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INVESTIGATION OF THE ELECTRONIC STATES OF ATOMS, MOLECULES, AND SOLIDS BY QUASIELASTIC KNOCK-ON OF AN ELECTRON BY A FAST ELECTRON (e, 2e)

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Continuing earlier investigations [1,2] of the analogs of direct nuclear reactions in the atomic-molecular region, we wish to point out the great value of the quasielastic knock-on reaction (e, 2e). The difference from work on ionization [3] lies here in the fact that it is necessary to measure for coincidence the pulses from both final electrons (Fig. 1) at fixed emission angles (see [4] regarding the (p, 2p) reaction). We shall show with three examples (impulse approximation) that this makes it possible to obtain the Fourier transform of the wave function of the knock-on electron and its binding energy. In paragraphs 1 and 2 we shall assume that the electron energies are equal ($E_1 = E_2$) and that the angles φ_1 and φ_2 are also equal (complanar symmetrical case).

1. H_2 molecule, final ion H_2^+ in state $1\sigma_g$:

$$\frac{d^2\sigma}{d\Omega_1 dE_1} \sim \left[\frac{q^2a_0^2 + \hbar^2 Z_{eff}^2}{\hbar^2 a_0^2}\right]^{-4}\left[\frac{x + \sin x}{x}\right]\left(\frac{d\sigma}{d\Omega_1}\right)_{free} W_n \qquad (1)$$

The cross section for free e-e scattering $(d\sigma/d\Omega_1)_{free}$ is tremendous, $\approx 10^{-21}$ cm²/sr at $E_0 \simeq 5$ keV ($\varphi_1 = 45°$), so that the targets must be unusually thin (100-Å films or equivalent gas jets). Further, $Z_{eff} \simeq 1.2$ (Heitler-London function), $x = qR/\hbar$, a_0 - Bohr radius, R - distance between nuclei in H_2, $\vec{q} = \vec{p}_1 + \vec{p}_2 - \vec{p}_0$, and W_n - probability of production of H_2^+ in the n-th vibrational state. W_n = 0.06, 0.2, and 0.3 for n = 0, 1, and 2. In the general case the ratio of the heights of the maxima in the spectrum of the energies $E_1 + E_2$ determines the spectrum of the genealogical connection [5] between the ground state of the target and the different hole states of the final ion.

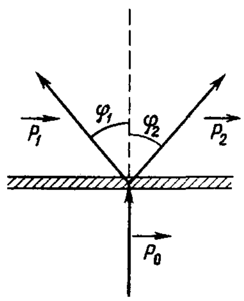

Fig. 1

2. Free electrons in a metal (plane waves):

$$\frac{d^2\sigma}{d\Omega_1 dE_1} \sim n\begin{pmatrix} p_x = p_y = 0, \quad p_z = p = 2p_{1z} - p_0 \\ \epsilon = 2E_1 - E_0 \end{pmatrix} E_1 \left(\frac{d\sigma}{d\Omega_1}\right)_{free} \tag{2}$$

Here $n(\begin{smallmatrix}\vec{p}\\ \epsilon\end{smallmatrix}) = 2$ if one of the occupied states has a quasimomentum $\vec{p}$ and an energy ϵ, and $n = 0$ in all other cases. If p and ϵ are specified ($|p| \ll p_0$), then the coincidences will be registered at $\varphi = \pi/4 - p/p_0$ and $E_1 = (E_0 + \epsilon)/2$. The non-complanar asymmetrical case gives a connection between ϵ and p even for an arbitrary direction of $\vec{p}$ in the single crystal.

3. Strong coupling with the lattice (Bloch's sums):

$$\frac{d^4\sigma}{d\Omega_1 d\Omega_2 dE_1 dE_2} \sim n\begin{pmatrix} \vec{p} = \vec{p}_1 + \vec{p}_2 + \vec{a}_i - \vec{p}_0 \\ \epsilon = E_1 + E_2 - E_0 \end{pmatrix} \delta_{p+k, a_i} |g_{at}(\vec{k} = \vec{p}_0 - \vec{p}_1 - \vec{p}_2)|^2 \sqrt{E_1 E_2} \left(\frac{d\sigma}{d\Omega_1}\right)_{free} \tag{3}$$

Here a_i is one of the reciprocal-lattice vectors, $g_{at}(\vec{k}) = \int[\exp(i\vec{k}\cdot\vec{r})\varphi(\vec{r})d\vec{r}$, and $\varphi(\vec{r})$ is the wave function of the electron in the atom.

Thus, at energy $E_1 + E_2$ corresponding to the bottom of the band ($p = 0$), we have a series of pointlike spots corresponding to $\vec{k} = \vec{a}_1, \vec{a}_2, \ldots$ (Laue). On going away from the bottom of the band, each of the spots $\vec{k} = \vec{a}_i$ becomes (irregularly) spherical with angular radius $\simeq p/p_0$.

The great difference between formulas (2) and (3) will probably make it possible to investigate the single plane-wave approximation in metals, molecular orbitals in molecular crystals, or localization of "ferromagnetic" d-electrons in metals of the Fe group and ferrites. All the occupied bands in metals, alloys, ionic crystals, etc. are admissible. The required accuracy in the measurement of E_0, E_1, and E_2 is $\simeq 0.1 - 0.2$ eV [6]. Allowance for the distortion of the wave and the departure from the mass shell, and the use of more realistic wave functions of the many-electron problem, will be discussed in a later detailed article.

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