Compton scattering beyond the impulse approximation

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We treat the nonrelativistic Compton scattering process in which an incoming photon scatters from an *N*-electron many-body state to yield an outgoing photon and a recoil electron, without invoking the commonly used frameworks of either the impulse approximation (IA) or the independent particle model (IPM). An expression for the associated triple differential scattering cross section is obtained in terms of Dyson orbitals, which give the overlap amplitudes between the *N*-electron initial state and the $(N-1)$ electron singly ionized quantum states of the target. We show how in the high-energy transfer regime, one can recover from our general formalism the standard IA based formula for the cross section which involves the ground-state electron momentum density of the initial state. Our formalism will permit the analysis and interpretation of electronic transitions in correlated electron systems via inelastic x-ray scattering spectroscopy beyond the constraints of the IA and the IPM.

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I. INTRODUCTION

Compton scattering is unique among spectroscopic techniques in that it allows direct experimental access to the ground-state electron momentum density (EMD) $\rho(\mathbf{p})$ of the target many-body system.[1,2] Recent high-resolution Compton scattering studies using synchrotron light sources have revealed interesting electron correlation effects in a number of materials.[3–12] The experimental work has been concentrated largely on the measurement of the double differential scattering cross section (for detecting energy transfer and solid angle of the outgoing photon), which yields the so-called Compton profile (CP) related to the two-dimensional (2D) integral of the EMD,

$$J(p_z)=\int\int \rho(\mathbf{p})dp_x dp_y, \tag{1}$$

or equivalently a one-dimensional projection of the EMD along the direction of the scattering vector p_z of the incident photon.

Form (1) which is used in much of the existing analysis of CP's is obtained within the framework of the impulse approximation (IA).[13,14] The fundamental scattering process considered in the IA is the scattering of a photon from a collection of free electrons. The IA is expected to be valid when the energy transferred in the scattering process is much larger than the binding energy of the electronic states involved. By its very nature, Eq. (1) lacks a systematic way of taking account of deviations from the IA.

With this motivation, our purpose in this paper is to consider the general scattering event in which the incoming photon is scattered from a bound many-electron system. We evaluate the resulting partial triple differential scattering cross section rigorously in terms of the so-called Dyson orbitals, which involve overlap of the *N*-body initial state wave function with the $(N-1)$ body wave function of the singly ionized final state with an ejected electron. The physically relevant triple differential scattering cross section is then obtained by summing over final (ionic) states and the steps necessary to recover the IA are clarified. By going beyond the IA, our study provides a systematic scheme for understanding electronic structure and correlation effects via inelastic x-ray scattering (IXS), away from the deeply inelastic regime.

In this connection, it is important to recognize that the standard Compton scattering experiment does not involve the measurement of the kinematics of the outgoing (recoil) electron. This is the reason for the appearance of the 2D integral and the concomitant loss of information about $\rho(\mathbf{p})$ in Eq. (1). As was pointed out first by Kaplan and Yudin[15] on the basis of their theoretical studies[16] of Compton scattering on bound electrons of light atoms and molecules, the full three-dimensional (3D) EMD can be determined if the characteristics of the scattered photon and the ejected electron are measured in coincidence. The authors[15,16] have also shown that, if the ejected electrons are selected by energy, the EMD associated with individual electronic states can in principle be obtained. We note that the EMD can also be probed directly via $(e,2e)$ experiments in which an incident electron of well-defined energy is scattered from the target and the kinematics of both the scattered and the recoil electron are measured.[17–20]

Although coincidence experiments were undertaken quite early,[21,22] results for 3D EMD were first reported by Bell and collaborators;[23–28] see also related work of Itoh and collaborators.[29,30] Since the cross section for an incident photon to scatter into an outgoing electron and a photon is measured, such a measurement is often referred to as a $(\gamma,e\gamma)$ experiment. From a formal viewpoint, the $(\gamma,e\gamma)$ experiment provides a measurement of the triple differential scattering cross section, for which we present in this paper a rigorous many-body expression .

For interpreting experimental CP's using the IA based formula (1), actual computations in the literature largely employ the independent particle model (IPM). The many-electron wave function underlying the IPM is built from Slater determinants of single-electron orbitals obtained usually via unrestricted Hartree-Fock approach or various versions of the

density-functional theory (DFT). With a growing interest in applying IXS for investigating electronic transitions in highly correlated systems using synchrotron light sources, we should keep in mind that one will need to take account of deviations not only from the IA but also from the IPM. Even in the relatively simple case of Li, substantial deviations in the EMD predicted by the local-density approximation have been implicated in explaining the observed discrepancies between the computed and measured CP's.[31]

Concerning other relevant literature related to the issue of going beyond the IA, several studies have considered the accuracy of the IA in describing core Compton profiles,[32–39] including work on hydrogenic orbitals,[32–36] and studies within the Hartree-Fock[38] as well as the DFT framework.[39] A general method for introducing final-state-interaction effects has been discussed by Sears[40] in the context of deep-inelastic neutron scattering. This work also discusses the Björken-scaling and *y*-scaling properties of the IA which have been particularly useful in particle physics. Recently, high-resolution valence CP's of Li at a relatively low photon energy of 8-9 KeV were considered in Refs. 41 and 42. The observed asymmetries in shape and smearing of the Fermi surface features in the CP's were attributed to the breakdown of the IA. It is further shown that these discrepancies in Li can be understood in terms of a finite width of the final state spectral function.[43] To our knowledge, all previous work concerning the breakdown of the IA has been dedicated to understanding the double differential scattering cross section. The present study focuses on the elementary $(\gamma, e\gamma)$ scattering process and provides a clearer picture of the many-body effects and their connection with the IA and the IPM.

An outline of this paper is as follows. These introductory remarks are followed in Sec. II A with a rigorous treatment of the partial triple differential scattering cross section in terms of Dyson orbitals. Section II B addresses the question of summing over final states to obtain the total triple differential cross section and how it reduces to the IA result proportional to the EMD. Section III makes a few concluding remarks.

II. GENERAL EXPRESSIONS FOR TRIPLE DIFFERENTIAL SCATTERING CROSS SECTION

A. Partial triple differential cross section

We consider the nonrelativistic elementary scattering process in which the incoming photon of energy ω_1 (here and throughout this paper, natural units, $\hbar = c = 1$, are assumed implicitly) and momentum $\mathbf{k}_1$ scatters from the *N*-electron many-body ground state of the solid (or molecule) with energy $E_0(N)$. The final state consists of an outgoing photon with energy ω_2 and momentum $\mathbf{k}_2$; the $(N-1)$ electron ionized state of the solid (or molecule) characterized by quantum number *n* and energy $E_n(N-1)$; a recoil electron carrying kinetic energy $E_e^{(n)}$ and momentum $\mathbf{p}_n$. We assume that the momentum transferred to the ionic system is $\mathbf{q}$ and the associated kinetic energy is neglected given the large mass of the target. The scattering process is illustrated schematically in Fig. 1(a). The total momentum $\mathbf{k}$ transferred through the scattering of the photon is

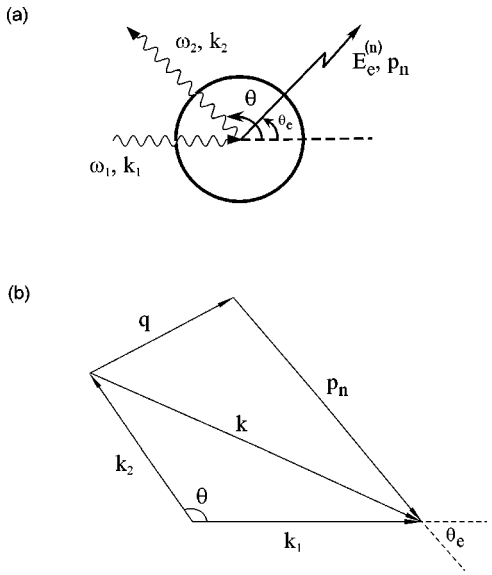

FIG. 1. (a) Schematic diagram of the elementary scattering event involved in the Compton scattering process. The incoming photon scatters from the target to produce an outgoing photon and an electron and leaves the singly ionized target (not shown) in a definite quantum state denoted by index *n*. The notation for kinematic variables is obvious. (b) Momentum conservation in the process of (a), where $\mathbf{q}$ is the momentum transferred to the ionized target.

$$\mathbf{k} = \mathbf{k}_1 - \mathbf{k}_2 = \mathbf{q} + \mathbf{p}_n , \tag{2}$$

where the second equality gives the momentum-conservation condition, which is shown also in Fig. 1(b).[44]

Care is needed in formulating the energy-conservation condition. In the standard treatment of the Compton scattering process, one assumes independent electrons with various one-particle energies. However, the preceding discussion makes it clear that the general interacting system is more naturally characterized via the quantum number *n* of the ionized target. Therefore the relevant binding energy $E_b^{(n)}$ is

$$E_b^{(n)} = E_n(N-1) - E_0(N) \tag{3}$$

in terms of the ground-state energy of the *N*-particle system and that of the $(N-1)$ particle ionized target. In the one-particle approximation, $E_b^{(n)}$ will correspond to the energy of the orbital from which the outgoing electron is ejected. The energy conservation then yields

$$\omega_1 - \omega_2 = E_b^{(n)} + E_e^{(n)} . \tag{4}$$

In addition to energy and momentum, the total spin is also conserved in the scattering process. If the target is initially in a $S=0$ state, then the final state will also be a singlet.

As shown in Ref. 14, in the high-energy transfer region, where $\omega_1 - \omega_2 \gg E_b^{(n)}$, the interaction between the electromagnetic field and the target can be approximated by[45]

$$V_{int} = \frac{e^2}{2mc^2}\mathbf{A}^2, \tag{5}$$

where **A** is the vector potential of the field. Using this form of the interaction, the expression for the double-differential Compton scattering cross section in the IA was obtained in Ref. 14. The IA corresponds in effect to modeling the scattering process as an elastic collision between a photon and an electron of a particular momentum with the target being represented by a distribution of such independent electronic states.

More relevant for our purposes is the treatment of Refs. 15 and 16. These authors obtain the cross section for the elementary Compton scattering process (in which the ion is left behind in a specific quantum state) from a many-body molecular system in the nonrelativistic $\mathbf{A}^2$ approximation of Eq. (5). It is natural to refer to such a cross section as a *partial* triple differential scattering cross section (PTDSC), since the total triple differential scattering cross section (TTDSC) is obtained by summing the PTDSC over final states (see Sec. II B). The expression for the PTDSC is[15,16]

$$\frac{d^3\sigma_n}{d\omega_2 d\Omega_2 d\Omega_e} = \frac{r_0^2}{2}(1+\cos^2\theta)\frac{\omega_2}{\omega_1}|M^{(n)}|^2 \times \delta(\omega_1-\omega_2-E_b^{(n)}-E_e^{(n)}), \tag{6}$$

where the δ-function reflects the energy-conservation law in Compton scattering, $r_0=e^2/mc^2$ is the classical electron radius, θ is the scattering angle, and

$$M^{(n)}=\left\langle \Psi_f^{(n)}(\mathbf{x}_1,\ldots,\mathbf{x}_N)\left|\sum_{\nu=1}^{N}\exp(i\mathbf{k}\mathbf{r}_\nu)\right|\Psi_i(\mathbf{x}_1,\ldots,\mathbf{x}_N)\right\rangle \tag{7}$$

is the transition matrix element calculated with N-electron wave functions of initial and final states of the target. Note that expression (6) for the PTDSC assumes an implicit summation over the vibrational states within the framework of the Born-Oppenheimer approximation;[16,46] in any event, it will be difficult to resolve vibrational levels in the Compton scattering regime.

The antisymmetry of the many-electron wave function implies that the contribution from each term in expression (7) is the same. Therefore, we may replace the summation over ν by the last term, which corresponds to the ejection of the Nth electron, yielding

$$M^{(n)}=N\langle\Psi_f^{(n)}(\mathbf{x}_1,\ldots,\mathbf{x}_N)|\exp(i\mathbf{k}\mathbf{r}_N)|\Psi_i(\mathbf{x}_1,\ldots,\mathbf{x}_N)\rangle. \tag{8}$$

We assume now that the initial state possesses a total spin $S=0$, as is the case in most nonmagnetic materials. The final state will then be a singlet state (due to spin conservation in the Compton scattering process) and the associated antisymmetric singlet wave function can be represented as[47]

$$\Psi_f^{(n)}(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\hat{\mathcal{A}}\frac{1}{\sqrt{2}}[\Psi_{n\alpha}(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\psi_{\mathbf{p}\beta}(\mathbf{x}_N) - \Psi_{n\beta}(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\psi_{\mathbf{p}\alpha}(\mathbf{x}_N)]. \tag{9}$$

Here $\psi_{\mathbf{p}\sigma}(\mathbf{x}_N)$ is the wave function of the ejected electron with momentum $\mathbf{p}_n$ and spin projection σ that can accept only two values: $\sigma=1/2$ denoted by α and $\sigma=-1/2$ by β. $\Psi_{n\alpha}$ and $\Psi_{n\beta}$ are the two doublet components of the $(N-1)$-electron ionic wave function in the nth quantum state (in the one-electron picture, this describes an ion with a hole in the nth shell). The ionic states are the eigenstates of the $(N-1)$-electron Hamiltonian. $\hat{\mathcal{A}}$ is an antisymmetrization operator given by

$$\hat{\mathcal{A}}=\frac{1}{\sqrt{N}}\left(1-\sum_{\nu=1}^{N-1}P_{\nu N}\right), \tag{10}$$

where the permutation $P_{\nu N}$ transposes the ejected Nth electron with the νth electron in the ion.

Substituting the final state wave function (9) into Eq. (8) and invoking the condition of strong orthogonality

$$\langle[\Psi_{n\alpha}(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\psi_{\mathbf{p}\beta}(\mathbf{x}_N) - \Psi_{n\beta}(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\psi_{\mathbf{p}\alpha}(\mathbf{x}_N)]|\Psi_i(\mathbf{x}_1,\ldots,\mathbf{x}_N)\rangle=0 \tag{11}$$

for all i, we obtain

$$M^{(n)}=\sqrt{\frac{N}{2}}\langle[\Psi_{n\alpha}(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\psi_{\mathbf{p}\beta}(\mathbf{x}_N) - \Psi_{n\beta}(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})\psi_{\mathbf{p}\alpha}(\mathbf{x}_N)] \times|\exp(i\mathbf{k}\mathbf{r}_N)|\Psi_i(\mathbf{x}_1,\ldots,\mathbf{x}_N)\rangle. \tag{12}$$

This can be represented in terms of the Dyson spin orbitals,[48–52] defined by

$$g_n(\mathbf{x}_N)=\sqrt{N}\int\Psi_n(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1})^* \times\Psi_0(\mathbf{x}_1,\ldots,\mathbf{x}_N)d\mathbf{x}_1,\ldots,d\mathbf{x}_{N-1}, \tag{13}$$

where the integration over $d\mathbf{x}_i$ includes a summation over the spin coordinates. The Dyson spin orbitals $g_n(\mathbf{x}_N)$ may thus be thought of as generalized overlap amplitudes between the ground state and the ionized states of the many-body system. They naturally appear in the spectral resolution of the one-particle Green function,[53,54] and have been exploited successfully in some studies of ionization of atomic and molecular systems by electromagnetic radiation or fast electrons.[55–57] Note that, in general, Dyson orbitals do not form an orthonormal set. Some authors[52] define Dyson orbitals without the prefactor of $\sqrt{N}$. The Dyson spin orbital with the spin projection σ may be written in terms of the spin function $\sigma(\zeta)$ as

$$g_n(\mathbf{x}_N)=g_n(\mathbf{r}_N,\sigma(\zeta_N))=g_n(\mathbf{r}_N)\sigma(\zeta_N). \tag{14}$$

The wave function of the ejected electron similarly is

$$\psi_{\mathbf{p}_n\alpha}(\mathbf{x}_N)=\psi_{\mathbf{p}_n}(\mathbf{r}_N)\alpha(\zeta_N). \tag{15}$$

Introducing definition (13) into Eq. (12) and performing spin integration, we obtain a compact general expression for the transition matrix element

$$M^{(n)}=\sqrt{2}\int g_n(\mathbf{r})\exp(i\mathbf{kr})\phi^*_{\mathbf{p}_n}(\mathbf{r})d\mathbf{r}. \tag{16}$$

In the region of large energy transfer, Eq. (16) provides an exact expression for the matrix element in terms of the Dyson orbital $g_n(\mathbf{x}_N)$ and the wave function of the ejected electron in the potential field of the ion. Electron correlation effects enter through $g_n(\mathbf{x}_N)$ and can be included in any particular scheme to the extent to which these are incorporated in the computation of this quantity. In general, Dyson orbitals can be expanded into linear combinations of Hartree-Fock or other one-particle wave functions. In the so-called diagonal approximation, the Dyson orbital is equal to the square root of the pole strength times the HF orbital,[50,52] and can be calculated using special code[58] implemented into the *Gaussian 98* program suite;[59] see also Ref. 60.

Under the condition $\omega_1-\omega_2\gg E_b^{(n)}$, the wave function of ejected electron $\phi_{\mathbf{p}_n}(\mathbf{r})$ may be approximated as a plane wave

$$\phi_{\mathbf{p}_n}(\mathbf{r})=\frac{1}{(2\pi)^{3/2}}\exp(i\mathbf{p}_n\mathbf{r}), \tag{17}$$

allowing the transition-matrix element to be expressed via the Dyson orbital $g_n(\mathbf{q})$ in momentum space

$$M^{(n)}=\frac{1}{2\pi^{3/2}}\int g_n(\mathbf{r})\exp(i\mathbf{qr})d\mathbf{r}=\sqrt{2}\ \ g_n(\mathbf{q}), \tag{18}$$

Here, $\mathbf{q}=\mathbf{k}-\mathbf{p}_n$ is the momentum transferred to the ion. Since the ejected electron is considered as being free (with energy $p_n^2/2m$), the absolute value of the vector $\mathbf{p}_n$ is completely determined by the energy-conservation law and is equal to

$$p_n=\sqrt{2m(\omega_1-\omega_2-E_b^{(n)})}. \tag{19}$$

The direction of the vector $\mathbf{p}_n$ is undetermined so that only the maximum and minimum values of the vector $\mathbf{q}$ are constrained as follows:

$$|k-p_n|\leqslant q\leqslant k+p_n\,. \tag{20}$$

In this sense, vector $\mathbf{q}$ involves an implicit dependence on the index n.

Using Eqs. (18) and (6), we obtain the final expression for the PTDSC with the ion created in a definite electronic state n as

$$\frac{d^3\sigma_n}{d\omega_2 d\Omega_2 d\Omega_e}=r_0^2(1+\cos^2\theta)\frac{\omega_2}{\omega_1}|g_n(\mathbf{q})|^2 \times\delta\left(\omega_1-\omega_2-E_b^{(n)}-\frac{p_n^2}{2m}\right). \tag{21}$$

Note that here the IPM is not invoked. In the IPM, the Fourier component of the Dyson orbital in Eq. (21) reduces to the Fourier component of the Hartree-Fock or the Kohn-Sham orbital from which the electron is removed. Moreover, aside from the use of the plane-wave form (17) for the ejected electron wave function, expression (21) does not invoke the impulse approximation.

The determination of the PTDSC in Eq. (21) requires measurements of the angular and energy characteristics of both the scattered photon and the ejected electron taken in coincidence. In order to understand the relevant experimental geometries, it is helpful to refer to the momentum-conservation condition depicted in Fig. 1(b). Kaplan and Yudin[15] suggested a scheme in which the characteristics of the outgoing photon beam [i.e., the angle θ and energy ω_2 in Fig. 1(a)] are fixed, but the angle θ_e of the ejected electron is varied to access different $\mathbf{q}$ values. The fixed value of ω_2 should be selected near the peak of the Compton line[15,16] (i.e., close to the value given by the Compton formula for the scattering from a free electron at rest). By measuring the energy of the ejected electron then, one can, in principle, select the specific quantum state n involved in the scattering process through the energy-conservation condition (4). Another approach, followed more recently by Itoh and collaborators, is to fix the position of the electron as well as the photon detector [i.e., the angles θ and θ_e in Fig. 1(a)], but energy analyze both the scattered photon and the recoil electron in coincidence.[29,30]

B. Summation over final states

The TTDSC is obtained from Eq. (21) by summing over the available final states n as[61]

$$\frac{d^3\sigma}{d\omega_2 d\Omega_2 d\Omega_e}=r_0^2(1+\cos^2\theta)\frac{\omega_2}{\omega_1} \times\sum_n\ |g_n(\mathbf{q})|^2\delta\left(\omega_1-\omega_2-E_b^{(n)}-\frac{p_n^2}{2m}\right). \tag{22}$$

In the high-energy transfer region, $\omega_1-\omega_2\gg E_b^{(n)}$, the binding energy in the δ-function on the right-hand side may be neglected,[62] so that the absolute value of momentum $\mathbf{p}_n$ in Eq. (19) becomes independent of n and the summation over n simplifies to yield

$$\sum_n\ |g_n(\mathbf{q})|^2\delta\left(\omega_1-\omega_2-E_b^{(n)}-\frac{p_n^2}{2m}\right) =\delta\left(\omega_1-\omega_2-\frac{p_e^2}{2m}\right)\sum_n\ |g_n(\mathbf{q})|^2, \tag{23}$$

where $\mathbf{p}_n$ is replaced by $\mathbf{p}_e$ to emphasize that the momentum of the outgoing electron is independent of state n.

The sum of $|g_n(\mathbf{q})|^2$ over all occupied states n can be expressed via the one-particle reduced density matrix[63–65] for an N-electron system defined as

$$\Gamma_1(\mathbf{r};\mathbf{r}')=N\int\ \ \Psi(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1},\mathbf{r},\zeta)^* \times\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_{N-1},\mathbf{r}',\zeta)d\mathbf{x}_1,\ldots,d\mathbf{x}_{N-1}d\zeta. \tag{24}$$

In the momentum space

$$\Gamma_1(\mathbf{q};\mathbf{q}) = \frac{1}{(2\pi)^3}\int \Gamma_1(\mathbf{r},\mathbf{r}')\exp[i\mathbf{q}(\mathbf{r}-\mathbf{r}')]d\mathbf{r}d\mathbf{r}'. \tag{25}$$

We now recall the following decomposition of the one-particle reduced density matrix:[54]

$$\Gamma_1(\mathbf{r};\mathbf{r}') = \sum_n g_n(\mathbf{r})g_n(\mathbf{r}')^*. \tag{26}$$

Substituting this decomposition into Eq. (25), one obtains

$$\sum_n |g_n(\mathbf{q})|^2 = (2\pi)^3\Gamma_1(\mathbf{q};\mathbf{q}) \equiv (2\pi)^3\rho(\mathbf{q}). \tag{27}$$

Thus, in the high-energy transfer region, the TTDSC is directly related to the 3D EMD as follows:

$$\frac{d^3\sigma}{d\omega_2 d\Omega_2 d\Omega_e} = (2\pi)^3 r_0^2(1+\cos^2\theta)\frac{\omega_2}{\omega_1}\rho(\mathbf{q}) \times \delta\left(\omega_1-\omega_2-\frac{p_e^2}{2m}\right). \tag{28}$$

It is this TTDSC that is measured in the $(\gamma,e\gamma)$ experiments by Bell and collaborators,[26–28] issues of experimental resolution notwithstanding. Note, however, that there is an interesting difference in the way the momentum density factor ρ occurs in Eq. (28) compared to the analytical expressions employed by Refs. 26–28. In our case, the EMD $[\rho(\mathbf{q})]$ is sampled at the momentum

$$\mathbf{q} = \mathbf{k} - \mathbf{p}_e, \tag{29}$$

which is the momentum transferred to the ion, whereas in the cross section of Refs. 26–30, the EMD involved is $\rho(\mathbf{p})$, where $\mathbf{p}$ is the initial momentum of the electron before scattering. The reason is that the study of Refs. 26–28 is based on the formulas of Ribberfors[66] for double differential cross sections in the IA. As already noted, in the IA the scattering is the same as for free electrons, but weighted with the probability with which the plane-wave state of momentum $\mathbf{p}$ occurs in the ground state. For a system of bound particles, this picture does not constitute a useful starting point, and our more general treatment indicates that the quantity that occurs naturally is the momentum $\mathbf{q}$ transferred to the ion. Nevertheless, in the IA, the two pictures are equivalent because in this regime, from momentum conservation, one obtains

$$\mathbf{p}+\mathbf{k}_1 = \mathbf{p}_e+\mathbf{k}_2 \tag{30}$$

or equivalently

$$\mathbf{p} = \mathbf{p}_e - \mathbf{k}. \tag{31}$$

Comparing Eqs. (29) and (31), we see that in the high-energy transfer limit, $\mathbf{q}$ and $\mathbf{p}$ differ only by direction (they are opposite), as the outgoing electron loses all memory of the bound state it came from. The range of q in formula (20) becomes

$$0 \leqslant q \leqslant 2k. \tag{32}$$

Thus, the maximum momentum transferred to the ion is given by $2k$. In the IA, $2k$ may be interpreted as the highest momentum of an electron in the initial system that can be ejected.

III. SUMMARY AND CONCLUSIONS

We start by considering the elementary process involved in Compton scattering, namely, the scattering of an incoming photon from the ground state of an N-electron target to yield a final state containing a singly ionized target with $(N-1)$ electrons in a specific quantum state together with an outgoing photon and an ejected electron. The associated PTDSC is obtained rigorously without resorting to the approximations inherent in either the IA or the IPM. It is shown that the PTDSC can be expressed in terms of the Dyson orbitals, which give the overlap between the wave function of the ground state of the N-electron initial system with the $(N-1)$ electron ionized final state wave function.

The TTDSC is then obtained by summing over final states, which is equivalent to summing over the occupied Dyson orbitals. Interestingly, in our general treatment, the momentum that plays a fundamental role in the formula for the cross section is the momentum $\mathbf{q}$ transferred to the ion in the scattering process and not the momentum $\mathbf{p}$ associated with the electronic system as is the case in the IA based treatment. We show how in the limiting case of the high-energy transfer regime, our formalism reduces to the standard IA description. Although our treatment is nonrelativistic, extension to the relativistic case is straightforward by using relevant results in the literature.[66,67] Our formalism will permit the analysis and interpretation of electronic transitions in correlated electron systems via IXS beyond the constraints of the IA and the IPM. Applications of the present formalism are in progress.

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