lifetime measurements, the basic method of positron annihilation spectroscopy [Barbiellini *et al.*, 1997].

Various theoretical calculations have been reported for the *angular correlation* of electron-positron pair annihilation [McEachran *et al.*, 1980; Bousahla *et al.*, 2004], using a different approximation methods. While the experimental measurements in that field was very limited and old done by [Brisco *et al.*, 1968], so far as we know.

2. Theory

The Hartree-Fock method [Landau, 1990] is the method we'll depend it in our treatment of the effective potential and the density parameters. This method is an extension to the distribution of low-energy interacting of electrons (positrons) from atoms by Morse & Allis[Temkin, 1959]. One limitation of their wave function, however, is its inability to take account of the reaction of the scattered electron back on the atom; i.e., the method does not seem to include the polarization effects [Temkin, 1959].

We write the wave function for the total system atom plus positron as:

$$\Psi_{\ell m}(r_1, r_2, ..., r_N; r) = \phi_A(r_1, r_2, ..., r_N; r) U_{k\ell m}(r) \quad \text{------------------(1)}$$

Where (ℓ) and *(m)* are the eigenvalues of the total orbital angular momentum and its z-component, and (ϕ_A) is the wavefunction for a certain atom in its ground state. $(U_{k\ell m}(r))$ represent the free positron wavefunction.

Writing

$$U_{k\ell m}(r) = \frac{u_{k\ell}(r)}{r} Y_{\ell m}(\Omega) \quad \text{--------------------------------(2)}$$

Where $Y_{\ell m}(\Omega)$ is the spherical harmonic, and $U_{k\ell m}(r)$ is normalized to correspond asymptotically to a density of one positron per unit volume, i.e.

$$u_{k\ell}(r) \underset{r\to\infty}{\sim} \frac{\sqrt{4\pi(2\ell+1)}}{k} \sin(kr - \frac{\ell\pi}{2} + \delta_\ell) \quad \text{-----------------(3)}$$

One of the interested quantities in the electron-positron interaction is the *angular correlation* of the two gamma rays produced when the pair annihilates. The *angular correlation* as a function of (q_z), the z-component of he linear momentum of the electron-positron pair, is given by [Drachman, 1969]:

$$P(q_z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} S(q) dq_x dq_y \quad \text{-------------------------------(4)}$$

Where

$$S(q) = \sum_{i=1}^{N} \int \left| \int e^{iq.r_i} \Psi_{\ell 0}(r_1, r_2, ..., r_N) \right|^2 d\tau_i^{-1} \quad \text{----------------(5)}$$

Where $(d\tau_i^{-1})$ indicates all variables except those included in $(d\tau_i)$. We are interested in the *angular correlation* for zero-energy positrons and hence only the $(\ell = 0)$ term in equ.(5) contributes.

Substituting equ.(1) in equ.(5) subject to the above remarks yields

$$S(q) = 2\left[\int_0^\infty j_0(qr)P_{1s}(r)u_{ks}(r)dr\right]^2 + \left[\int_0^\infty j_0(qr)P_{2s}(r)u_{ks}(r)dr\right] \times \left[\int_0^\infty j_0(qr)P_{2s}(r)u_{ks}(r)dr\right] \text{--------(6)}$$

Where (P_{1s}) and (P_{2s}) are the radial parts of the Hartree-Fock orbitals of (ϕ_A), and $(j_{\ell=0}(qr))$ is the usual spherical Bessel function. Changing to cylindrical polar coordinates, then equ.(4) will becomes:

$$P(q_z) = 2\pi\int_{q_z}^\infty S(q)qdq \quad \text{--------------------------(7)}$$

In this work we will plot the *angular correlation* (P) as a function of (θ) (the angle between the two gamma rays) where $(\sin\theta \approx \frac{P_z}{mc})$ or $(\theta \approx \frac{\hbar q_z}{mc} \approx \frac{q_z}{137})$ in atomic units. $(P(\theta))$ is normalized to unity at $(\theta = 0)$ so that the normalization of $(u_{k\ell})$ is unimportant.

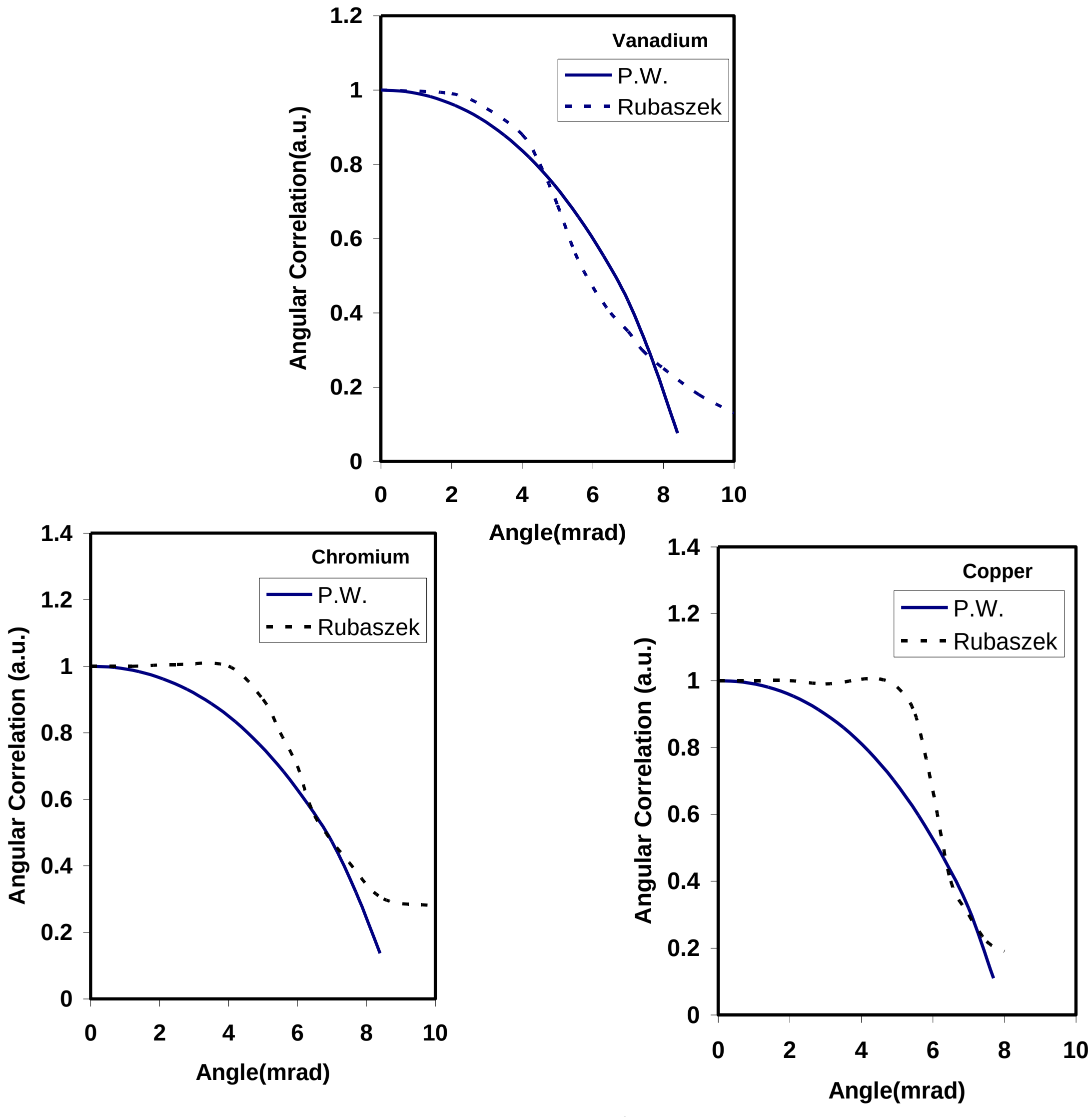
3. Results & Discussion

Since electrons in atoms possess kinetic energy, if an entering positron with certain energy annihilates with an electron in atom, the center of mass of the pair would not in general be at rest at the time of annihilation. The component (P_z) of the center of mass momentum of the annihilation pair perpendicular to the direction of emission of gamma rays deflect the photon propagation direction from their mutually opposite direction by angle (θ).

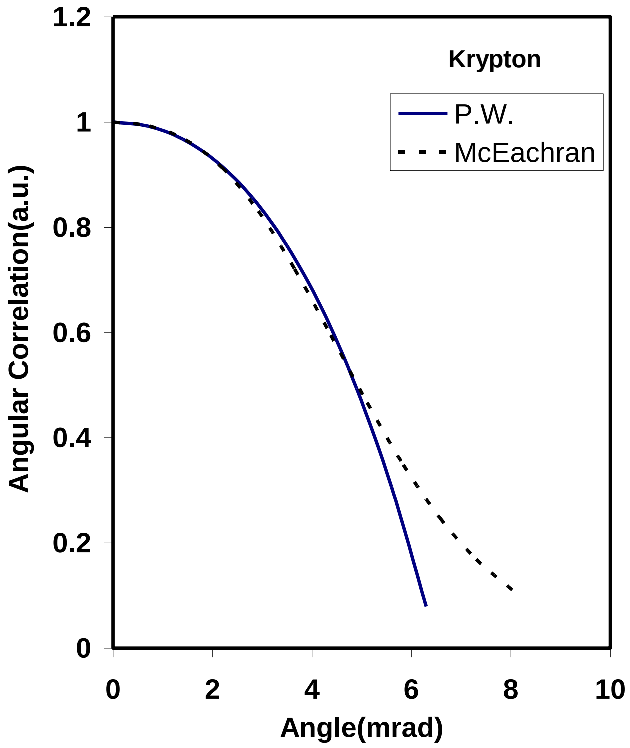
In figure(1) we present our results of the *angular correlation* for (V, Cr & Cu)-atoms compared with theoretical calculations of [Rubaszek et al.,2001; Rubaszek et al.,2002]. In figure(2) our results of $(P(\theta))$ for (Kr & Xe)-atoms compared with the theoretical data of [McEachran et al.,1980]. The agreement between our results and those we compared with, was good for (Kr & Xe)-atoms, and reasonable for (V, Cr & Cu)-atoms. Furthermore, the figures shows that the agreement between our calculations and the experiment and theory is very good at small values of (θ) but there are systematic deviation at large values of (θ).

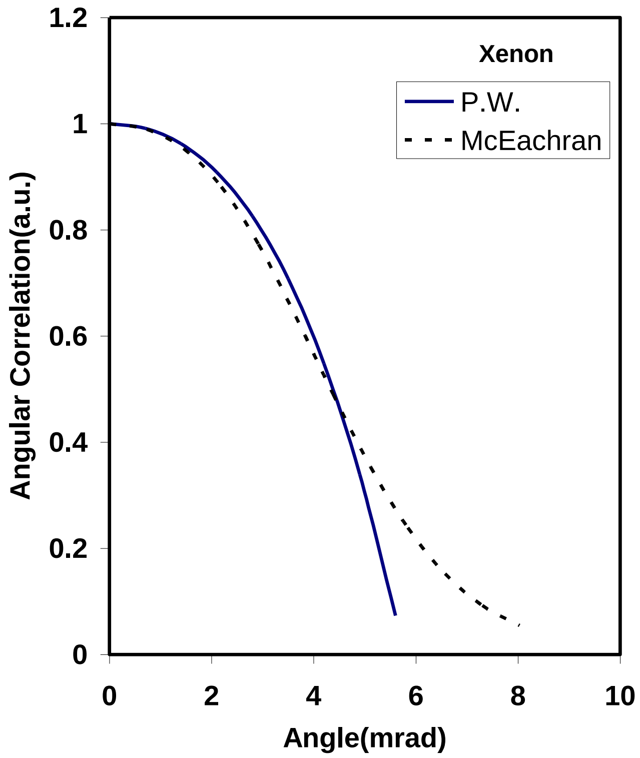
The shape of our curves in figures (1) & (2) have a similar behavior for all atoms, i.e. quite smooth and rising very steeply as zero angle is approached. Furthermore, we noticed that $(P(\theta))$ depends much more critically on the actual form of the total wave function and hence is likely to be more affected by the approximation made. In this work we concentrate on a various groups of atoms represented by two of the noble atoms and metals like (V, Cr & Cu)-atoms. Where the value of $(P(\theta))$ for (V, Cr & Cu) need for a fitting process to made a some approximation with the compared data.

The Hartree-Fock approximation proved their success in getting a good results of the angular correlation from calculating the density functions for the systems under study. As we noticed the agreement was fine for the comparison with the other approximations theories, such as the polarized orbital method of [McEachran *et al.* 1980] and the local density approximation of [Rubaszek *et al.*, 2001 ; Rubaszek *et al.*, 2002].



Figure(1): The Angular Correlation for (V, Cr, & Cu)-Atoms the solid curve represent the present work, the dashed curve represent the [Rubaszek et.al.,2001; Rubaszek et.al.,2002]data.





Figure(2): The Angular Correlation for (Kr,Xe)-Atoms the solid curve represent the present work, the dashed curve represent the [McEachran et.al.,1980]data.

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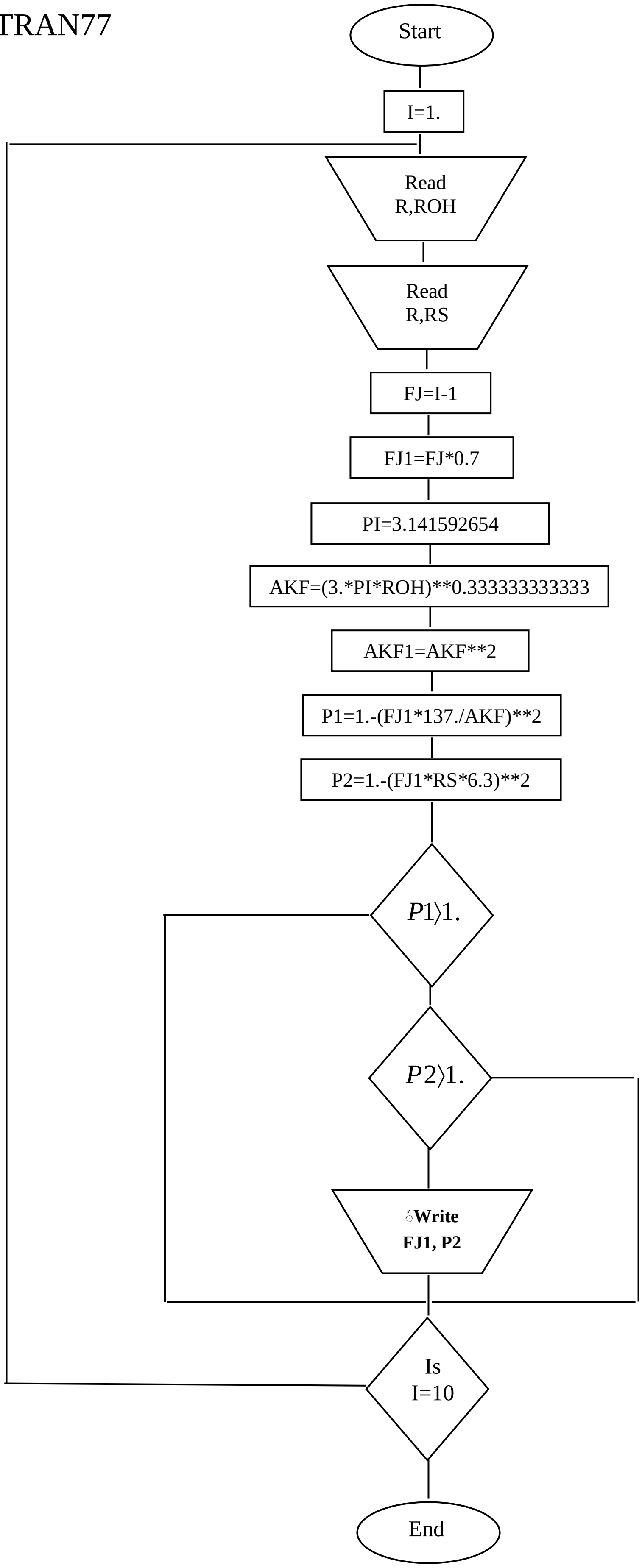
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Read
R,RS
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FJ1=FJ*0.7
PI=3.141592654
AKF=(3.*PI*ROH)**0.333333333333
AKF1=AKF**2
P1=1.-(FJ1*137./AKF)**2
P2=1.-(FJ1*RS*6.3)**2
P1⟩1.
P2⟩1.
Write
FJ1, P2
Is
I=10
End