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Collinear Angular Correlation of Gamma Rays from Positron Annihilation in Magnetically Quenched Ionic Crystals

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The general formula for collinear angular correlation of y-rays, which originate from positron annihilation, is derived,and its applicability in analyzing F-centers, in magnetically quenched ionic crystals, is demonstrated.

Deriva-se a expressão geral para a correlação angular, colinear, de raios gama, que da aniquilação de positrons se originam. Mostra-se , outrossim, sua aplicabilidade à análise, de centros-F, em cristais iônicos magneticamente "enfraquecidos".

1. INTRODUCTION

The positrons have long been used as probes in studying the electronic structure of solids[1,2]. As the positron comes off the source (usually ones uses Na^{22} as the source), then, because of its high energy, it reaches the interior of the sample, whose electronic state is being studied. Furthermore, due to the strong coupling of the charge particle with the optical band phonons, especially in the case of ionic crystals, the positron is quickly thermalized inside the sample. The time for its thermalization is much shorter than life-time for annihilation which is of the order of 10^{-10} sec. The reason, for the positron life-time to have such an order of magnitude, is found in the two

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following facts. (i) Non formation of positronium because of the lack of Ore gap for the positron in ionic crystals. (ii) The thermalized positron wave function is concentrated about the negative ion, with its maximum at about the radius of the ion.

Once the positron arrives at the vicinity of negative ions, its small thermal energy can be neglected, and the process of annihilation can be assumed to take place from the ground state, of the positron - electron system, plus the crystals. The direct measurable quantities, for this annihilation process, are the positron-electron annihilation rate and the angular correlation of the y-rays. The measurement of the annihilation rate $\Gamma_{2\gamma}$ or $\Gamma_{3\gamma}$ provides information about the electron density at the point where the positron is being annihilated, while the measurement of the angular correlation of the y-rays gives information on the electron states of the negative ions. Recently, a series of investigations have been carried out for the cases of positron annihilation in magnetically quenched ionic crystals[3,4]. It was found that the magnetic quenching of the positron decay, in alkalei halides, exhibits a second spectral component which is presumably caused by a positronium-like system. As for the measurement of the angular correlation of two y-rays, a significant raise in the collinear amplitude was found when the colored ionic crystal was placed in a magnetic field of the order of 10^4 gauss[5].

In this paper, we shall only discuss the two y-rays angular correlation, and provide a general formulation of the collinear angular correlation amplitude of positron annihilation in magnetic quenched ionic crystals. An analytical expression for $N(\theta=0)$ is derived in the next two Sections. The application to the specific case will be found in the last Section.

2. GENERAL DERIVATION OF THE ANGULAR CORRELATION FUNCTION

In this Section, we consider the angular correlation of two y-rays from positron annihilation, in the state of lowest crystal momentum, with the halide electron represented by the Bloch wave function over the entire crystal lattice. As explained in the Introduction, the positron lingers around for a while, at the vicinity of the halide ion, before being annihilated, and its wave function is represented by $1/\sqrt{N}$ times the normalized wave function $\phi_{e+}(\vec{r})$ of a positron bound to the halide ion. N denotes the total number of halide ions in the crystal. The electron Bloch wave function with crystal momentum $\hbar\vec{K}$ is given by $(1/\sqrt{N})\ e^{i\vec{K}.\vec{r}}\ \psi_{e^-}(\vec{r})$. The total momentum, $\hbar\vec{k}$, sarried off by the annihilating γ-rays, is equal to the momentum of the e^+e^- system. Hence, the probability amplitude of having the two γ-rays with total momentum $\hbar\vec{k}$, denoted by $f(\vec{k})$, is the Fourier transform of the product of positron and electron wave functions, i.e.,

$$f(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int e^{-i\vec{k}.\vec{r}} \sum \frac{1}{N} e^{i\vec{K}.\vec{r}}\ \psi_{e^-}(\vec{r})\ \phi_{e^+}(\vec{r})\ d^3r$$

$$= \sum_n \frac{1}{(2\pi)^{3/2}} \frac{1}{N} \int e^{-i\vec{k}.\vec{r}'} \psi_{e^-}(\vec{r}')\ \phi_{e^+}(\vec{r}')\ e^{-i(\vec{k}-\vec{K}).\vec{r}_n}\ d^3r', \tag{1}$$

The 2nd. expression, for $f(\vec{k})$, is obtained by shifting the origin of the integration coordinates to the n–th halide ion in the crystal. The probability $|f(\vec{k})|^2$ is then given by

$$|f(\vec{k})|^2 = \sum_{n,m,K} \frac{1}{(2\pi)^3} \frac{1}{N^2} e^{-i(\vec{k}-\vec{K})\cdot(\vec{r}_n-\vec{r}_m)} \left| \int e^{-i\vec{k}.\vec{r}} \phi_{e^+}(\vec{r}) \psi_{e^-}(\vec{r}) d^3r \right|^2 . \tag{2}$$

Since the sum over the entire reciprocal space, $\vec{K}$, in Eq. (2), gives

$$\sum_{n,m} e^{-i\vec{K}.(\vec{r}_n-\vec{r}_m)} = N\ \delta_{nm}\ , \tag{3}$$

that equation reduces to

$$|f(\vec{k})|^2 = \frac{1}{(2\pi)^3} \left| \int e^{-i\vec{k}.\vec{r}} \phi_{e^+}(\vec{r}) \psi_{e^-}(\vec{r}) d^3r \right|^2 . \tag{4}$$

The wave functions involved in the above equation are only those of the system of the positron-electron pair. Therefore the result can be used for any system of the positron-electron pairs in annihilation. As an example, positron annihilation in a colored ionic crystal, in which the trapped electron, at the color center plays the role of the halide electron of a pure ionic crystal, will be discussed in detail later on.

The angular correlation $N(\theta)$ is obtained from the above equation by an integration over the whole space of k_x and k_y, i.e.,

$$N(\theta) = N(k_z/mc) = \int |f(\vec{k})|^2 \; dk_x dk_y \; . \tag{5}$$

This conection stems from the fact that in the measurement of the momentum distribution of the photons, a long slit of the photon detector is moving along a part of a circular track the sample being located at the center of the circle, and the long slit perpendicular to the circle. Therefore, the distribution, with respect to only one cartesian component, is experimentally available.

3. COLLINEAR ANGULAR CORRELATION

We shall derive, in this Section, a general analytical expression for the collinear angular correlation in the case of positron annihilation in magnetically quenched ionic crystals. The result will be equally applicable in analyzing positron annihilation with color centers, as explained in the previous Section. Let us, now, consider the case that the magnetic field is applied to the sample crystal with the field in the z-direction. The electron wave function, can, then, be cast into the following form:

$$\psi_{e^-}(\vec{r}) = \chi_e(\xi,\eta) e^{im\phi} \quad , \tag{6}$$

where ξ, η and ϕ are parabolic coordinates, and m takes only integral values.

As for the positron, in a magnetic field of the order of 10 k gauss, the thermal energy of the positron can be neglected compared with the eigenenergy, of the charged particle, in a magnetic field of the above mentioned strength. Furthermore, the positrons, in the " Swiss cheese model"[6] for a ionic crystal, are mostly degenerated in the lowest cyclotron orbit, and the wave function of the positron depends only upon the variables 5 and η, namely, $\phi_{e^+}(\vec{r}) = \phi_{e^+}(\xi,\eta)$. The function $f(\vec{k})$, when expressed in parabolic coordinates, becomes

$$f(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int e^{-i\vec{k}.\vec{r}(\xi,\eta,\phi)} \phi_{e^+}(\xi,\eta)\chi_{e^-}(\xi,\eta) e^{im\phi} \frac{\xi+\eta}{4} \, d\xi d\eta d\phi \ . \tag{7}$$

For the purpose of arriving at the collinear angular correlation, we restrict our attention to the dependence of the f function on the transverse momentum, $\vec{k}_t$. From Eq.7, we have

$$f(\vec{k}_t,0) = \frac{1}{(2\pi)^{3/2}} \int e^{-ik_t\sqrt{\xi\eta}\cos\phi} \phi_{e^+}\chi_{e^-} e^{im\phi} \frac{\xi+\eta}{4} d\xi d\eta d\phi \ . \tag{8}$$

By means of an integral representation of Bessel functions, namely,

$$J_m(x) = \frac{1}{2\pi(i)^m} \int e^{i(x\cos\phi - m\phi)} \, d\phi, \tag{9}$$

$f(\vec{k}_t,0)$ takes the following expression:

$$f(\vec{k}_t,0) = \frac{i^m}{(2\pi)^{1/2}} \int J_m(k_t\sqrt{\xi\eta}) \ \phi_{e^+}\chi_{e^-} \frac{\xi+\eta}{4} \, d\xi d\eta \ . \tag{10}$$

Integrating over the transverse components of $\vec{k}_t$ and taking $k_P=0$, the collinear angular correlation can be easily found, with the help of Eq.10, to be

$$N(0)=\frac{1}{2\pi}\int J_m(k_t\sqrt{\xi\eta})J_m(k_t\sqrt{\xi'\eta'})\phi_{e^+}(\xi,\eta)\phi^*_{e^+}(\xi',\eta')\chi_{e^-}(\xi,\eta)\chi^*_{e^-}(\xi',\eta')\,.$$

$$\cdot\ \frac{\xi+\eta}{4}\,\frac{\xi'+\eta'}{4}\,d\xi d\xi' d\eta d\eta' d^2k_t \quad . \tag{11}$$

To simplify the above expression one makes the following substitutions:

$$u = \sqrt{\xi\eta} \quad , \tag{12a}$$

$$v = \frac{1}{2}(\xi-\eta), \tag{12b}$$

and perform the $\vec{k}_t$ integration in polar coordinates:

$$N(0) = \int J_m(k_t u)\ J_m(k_t u')\phi_{e^+}(u,v)\phi^*_{e^+}(u',v')\,.$$

$$\cdot\chi_{e^-}(u,v)\chi^*_{e^-}(u',v')udu\ u'du'dv\ dv'\ k_t dk_t \tag{13}$$

Using the identity,

$$\int_0^\infty kJ_m(kx)J_m(kx')dk = \frac{1}{x}\,\delta(x-x'), \tag{14}$$

one can put Eq,(12), in mure compact form, as follows:

$$N(0)=\int\phi_{e^+}(u,v)\phi^*_{e^+}(u,v')\chi_{e^-}(u,v)\chi^*_{e^-}(u,v')dvdv'udu\ . \tag{15}$$

4. APPLICATION TO F-CENTERS IN IONIC CRISTALS

This Section is devoted to the discussion of F-centers in the ionic crystals. Some analyses have been done for the case of color centers in alkali halides[7,8,9]. Among the two model potentials recently proposed in the theoretical study of positron annihilation from F-centers, the hydrogenic model potential seems in better agreement with experiment[9]. Therefore, we shall discuss the collinear angular correlation for this particular model, in which the wave function is a familiar one. Suppose that a positron, at the lowest cyclotron level, annihilates with the ground-state electron which is trapped in the F-center. Then, $N(0)$ in Eq. (15) takes the following expression:

$$N(0) = \frac{1}{\pi^2}\int \left(\frac{eH}{\hbar c}\right)\exp\left(-\frac{eH}{2\hbar c}u^2\right).\exp\left[-\frac{1}{\beta}(u^2+v^2)^{1/2}\right]\cdot$$

$$\cdot\exp\left[-\frac{1}{\beta}(u^2+v'^2)\right]du\,dv\,dv' , \qquad (16)$$

where $\beta(=\hbar^2\sqrt{8\Delta E}/\sqrt{3}\,m)$ is the radius of the ground state electron orbit, at the color center, and ΔE is taken from the maximum of the F-band. The above integation, in Eq. (16), can be simplified by letting $v=u\zeta$ and $v'=u\zeta'$, and performing the u-integration by using the saddle-point approximation. After some analytic details, one obtains

$$N(0) \simeq C\, e^{-\varepsilon}\, \varepsilon/\sqrt{1+\varepsilon} \quad . \qquad (17)$$

Here, C is a constant (independent of the external field H), and the parameter ε stands for $eH\beta^2/2\hbar C$. The two γ-rays, collinear angular correlation, in the hydrogenic model potential of the F-center, increases monotonically as $\varepsilon<1$; namely; when the radius of the positron orbit is smaller than that of the electron, and it falls of as $\varepsilon>1$. The dependence of the collinear angular correlation, on the external magnetic field will provide another criterion for the preference in selecting the model potential. For instance, the Krumhansl - Schwartz Potential can also be analyzed in a similar manner by resorting to numerical computations, which, however, is beyond the scope of the present paper.

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