Angular correlation theory for double photoionization in a rare-gas atom

Dipankar Chattarji and Chiranjib Sur
Department of Physics, Visva Bharati, Santiniketan 731 235, India
(Received 21 May 2001; published 11 December 2001)

We consider the process of double photoionization (DPI) in a rare-gas atom as a two-step process, namely, (i) photoionization in an inner shell followed by (ii) the emission of an Auger electron from an outer shell. An angular correlation function for the two emitted electrons is defined by analogy with the theory of angular correlation in nuclear physics. An expression is obtained for this angular correlation function by a statistical method that makes use of the density and efficiency operators. The latter takes care of the attenuation of the probability of detection of an electron due to the geometrical properties of the detector. Theoretical values of the angular correlation function are obtained for DPI in xenon and these are shown to be in good agreement with the experimental results given by Kämmerling and Schmidt [J. Phys. B **26**, 1141 (1993)].

DOI: 10.1103/PhysRevA.65.012702 PACS number(s): 32.80.Hd, 32.80.Fb, 03.65.Ta, 79.20.Fv

I. INTRODUCTION

The theory of angular correlation was originally formulated in nuclear physics. This was done for two possible kinds of phyical situations.

(i) Angular correlation of successive nuclear radiations emitted by a radioactive nuclear species, e.g., a γ-γ cascade.

(ii) Angular correlation of the successive nuclear radiations resulting from the more general case of a nuclear scattering process.

The earliest paper on this subject was written by Hamilton [1] for the case of a γ-γ cascade. Later on, Gardner [2] wrote down the angular correlation function using the wave functions of the states occurring in a cascade decay. Racah [3] obtained, thereafter, a simple expression for the angular correlation function in terms of the angle between the directions of emission of the two successive radiations emitted by a nucleus. He did not worry about the history of this nucleus, and his theory held regardless of whether the emitted radiations consisted of bosons or fermions. Subsequently, Biedenharn and Rose [4] extended Racah's work to give a general form of the angular correlation function for the successive nuclear radiations. About the same time, Coester and Jauch [5] gave a theory in the more general context of nuclear reactions. Their paper gives a derivation of the angular correlation function that brings out the statistical nature of the problem. Later, Devons and Goldfarb [6] wrote a detailed review of angular correlations up to that point.

In our problem, a rare-gas atom absorbs a photon having specified properties, i.e., energy, spin etc. As a result, the atom emits a photoelectron giving rise to a singly charged ion. This ion now deexcites by emitting an Auger electron. This yields a doubly charged residual ion. Note two basic features of this problem.

(i) The initial atomic state is randomly oriented (an improper state).

(ii) Only limited information is available about the emitted electrons, usually their directions of motion.

The density matrix or statistical matrix ρ was introduced into quantum mechanics to provide for the discussion of just such a situation [7,8]. It forms an important ingredient of the nuclear theory of angular correlations. It will naturally figure in our atomic theory of angular correlations as well.

In Sec. II we shall try to construct an angular correlation function for the atomic problem outlined above. This is done in Sec. II A using a statistical approach. In Sec. III we report our calculation for the xenon atom that was experimentally studied by Schmidt and his co-workers [9].

II. AN ANGULAR CORRELATION THEORY FOR ATOMS: THE DOUBLE-PHOTOIONIZATION PROBLEM

Double photoionization (DPI) occurs when an atomic target consisting of rare-gas atoms is irradiated with photons from an advanced light source, e.g., a synchrotron, and an atom emits two electrons in quick succession. In the case where the time interval between the emission of these two electrons is very small, one could think of DPI as a one-step process. A considerable amount of work has already been done on this [10,11]. However, in the case where the time interval between the successive emission of the two electrons is substantially longer than the time taken by the photoelectron to leave the interaction zone, DPI may be regarded as a two-step process [12]. This in its turn will depend on the energy imparted to the atomic system by the incident photon.

We shall now try to construct a theory for the two-step process described above, keeping in view the earlier work done in nuclear physics. Since this is a two-step process mediated by electromagnetic interaction at two vertices, we expect it to be a second-order process as compared to normal photoionization (PI). Hence the probability of its occurrence will be much lower than that of PI, and its detection will call for a much greater precision.

Consider a randomly oriented rare-gas atom in a $^1S^e$ state. It absorbs a photon and after a certain time interval emits a photoelectron from an inner shell, giving a single-vacancy ionic state. This intermediate ionic state now deexcites by emitting an Auger electron, typically from an outer shell, giving rise to a two-vacancy final state [12]. So our process amounts to

$$h\nu + \mathbf{A} \rightarrow \mathbf{A}^+ + e_1^- \rightarrow \mathbf{A}^{2+} + e_1^- + e_2^- . \qquad (1)$$

The initial state of our system is characterized by the set of quantum numbers $(J_a M_a \alpha_a)$, or by virtual quantum num-

bers $(J'_aM'_a\alpha'_a)$ arising from a possible interaction with other atoms and electrons. Here (J_aM_a) or $(J'_aM'_a)$ are angular momentum quantum numbers, and α_a,α'_a denote the set of remaining quantum numbers characterizing the system.

We wish to obtain an angular correlation function for the two emitted electrons in terms of the angle θ between their directions of emission.

The method of efficiency and density operators

We now approach the problem of angular correlation from a statistical standpoint. We note that there is a certain probability for the atom to attain the final state given above. This is described by the appropriate matrix element of the density or statistical operator ρ as defined in the literature [7,13]. Now, even if the atom goes over to the final state, because of the finite size of our detecting equipment and other limiting factors, this event may or may not be detected. There is thus a certain probability $\epsilon(0\leqslant\epsilon\leqslant 1)$ that the event will be detected. This probability is represented by the efficiency operator ε that will depend on the size, position, and geometrical arrangement of the detecting equipment.

Now, how does the angular correlation function relate to the operators ρ and ε? We shall try to answer this question in the following manner. We start out by defining

$$\bar{\varepsilon}=\sum_Q \varepsilon_Q\langle Q|\rho|Q\rangle=\sum_Q \varepsilon_Q\rho_{QQ}=\mathrm{Tr}(\varepsilon\rho). \tag{2}$$

Here ε_Q is the efficiency or probability of detection of the state described by quantum numbers Q, and ρ_{QQ} the probability of the system being in the particular state Q.

From the elements of statistical mechanics, we know that $\bar{\varepsilon}$ is the expectation value (or average value) of the efficiency operator ε [13]. We shall presently see that the angular correlation function is simply related to $\bar{\varepsilon}$.

Since $\bar{\varepsilon}$ is the trace of a matrix it is invariant under a unitary transformation in Hilbert space.

We now ask the question: what are the transformation properties of the matrices ε and ρ as we go from one unitary representation to another? It is easily seen that ε and ρ are tensor operators. Hence they are also called the efficiency and density (or statistical) tensors, respectively [5]. The fact that ε and ρ are both tensor operators makes them amenable to further analysis.

Since the initial atomic system is randomly oriented, we have that the rotational symmetry and angular momentum is conserved. Hence our state vectors are eigenvectors of J^2 and J_z. In such a case the matrix elements of a tensor operator have a simple geometric dependence on the magnetic quantum numbers. This is given by the Wigner-Eckart theorem.

Using this theorem we write the matrix element of the density operator as

$$\langle J_aM_a\alpha_a|\rho|J'_aM'_a\alpha'_a\rangle=\sum_{k_a\kappa_a}(-1)^{J'_a-M'_a}C^{J_aJ'_ak_a}_{M_aM'_a\kappa_a}\rho_{k_a\kappa_a}(J_a\alpha_a,J'_a\alpha'_a). \tag{3}$$

In Eq. (3) $C^{J_aJ'_ak_a}_{M_aM'_a\kappa_a}$ is a Clebsch-Gordan coefficient satisfying the triangle rule $k_a=J_a+J'_a$ and κ_a is the projection of k_a. Similarly, the matrix element of the efficiency operator is given by

$$\langle J_aM_a\alpha_a|\varepsilon|J'_aM'_a\alpha'_a\rangle=\sum_{k_a\kappa_a}(-1)^{J'_a-M'_a}C^{J_aJ'_ak_a}_{M_aM'_a\kappa_a}\varepsilon_{k_a\kappa_a}(J_a\alpha_a,J'_a\alpha'_a). \tag{4}$$

Using the unitarity property of Clebsch-Gordan coefficients, we get the density tensor of rank k_a with $(2k_a+1)$ components

$$\rho_{k_a\kappa_a}(J_a\alpha_a,J'_a\alpha'_a)=\sum_{M_aM'_a}(-1)^{M_a-M'_a}C^{J_aJ'_ak_a}_{M_aM'_a\kappa_a}\langle J_aM_a\alpha_a|\rho|J'_aM'_a\alpha'_a\rangle. \tag{5}$$

A similar expression can be obtained for the components of the efficiency tensor.

So the expectation value of ε becomes

$$\bar{\varepsilon}=\mathrm{Tr}(\varepsilon\rho)=\sum_{J_aJ'_a\alpha_a\alpha'_ak_a\kappa_a}\rho_{k_a\kappa_a}(J_a\alpha_a,J'_a\alpha'_a)\varepsilon^{\star}_{k_a\kappa_a}(J_a\alpha_a,J'_a\alpha'_a). \tag{6}$$

Our choice of phase [14] ensures that $\rho_{k_a\kappa_a}$ is a Hermitian tensor. It satisfies the relation

$$\rho^{\star}_{k_a\kappa_a}(J_a\alpha_a,J'_a\alpha'_a)=(-1)^{J'_a-J_a+\kappa_a}\rho_{k_a-\kappa_a}(J'_a\alpha'_a,J_a\alpha_a). \tag{7}$$

Some simplification yields the result

$$\rho_{k_a\kappa_a}(J_a\alpha_a,J'_a\alpha'_a)=\frac{\delta_{k_a0}\delta_{\kappa_a0}\delta_{J_aJ'_a}}{\sqrt{2J_a+1}}\langle J_c\|j_2\|J_b\rangle\times\langle J_c\|j'_2\|J_b\rangle^{\star}\langle J_b\|j_1\|J_a\rangle\langle J_b\|j'_1\|J_a\rangle^{\star}. \tag{8}$$

Here the symbol $\langle\|\|\rangle$ stands for a reduced matrix element.

The first decay, namely the photoionization process, is characterized by the relation

$$J_a=J_b+j_1. \tag{9}$$

Since the detection of the photoelectron and that of the singly charged ion are independent events, the joint probability of their detection is given by the product of the individual probabilities. Hence we can write

$$\langle J_a M_a \alpha_a|\varepsilon|J'_a M'_a \alpha'_a\rangle = \sum \langle J_b M_b \alpha_b|\varepsilon|J'_b M'_b \alpha'_b\rangle \times\langle j_1 \mu_1|\varepsilon|j'_1 \mu'_1\rangle \times C^{\star J_b j_1 J_a}_{M_b \mu_1 M_a} C^{J_b j'_1 J'_a}_{M'_b \mu'_1 M'_a}. \quad (10)$$

Here $(J_b M_b)$, $(J'_b M'_b)$ describe the intermediate state and α_b, α'_b denote the remaining quantum numbers. The summation in Eq. (10) extends over $M_b M'_b \mu_1 \mu'_1$.

Then

$$\varepsilon_{k_a \kappa_a}(J_a \alpha_a, J'_a \alpha'_a) = \sum_{k_1 \kappa_1 k_b \kappa_b} \varepsilon_{k_b \kappa_b}(J_b \alpha_b, J'_b \alpha'_b)\varepsilon_{k_1 \kappa_1}(j_1 j'_1) \times C^{\star k_b k_1 k_a}_{\kappa_b \kappa_1 \kappa_a} \sqrt{2J_a+1}\sqrt{2J'_a+1}\sqrt{2k_b+1} \times \sqrt{2k_1+1} \begin{Bmatrix} J_b & j_1 & J_a \\ J'_b & j'_1 & J'_a \\ k_b & k_1 & k_a \end{Bmatrix}, \quad (11)$$

with the relations

$$J_a = J_b + j_1, k_a = J_a + J'_a, k_b = J_b + J'_b$$

and

$$k_1 = j_1 + j'_1.$$

Since the intermediate singly ionized state decays into a residual doubly ionized atom and an Auger electron, we can factorize the efficiency operator of the singly ionized atom in terms of the efficiency operators of the residual doubly ionized atom and the Auger electron.

Since the residual doubly ionized atom is left in a sharp eigenstate with the quantum number J_c and no further measurement is made on it, we get the efficiency operator

$$\varepsilon_{k_c \kappa_c}(J_c \alpha_c, J'_c \alpha'_c) = \sqrt{2J_c+1}\,\delta_{k_c 0}\delta_{\kappa_c 0}\delta_{J_c J'_c}\delta_{\alpha_c \alpha'_c}. \quad (12)$$

A matrix element of the efficiency operator for each electron has the form

$$\varepsilon_{k_i \kappa_i}(j_i j'_i) = \sum_{\mu_i \mu'_i} (-1)^{j_i - j'_i} C^{j_i j'_i k_i}_{\mu_i - \mu'_i \kappa_i} \langle j_i \mu_i|\varepsilon|j'_i \mu'_i\rangle = \sum_{\mu_i \mu'_i \sigma_i \sigma'_i} (-1)^{j'_i - \mu'_i} C^{j_i j'_i k_i}_{\mu_i - \mu'_i \kappa_i} \langle j_i \mu_i|\Omega_i \sigma_i\rangle \times\langle \sigma_i|\varepsilon|\sigma'_i\rangle\langle \Omega_i \sigma'_i|j'_i \mu'_i\rangle, \quad (13)$$

with $i=1,2$. $i=1$ denotes the photoelectron and $i=2$ the Auger electron. Using the axis of the detector as the quantization axis for each detected electron, we get

$$\langle \Omega_i \sigma_i|j_i \mu_i\rangle = \sum_{\kappa_i} \langle 0\sigma_i|j_i \kappa_i\rangle D^{j_i \star}_{\mu_i \kappa_i}(\Re_i), \quad (14)$$

$D(\Re_i)$ is the corresponding rotation matrix for the ith electron.

Then Eq. (13) becomes

$$\varepsilon_{k_i \kappa_i}(j_i j'_i) = \sum_{\kappa'_i} c_{k_i \kappa'_i}(j_i j'_i) D^{k_i \star}_{\kappa_i \kappa'_i}(\Re_i), \quad (15)$$

where $c_{k_i \kappa'_i}(j_i j'_i)$ is the attenuation factor corresponding to the change in the state of polarization and is given by

$$c_{k_i \kappa_i}(j_i j'_i) = \Im \sum_{\mu_i \mu'_i} (-1)^{j'_i - \mu'_i} \langle 0\sigma_i|j_i \mu_i\rangle^\star \times\langle 0\sigma'_i|j'_i \mu'_i\rangle C^{j_i j'_i k_i}_{\mu_i - \mu'_i \kappa_i} \langle \sigma_i|\varepsilon|\sigma'_i\rangle. \quad (16)$$

The symbol $\Im$ represents a summation over the spin of the emitted electrons and depends on the characteristics of the detector. We now take the summation $\Im f(\sigma\sigma')$ to be equivalent to $\Sigma\langle\sigma|\varepsilon|\sigma'\rangle f(\sigma\sigma')$.

Making use of properties of Clebsch-Gordan coefficients and 9-j symbols, and also using the additivity of rotation matrices [14]

$$\sum_\nu D^k_{\nu \kappa_1}(\Re_1) D^{k\star}_{\nu \kappa_2}(\Re_2) = \sum_\nu D^k_{\nu \kappa_1}(\Re_1) D^k_{\kappa_2 \nu}(\Re_2^{-1}) = D^k_{\kappa_2 \kappa_1}(\Re_2^{-1}\Re_1), \quad (17)$$

we get

$$\overline{\varepsilon} = (2J_b+1)(-1)^{J_a + J_c - 2J_b} \times \sum (-1)^{k - j_1 - j_2} w(J_b J'_b j_1 j'_1, k J_a) \times w(J_b J'_b j_2 j'_2, k J_c) c_{k\kappa_1}(j'_1 j_1) c^\star_{k\kappa_2}(j_2 j'_2) D^k_{\kappa_1 \kappa_2}(\theta_1 \theta_2 \theta_3) \times\langle J_c\|j_2\|J_b\rangle\langle J_c\|j'_2\|J_b\rangle^\star\langle J_b\|j_1\|J_a\rangle\langle J_b\|j'_1\|J_a\rangle^\star. \quad (18)$$

In Eq. (18) the summation is over $j_1, j'_1, j_2, j'_2, k, \kappa_1$, and κ_2.

If the electrons are unpolarized, or if the detectors are insensitive to polarization, $\kappa_1 = \kappa_2 = 0$ and $D^k_{00}(\theta_1 \theta_2 \theta_3) = P_k(\cos\theta_2)$. We now identify the angle θ_2 with θ, the angle between the directions of emission of the photo-electron and the Auger electron. From the Hermitian character of the efficiency and density matrices, it follows that

$$c_{k\kappa}(jj') = (-1)^\kappa c^\star_{k\kappa}(j'j). \quad (19)$$

For our case $\kappa_1 = \kappa_2 = 0$, and

$$c_{k0}(jj') = \frac{\sqrt{2j+1}\sqrt{2j'+1}}{4\pi}(-1)^{j-(1/2)+k} C^{jj'k}_{(1/2)-(1/2)0}. \quad (20)$$

We can thus write

$$\overline{\varepsilon}=(-1)^{J_a+J_c-2J_b}\sqrt{2J_b+1}$$
$$\times\sum_k\,(-1)^{k-j_1-j_2}w(J_bJ_b'j_1j_1',kJ_a)w(J_bJ_b'j_2j_2',kJ_c)$$
$$\times\langle J_c\|j_2\|J_b\rangle\langle J_c\|j_2'\|J_b\rangle^\star\times\langle J_b\|j_1\|J_a\rangle$$
$$\times\langle J_b\|j_1'\|J_a\rangle^\star c_{k0}(j_1j_1')c_{k0}^\star(j_2j_2')P_k(\cos\theta). \tag{21}$$

Here k is an even integer ranging from zero to k_{max}, k_{max} being defined as follows. Let $\{\{j_1+j_1'\}_{max},\{j_2+j_2'\}_{max}\}_{min}=p$. Then $k_{max}=p$ if p is even and $k_{max}=p-1$ if p is odd. We now express $\langle J_c\|j_2\|J_b\rangle$ in terms of $\langle J_b\|j_2\|J_c\rangle$. Though the reduced matrix elements are neither real nor Hermitian, it happens that

$$\sqrt{2J_b+1}\langle J_a\|j\|J_b\rangle=(-1)^{J_a-j+J_b}\sqrt{2J_a+1}\langle J_b\|j\|J_a\rangle^\star. \tag{22}$$

This gives

$$\overline{\varepsilon}=\sum_k\,(-1)^{j_1+j_2}c_{k0}(j_1j_1')c_{k0}^\star(j_2j_2')\langle J_c\|j_2\|J_b\rangle$$
$$\times\langle J_c\|j_2'\|J_b\rangle^\star\langle J_b\|j_1\|J_a\rangle\langle J_b\|j_1'\|J_a\rangle^\star$$
$$\times w(J_bJ_b'j_1j_1',kJ_a)w(J_bJ_b'j_2j_2',kJ_c)P_k(\cos\theta). \tag{23}$$

If the finite size of the detector is taken into account, the efficiency of detection described by the matrix element of the efficiency operator must be changed slightly. Then we have to introduce z_k as the attenuation factor due to the finite size of the detector. We assume the detector to be axially symmetric [15,16]. The efficiency tensor described by Eq. (15) is now written as

$$\varepsilon_{k_i\kappa_i}(j_ij_i')=\sum_{\kappa_i'}\,z_{k_i}c_{k_i\kappa_i'}(j_ij_i')D^{k_i\star}_{\kappa_i\kappa_i'}(\Re_i). \tag{24}$$

So the expectation value in our case becomes

$$\overline{\varepsilon}=\sum_k\,z_k(1)_kz_k(2)(-1)^{j_1+j_2}c_{k0}(j_1j_1')c_{k0}^\star(j_2j_2')$$
$$\times\langle J_c\|j_2\|J_b\rangle\langle J_c\|j_2'\|J_b\rangle^\star\langle J_b\|j_1\|J_a\rangle\langle J_b\|j_1'\|J_a\rangle^\star$$
$$\times w(J_bJ_b'j_1j_1',kJ_a)w(J_bJ_b'j_2j_2',kJ_c)P_k(\cos\theta). \tag{25}$$

Note that the θ dependence of $\overline{\varepsilon}$ is contained in the function

$$W(\theta)=\sum_k\,z_k(1)_kz_k(2)(-1)^{j_1+j_2}c_{k0}(j_1j_1')c_{k0}^\star(j_2j_2')$$
$$\times w(J_bJ_b'j_1j_1',kJ_a)w(J_bJ_b'j_2j_2',kJ_c)P_k(\cos\theta). \tag{26}$$

We now define $W(\theta)$ to be the angular correlation function for the two emitted electrons where θ is the angular separation between their directions of emission [17]. It is clear that angular correlation between the directions of emission of the photoelectron and the Auger electron is a direct manifestation of the efficiency of the observing equipment. In Sec. III we shall see that the angular correlation function so defined agrees closely with the measured angular correlation in the DPI experiments on xenon [9]. This confirms that the observing equipment does play a role, introducing an element of probability that finds expression in the angular correlation function.

This definition will have to be modified if it is possible for the photoelectron to be emitted into more than one angular momentum channels. In Sec. III we shall see how this modification can be made.

Note that Eq. (26) holds formally not only for double photoionization in atoms, but also for two-step angular correlation experiments involving either fermions or bosons.

III. CALCULATION AND RESULTS

We consider the problem of DPI in xenon. The neutral xenon atoms are irradiated with a photon beam of energy 94.5 eV. This leads to photoionization in the $4d_{5/2}$ shell followed by an N_5-$O_{2,3}O_{2,3}\,^1S_0$ Auger decay. Using the dipole approximation the possible photoionization channels are $e4d_{5/2}\rightarrow\epsilon_pf_{7/2}$, $f4d_{5/2}\rightarrow\epsilon_pf_{5/2}$ and $g4d_{5/2}\rightarrow\epsilon_pp_{3/2}$, respectively. The Auger transition is characterized by only one partial wave $\epsilon_Ad_{5/2}$ [18]. These transitions are governed by the corresponding selection rules for photoionization and Auger transitions.

Since the initial photoionization process is not characterized by a single angular momentum quantum number but by angular momentum quantum numbers corresponding to three possible channels, the angular correlation function described in Sec. II A above will be modified. The total intensity will, however, remain unchanged. If the photoionization channels are described by the total angular momentum quantum numbers j_1^e, j_1^f and j_1^g and the Auger electron by j_2, then the expectation value of the efficiency operator becomes

$$\overline{\varepsilon(\theta)}=\overline{\varepsilon_e(\theta)}+\overline{\varepsilon_f(\theta)}+\overline{\varepsilon_g(\theta)}+\overline{\varepsilon_{ef}(\theta)}+\overline{\varepsilon_{fg}(\theta)}+\overline{\varepsilon_{ge}(\theta)}. \tag{27}$$

Here

$$\overline{\varepsilon_e(\theta)}=\sum_k\,z_k(1)z_k(2)(-1)^{j_1^e+j_2}c_{k0}(j_1^ej_1^e)c_{k0}^\star(j_2j_2)$$
$$\times|\langle J_c\|j_2\|J_b\rangle|^2|\langle J_a\|j_1^e\|J_b\rangle|^2$$
$$\times w(J_bJ_bj_1^ej_1^e,kJ_a)w(J_bJ_bj_2j_2,kJ_c)P_k(\cos\theta). \tag{28}$$

The expectation values $\overline{\varepsilon_f(\theta)}$ and $\overline{\varepsilon_g(\theta)}$ have the same form with $j_1^e\rightarrow j_1^f$ and $j_1^e\rightarrow j_1^g$ respectively. The quantity $\overline{\varepsilon_{ij}(\theta)}$ is an interference term arising from interaction between photoionization channels i and j $(i,j=e,f,g$ with $i\neq j)$.

$$\overline{\varepsilon_{ef}(\theta)}=\sum_k z_k(1)z_k(2)(-1)^{j_2}|\langle J_c\|j_2\|J_b\rangle|^2 \times\langle J_a\|j_1^e\|J_b\rangle\langle J_a\|j_1^f\|J_b\rangle \times[(-1)^{j_1^e}c_{k0}(j_1^e j_1^f)+(-1)^{j_1^f}c_{k0}(j_1^f j_1^e)]c_{k0}^{\star}(j_2 j_2) \times w(J_b J_b j_1^e j_1^f,kJ_a)w(J_b J_b j_2 j_2,kJ_c)P_k(\cos\theta), \tag{29}$$

$$\overline{\varepsilon_{fg}(\theta)}=\sum_k z_k(1)z_k(2)(-)^{j_2}|\langle J_c\|j_2\|J_b\rangle|^2 \times\langle J_a\|j_1^f\|J_b\rangle\langle J_a\|j_1^g\|J_b\rangle \times[(-1)^{j_1^f}c_{k0}(j_1^f j_1^g)+(-1)^{j_1^g}c_{k0}(j_1^g j_1^f)]c_{k0}^{\star}(j_2 j_2) \times w(J_b J_b j_1^g j_1^f,kJ_a)w(J_b J_b j_2 j_2,kJ_c)P_k(\cos\theta) \tag{30}$$

and

$$\overline{\varepsilon_{ge}(\theta)}=\sum_k z_k(1)z_k(2)(-1)^{j_2}|\langle J_c\|j_2\|J_b\rangle|^2 \times\langle J_a\|j_1^g\|J_b\rangle\langle J_a\|j_1^e\|J_b\rangle \times[(-1)^{j_1^e}c_{k0}(j_1^e j_1^g)+(-1)^{j_1^g}c_{k0}(j_1^g j_1^e)]c_{k0}^{\star}(j_2 j_2) \times w(J_b J_b j_1^e j_1^g,kJ_a)w(J_b J_b j_2 j_2,kJ_c)P_k(\cos\theta). \tag{31}$$

In $\overline{\varepsilon_e(\theta)}$, $\overline{\varepsilon_f(\theta)}$, and $\overline{\varepsilon_g(\theta)}$ k is the smallest even integer of the sets $\{2j_1^e,2j_2,2J_b\}$, $\{2j_1^f,2j_2,2J_b\}$ and $\{2j_1^g,2j_2,2J_b\}$ respectively. In $\varepsilon_{ef}(\theta)$, $\varepsilon_{fg}(\theta)$ and $\varepsilon_{ge}(\theta)$ k is the smallest even integer ($k\neq 0$) of the sets $\{j_1^e+j_1^f,2j_2,2J_b\}$, $\{j_1^f+j_1^g,2j_2,2J_b\}$, and $\{j_1^e+j_1^g,2j_2,2J_b\}$ respectively. We can now write

$$\overline{\varepsilon(\theta)}=|\langle J_c\|j_2\|J_b\rangle|^2[\omega_e(\theta)+\delta_1^2\omega_f(\theta)+\delta_2^2\omega_g(\theta) +\delta_1\omega_{ef}(\theta)+\delta_2\omega_{fg}(\theta)+\delta_1\delta_2\omega_{ge}(\theta)], \tag{32}$$

where

$$\delta_1=\frac{\langle J_a\|j_1^f\|J_b\rangle}{\langle J_a\|j_1^e\|J_b\rangle} \quad\text{and}\quad \delta_2=\frac{\langle J_a\|j_1^g\|J_b\rangle}{\langle J_a\|j_1^e\|J_b\rangle}. \tag{33}$$

Here

$$\omega_e(\theta)=\sum_k z_k(1)z_k(2)(-1)^{j_1^e+j_2}c_{k0}(j_1^e j_1^e)c_{k0}^{\star}(j_2 j_2) \times w(J_b J_b j_1^e j_1^e,kJ_a)w(J_b J_b j_2 j_2,kJ_c)P_k(\cos\theta), \tag{34}$$

$\omega_f(\theta)$ and $\omega_g(\theta)$ have the same form with $j_1^e\rightarrow j_1^f$ and $j_1^e\rightarrow j_1^g$ respectively. And

$$\omega_{ef}(\theta)=\sum z_k(1)z_k(2)(-1)^{j_2}[(-1)^{j_1^e}c_{k0}(j_1^e j_1^f) +(-1)^{j_1^f}c_{k0}(j_1^f j_1^e)]c_{k0}^{\star}(j_2 j_2) \times w(J_b J_b j_1^e j_1^f,kJ_a)w(J_b J_b j_2 j_2,kJ_c)P_k(\cos\theta), \tag{35}$$

$$\omega_{fg}(\theta)=\sum_k z_k(1)z_k(2)(-1)^{j_2}[(-1)^{j_1^f}c_{k0}(j_1^f j_1^g) +(-1)^{j_1^g}c_{k0}(j_1^g j_1^f)]c_{k0}^{\star}(j_2 j_2) \times w(J_b J_b j_1^g j_1^f,kJ_a)w(J_b J_b j_2 j_2,kJ_c)P_k(\cos\theta) \tag{36}$$

and

$$\omega_{ge}(\theta)=\sum_k z_k(1)z_k(2)(-1)^{j_2}[(-1)^{j_1^e}c_{k0}(j_1^e j_1^g) +(-1)^{j_1^g}c_{k0}(j_1^g j_1^e)]c_{k0}^{\star}(j_2 j_2) \times w(J_b J_b j_1^e j_1^g,kJ_a)w(J_b J_b j_2 j_2,kJ_c)P_k(\cos\theta). \tag{37}$$

The parameters δ_1 and δ_2 can be determined uniquely by comparison with the experiment [6]. Writing out the expression (32) in terms of Legendre polynomials, we get

$$\overline{\varepsilon(\theta)}=\aleph[a_0+a_2P_2(\cos\theta)+a_4P_4(\cos\theta)]. \tag{38}$$

Here

$$\aleph=|\langle J_c\|j_2\|J_b\rangle|^2|\langle J_a\|j_1^e\|J_b\rangle|^2,$$

and the coefficients are $a_0=z_0(1)z_0(2)(1+\delta_1^2+\delta_2^2)$, $a_2=z_2(1)z_2(2)(1.0204+0.751\delta_1^2+0.8\delta_2^2+0.269\delta_2+0.311\delta_1+0.733\delta_1\delta_2)$, and $a_4=z_4(1)z_4(2)(0.5510-0.122\delta_1^2)$. This gives

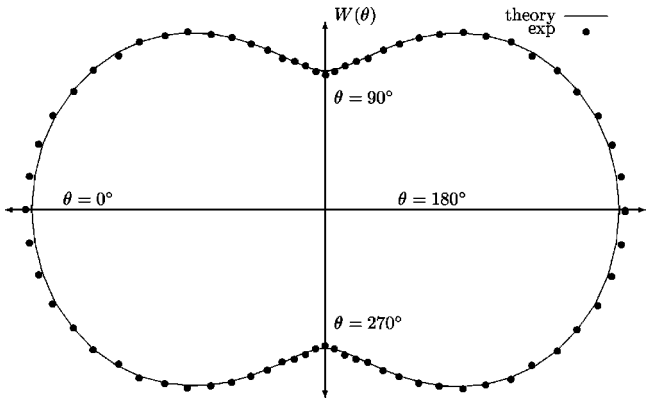

FIG. 1. A polar plot of our angular correlation function for DPI in Xenon is compared with the experimental polar plot given by Kämmerling and Schmidt [9].

$$\bar{\varepsilon} = \aleph'[1 + b_2 P_2(\cos\theta) + b_4 P_4(\cos\theta)], \tag{39}$$

where $b_2 = a_2/a_0 = 0.760$, $b_4 = a_4/a_0 = 0.042$, and $\aleph' = \aleph a_0 = |\langle J_c \| j_2 \| J_b \rangle|^2 |\langle J_a \| j_1^e \| J_b \rangle|^2 a_0$. We now define the angular correlation function for this case of channel mixing by writing

$$W(\theta) = [1 + b_2 P_2(\cos\theta) + b_4 P_4(\cos\theta)]. \tag{40}$$

Figure 1 gives the results of the comparison between our theoretical values and the experimental values [9]. It will be seen that our polar plot of $W(\theta)$ agrees quite closely with that given by Kämmerling and Schmidt [9] except for a small difference in the region around $\theta = 0°$ and $\theta = 180°$.

By using scattering theory with the appropriate boundary conditions, it is possible to obtain δ_1 and δ_2 without recourse to the experimental curves. This in its turn should give not only a_0, but also b_2 and b_4. This is the way our theory can be used to predict the value of the angular correlation function at any required angle. This would make our theory autonomous. In the absence of multichannel interaction, $\delta_1 = \delta_2 = 0$, Eq. (40) reduces to Eq. (26).

The expectation value $\bar{\varepsilon}$ turns out to be the product of a normalization factor depending on the reduced matrix elements and an angular factor. The simplicity of the latter is very striking. It seems as if the dynamical calculation involving the radial matrix elements is redundant. Of course this is not true, because to extract dynamical properties of the system, such as, triply differential cross sections we have to play with the normalizing factor. However, the very simplicity of the result hinges on the factorization of the problem into a dynamical part and an geometrical part depending on θ. This comes from the use of Wigner-Eckart theorem, which is a consequence of the fact that we are dealing with the matrix elements of tensor operators.

ACKNOWLEDGMENTS

One of the authors (D.C.) is deeply grateful to Professor Volker Schmidt for introducing him to the subject of double photoionization. C.S. would like to acknowledge the support provided by the University Grants Commission of India.

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