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Influence of correlations on the trajectories of zeroes of the matrix elements for bound–bound and bound–free transitions in electron scattering

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Abstract

The topology of the trajectories of the zeroes of the electron scattering matrix elements has been obtained in the Born approximation. At small-momentum transfer, K the behaviour of the trajectories depends on the positions and the number of Cooper minima. We demonstrate strong correlation effects in this K area. At the high momentum, the positions of the zeroes depend only slightly on the energy transfer to the atomic electron, and correlation effects are not important.

Keywords: Electron scattering; Generalized oscillator strengths; Matrix element; Born approximation; RPAE

Introduced by Bethe (1930), the generalized oscillator strengths (GOS) for the excitation (as well as the generalized oscillator strengths densities for the ionization) are proportional to the differential cross sections (DCS) for electron scattering from many-electron atoms and molecules, and thus can provide important information about the process. Particularly, accurate calculations of GOS are critically desirable for the normalization of measured relative cross sections, especially in the small-momentum transfer region where difficulty of reliable measuring were numerously reported (Vuskovic et al., 1982; Marinkovic et al., 1986,1992; Ismail and Teubner, 1995; Avdonina et al., 1999). The most sensitive test for the accuracy of the calculation can be a comparison of the theoretical and experimental results in the vicinity of the GOS extrema. It was shown for various excitation and ionization transitions in atoms (Marinkovic et al., 1999; Manson, 1971; Miller, 1973; Kruglova et al., 1977; Tong et al., 1989; Chen and Msezane, 2000; Msezane et al., 2002; Avdonina et al., 2005) that GOS's have a complicated structure, which is dominated by multiple minima due to zeroes of the correspondent electron scattering matrix elements in the dependence of the momentum transfer K as well as of the energy transfer ω. In this paper, we identify the location of the positions of the GOS's minima giving trajectories of the zeroes of the scattering matrix elements on the K and ω plane.

Since we are mostly interested in the region of small K, the topology of the nodal curves of the scattering matrix elements for different atoms and transitions has

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been obtained in the first Born approximation (FBA). (Recently, it was shown (Avdonia et al., 2005) that though at low input electron energies E the number and positions of the GOS's minima differ in many cases from the FBA predictions, it is still possible to use this approximation to accurately predict the position of the low K minima.) Our calculations involve plane waves for the initial and final states of the scattering electron and non-relativistic Hartree–Fock (HF) wave functions for the initial and final atomic electron states. We show that at small K the topology of the nodal curves depends on the positions and the number of Cooper minima, while at high K it only slightly depends on K. Influence of many-electron correlation effects on the trajectories is discussed using the non-relativistic random phase approximation with exchange (RPAE) (Amusia, 1990). Our results show substantial, quantitative though not qualitative, difference of FBA and RPAE results.

The GOS for excitation or density of GOS for ionization is defined in terms of the incident energy E, energy transfer ω, and momentum transfer K (Bethe, 1930) as (atomic units are used throughout)

$$\mathrm{GOS}(E,\omega,K)=\frac{\omega}{2}\frac{p_{\mathrm{i}}}{p_{\mathrm{f}}}K^2\sigma, \tag{1}$$

where p_{if} are the electron momenta before and after the collision, respectively, σ is the measured or calculated DCS: $\sigma=\mathrm{d}\sigma/\mathrm{d}\Omega$ for excitation and $\sigma=\partial^2\sigma/\partial\Omega\partial\omega$ for ionization. The momentum transfer K depends on E, ω, and the scattering angle θ

$$K^2=2E\left[2-\frac{\omega}{E}-2\sqrt{\left(1-\frac{\omega}{E}\right)}\cos\theta\right]. \tag{2}$$

In the FBA, DCS in Eq. (1) is obtained by averaging the square of the scattering amplitude over the magnetic sublevels of the initial state orbital angular momentum ℓ_{i} and summing it over the magnetic sublevels of the final state orbital angular momentum ℓ_{f}, so that GOS can be expanded as (Sobelman, 1979)

$$\mathrm{GOS}(\omega,K^2)=\frac{2\omega N_{\ell_{\mathrm{i}}}}{(2\ell_{\mathrm{i}}+1)}\sum_L(2L+1)K^{2(L-1)}\left|m^L_{\mathrm{fi}}(\omega,K^2)\right|^2, \tag{3}$$

where N_{ℓ_i} is the number of electrons in the initial state. Substitution of plane waves for the wave functions of the initial and scattered electrons and of one-electron HF approximation wave functions for the atomic electrons reduces the matrix element $m^L_{\mathrm{fi}}(\omega,K^2)$ of Eq. (3) to the expression

$$m^L_{\mathrm{fi}}(\omega,K^2)=\frac{\sqrt{(2\ell_{\mathrm{f}}+1)(2\ell_{\mathrm{i}}+1)}}{K^L}\begin{pmatrix}\ell_{\mathrm{f}} & L & \ell_{\mathrm{i}}\\ 0 & 0 & 0\end{pmatrix}\times\int_0^\infty R_{\mathrm{f}}(r)j_L(Kr)R_{\mathrm{i}}(r)r^2\mathrm{d}r \tag{4}$$

$R_{\mathrm{i}}(r)$ and $R_{\mathrm{f}}(r)$ are, respectively, the HF radial wave functions of the initial and final atomic electrons, and $j_1(Kr)$ is the spherical Bessel function. Non-zero values of the $3j$ symbol (Sobelman, 1979) in Eq. (4) correspond to the values of the total orbital angular momentum L of the electron–hole pair: $\ell_{\mathrm{f}}-\ell_{\mathrm{i}}\leqslant L\leqslant\ell_{\mathrm{f}}+\ell_{\mathrm{i}}$.

If $m^L_{\mathrm{fi}}(\omega,K^2)$ changes sign, it can result in a minimum in the total GOS in its dependence on either the momentum transfer or energy transfer. Note that for small-momentum transfer the reason for a minimum in GOS can be similar to the reason for a minimum in the optical oscillator strengths, the well-known Cooper minima (Fano and Cooper, 1968) for transitions in the photo processes (Manson, 1971). Since the GOS's reach the optical oscillator strengths at $K=0$ (Lassettre et al., 1969), the existence of a Cooper minimum leads to a minimum in the GOS, considered as a function of the energy ω. There can be other GOS minima, which are not associated with OOS minima, but are related to the interaction operator in the matrix element (Bessel operator in the FBA). The roots of $m^L_{\mathrm{fi}}(\omega,K^2)=0$ form curves in the K–ω plane (trajectories).

We can see from Eqs. (3) and (4) that when $K\to0$ the optically allowed GOS approach the optical oscillator strength, but the optically forbidden GOS ($L\neq1$) approach zero. Therefore, at small K the most important contribution in the sum for GOS in Eq. (3) is given by dipole transitions ($L=1$). With increase of K, the more important role is played by monopole transitions (Amusia et al., 1975). With farther increase of K, the relative contribution of dipole and monopole transitions in GOS decreases, and the contributions of quadrupole and higher order transitions increases (note, that at small K both monopole and quadrupole GOSs are proportional to K^2). Here we restrict our calculations by consideration of the most important at small K dipole and monopole transitions.

We start from the dipole transitions: $3\,\mathrm{s}\to(\mathrm{n},\varepsilon)\mathrm{p}\ {}^1\mathrm{P}$ in Na and $6\,\mathrm{s}\to(\mathrm{n},\varepsilon)\mathrm{p}\ {}^1\mathrm{P}$ in Ba. In Fig. 1, we show sets of nodal curves of GOS's for $3\,\mathrm{s}\to(\mathrm{n},\varepsilon)\mathrm{p}\ {}^1\mathrm{P}$ transition in Na on K and ejected electron energy ε plane ($\varepsilon=\omega+E_{\mathrm{i}}$, where E_{i} is the energy of the initial atomic electron). Note, that according to the Born approximation, the range of possible values of K becomes narrower with decreasing electron scattering energy E. In Fig. 1, we show how the physical region of possible K and ε narrows when E changes from $E=100$ to $E=40\,\mathrm{eV}$, so only three first nodal curves become important at this last energy. It means that with decreasing E, fewer minima are exposed in the physical region of the GOS curves.

At small K the topology of the nodal curves depends on the position of the Cooper minima (Manson, 1971; Tong et al., 1989) in the corresponding photoionization cross section. In Fig. 2 we show the zero of the photoionization matrix element (in the length form), which corresponds to