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Manifestations of Collective Properties of the Degenerate Electron Gas in the $(e, 2e)$ Quasielastic Knockout Process*

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It is shown that quasielastic knockout $(e, 2e)$ of electron by a fast electron from a thin solid film presents direct information about both the $\vec{k}$ and ω dependence of the single-particle, spectral-weight function $A(\vec{k},\omega)$ of target electrons. We discuss the expected manifestation of Mahan-Nozières edges and their plasmon satellites in an $(e, 2e)$ experiment side by side with that of plasmaron hole states.

The high-energy, quasielastic knockout of nucleons or nucleon clusters [$(p, 2p)$, (p, pd), etc.] is a powerful tool for nuclear-structure research.[1] Several years ago the $(e, 2e)$ quasielastic knockout process was proposed by Smirnov and one of the authors[2] for the investigation of electron wave functions in atoms, molecules, and thin solid films. Its advantage in comparison with the methods of positron annihilation and Compton scattering profiles[3] consists in the possibility of obtaining the momentum distribution of the target electron for the fixed value of its binding energy side by side with the fixed orientation of its quasimomentum in a monocrystal. The disadvantage of the $(e, 2e)$ method is that it cannot be used for the investigation of thick solid ($d > 250$ Å) or liquid targets.

Subsequent papers have exhibited both various theoretical aspects of the problem mentioned[4-6] (in particular the manifestation of the band structure of solids[2,5,6]) and the first experimental results for solid[7] and gas[8] targets (with the best energy resolution at present[8] $\Delta E \simeq 1-2$ eV). Rather rapid further experimental progress is to be expected.

The first problem considered in the present paper concerns the Mahan-Nozières edges[9] and their plasmon satellites.[10] The main difference between the $(e, 2e)$ process and x-ray absorption considered earlier[9,10] is that the final electron is not near the Fermi surface but is ejected into the high-energy (a few keV) continuum described by plane waves. Thus only the polarization of the degenerate electron gas by the suddenly appearing deep hole is present as a collective effect (high-energy x-ray photoemission would be, of course, similar in this respect). In terms of Ref. 9 we obtain information about singularities of the deep-electron spectral-weight function $Z(\omega)$ itself.

For describing this effect we should generalize the formulas of our previous papers.[2,6] Namely, we should replace the quantity $\delta(\omega - \epsilon_{\vec{p}})\,\delta_{\vec{k}\vec{p}}$ entering into equations for the Sommerfeld model of a degenerate electron gas[2,6] by the general electron spectral-weight function $A(\vec{k}, \omega)$.[11] We obtain

$$\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dE_1 dE_2 d\omega} = \frac{2mk_2}{(2\pi\hbar)^3}\left(\frac{d\sigma}{d\Omega_1}\right)^{\text{free}}_{\text{lab}} NV\delta(E_0 - E_1 - E_2 - \omega)A(\vec{k}, \omega) \qquad (1)$$

as the $(e, 2e)$ cross section for a unit crystal volume containing N electrons (V is the volume of the

elementary cell of the crystal). Here $\vec{k} = -\vec{k}_0 + \vec{k}_1 + \vec{k}_2$ is the momentum of the target electron fixed by both the geometry of experiment and the chosen values of the energies E_1 and E_2 of the two final electrons; ω is the binding energy of the knocked-out electron.

We can see that the quantity $A(\vec{k}, \omega)$ represents nothing else but a general expression for the $(e, 2e)$ form factor—the $(e, 2e)$ method gives us information just about true particles (not quasiparticles), i.e., about the single-particle spectral-weight function $A(\vec{k}, \omega)$.

For the case of a deep hole we obtain from Eq. (1)

$$\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dE_1 dE_2 d\omega} = \text{const} \times k_2 \left(\frac{d\sigma}{d\Omega}\right)^{\text{free}}_{\text{lab}} \delta(E_0 - E_1 - E_2 - \omega) |\varphi_l(k)|^2 Z(\omega), \tag{2}$$

where $\varphi_l(k)$ is the wave function of the deep hole. The shapes of a deep-hole level maximum and its plasmon satellites are determined by the ω dependence of the function[9,10]

$$Z(\omega) = \sum_n (e^{-a} a^n / n!) A(\omega - \omega_0 - n\omega_p) \tag{3}$$

(the plasmon dispersion is omitted here for the sake of brevity),

$$A(X) \sim |X|^{-(1-\alpha)} \theta(X), \quad \alpha = 2\sum_l (2l+1)(\delta_l/\pi)^2,$$
$$a = \omega_p^{-1} \sum_{\vec{q}, q<q_c} |V_{\vec{q}}|^2 q^2 / 8\pi e^2, \tag{4}$$

where ω_p is the plasmon energy and q is a plasmon momentum (we assume $\langle q^2 \rangle \ll \langle k^2 \rangle$). The values of $1 - \alpha$ are 0.80, 0.87, and 0.98 for Li,[12] Na,[12] and Cu,[13] respectively.

If we compare the singularities (4) with those of x-ray absorption (in fact, they are finite sharp maxima[14] of asymmetrical shape),[9,10]

$$B(\omega) \sim |\omega|^{-\alpha_l}, \quad \alpha_l = 2\delta_l/\pi - \alpha, \tag{5}$$

we see a noticeable difference even if both values $1 - \alpha$ and α_l are positive. But the difference becomes drastic if $1 - \alpha > 0$ but $\alpha_l < 0$, as happens, say, in the s-p transitions in lithium, sodium, and some other metals.[12] Here the threshold singularity of x-ray absorption enters as a threshold suppression ($\alpha_1 \simeq -0.1$).

The experimental check of predictions concerning Mahan-Nozières edges would require an energy resolution in the $(e, 2e)$ method of $\Delta E \simeq 0.5$ eV which is comparable to the best present experimental resolution for gas targets. The intensity of plasmon satellites in comparison with that of the ground state should not depend on the initial energy value E_0. In a (e, e') or (γ, γ') scattering experiment on a Li or Na target it is possible to observe a true singularity extending measurements to relatively large scattering angles[15]; however, the physics in this case is very different.

Of course, we should not limit ourselves to the deep holes. The holes in the conduction band itself should also be investigated. The most interesting phenomena here are probably the plasmaron states[16] which appear as both $\vec{k}$ and ω singularities of $A(\vec{k}, \omega)$ in Eq. (1). They are separated from the bottom of the conduction band by an energy $\simeq 1\omega_p$ and should be easily seen in the $(e, 2e)$ experiment.

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Transition Probabilities and Overlap-Covalency Effects in the X-Ray Photoemission Spectra of Transition-Metal Compounds: ReO_3

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Differences in photoelectric transition probabilities have an important effect on the interpretation of x-ray photoemission spectra of transition-metal compounds with pronounced overlap-covalency effects. It is shown that the apparent discrepancy between the x-ray–photoemission valence-band data for ReO_3 and the theoretical density-of-states curve is resolved if one considers only the 5*d* component of the density of states.

It is shown in this communication that valence-band spectra of transition-metal compounds obtained by x-ray photoemission spectroscopy (XPS) may be grossly distorted by transition-probability effects. These effects are so severe that erroneous conclusions can be drawn from straightforward comparisons between XPS data and theoretical density-of-states curves. The fact that, for example, the strength of a rare-earth 4*f*-electron signal is strongly photon-energy dependent is, of course, well known. Similarly, it has been suggested that the small discrepancies which are found between theoretical and experimental band structures of the noble metals are due to increasing *s* admixture into the lower part of the *d* band.[1] As an example of rather more drastic effects we consider ReO_3.

The electronic structure of this cubic, metallic compound[2] has been the subject of a number of investigations.[3-6] In Fig. 1 we show the ReO_3 density of states from Ref. 3, smoothed by a 0.55-eV Gaussian, which corresponds to the resolution function of the spectrometer used to obtain the XPS data discussed below. This band structure successfully accounts for both the optical properties and the Fermi-surface dimen-

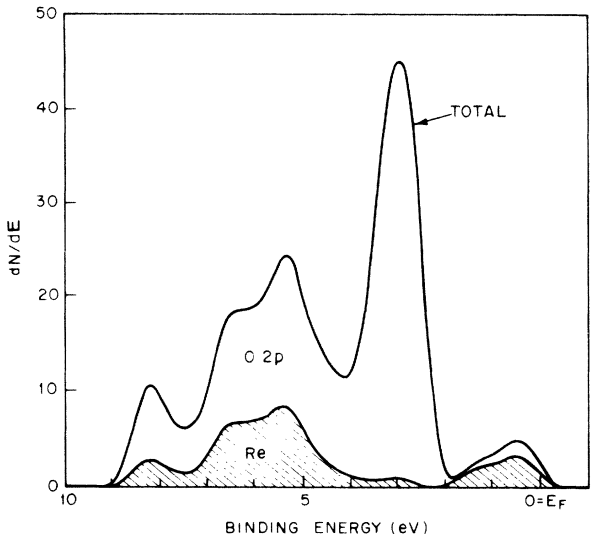

FIG. 1. Calculated density of states of ReO_3 from Ref. 3 smoothed by a 0.55-eV Gaussian. The shaded area indicates the Re 5*d* contribution.