Quasielastic knockout of atoms from molecules by high-energy atoms

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The general theory is set forth for the quasielastic knockout of atoms from molecules by fast atoms with energy of the order of 500 eV ($A+(BC)\rightarrow A+B+C$). The theory is based on the adiabatic approximation and is illustrated by the example of knockout of a hydrogen atom from the molecules H_2O and H_2. It is pointed out that measurement in coincidence of the angular correlation between the two final particles gives partial momentum distributions (form factors) of the knocked out atoms in the molecule. The appearance of the form factor depends substantially on the nature of the wave function of the excited vibrational state of the final radical, which also may be unstable. Thus, the method of quasielastic knockout can serve as a unique means of investigation of the properties of molecular radicals. An experiment with ions is also possible, $A^{++}+(BC)\rightarrow A^{+}+B^{+}+C$, but its interpretation is more difficult.

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1. INTRODUCTORY REMARKS

The substantial achievements of the method of quasielastic knockout of an electron by an electron, $(e, 2e)$ at high energies in the keV range[1] show that this new method is a powerful means of studying wave functions of individual atoms and molecular orbitals and will stimulate further theoretical and experimental study of the possibilities of use of the methods of high energy nuclear physics in the atomic and molecular region.

In the present work we develop the theory of quasielastic knockout of atoms from molecules by fast electrically neutral particles and propose a new type of experiment, utilizing the coincidence technique, for direct study of the Fourier spectrum of the vibrational function of the initial molecule on the basis of the variable of motion of the knocked out atom with respect to the residual molecule for a specified fixed vibrational state of this final molecule or radical. In this way it is possible to study any vibrational states of the final molecule, including even unstable radicals, since the Fourier spectrum under discussion is extremely sensitive to the wave function of this final vibrational state.

This question was posed by us at one time in preliminary form,[2] but was not developed, since the experimental technique at that time did not permit such studies to be carried out. However, the state of the art has changed radically in the course of fourteen years. In the first place, the coincidence technique has been developed for $(e, 2e)$ experiments which are similar in their physics.[1] Secondly, the time-of-flight method has been mastered for measurement of the velocities of neutral atoms.[3] In the third place, efficient detectors of neutral atoms have been suggested.[4] Further, there is the possibility of identifying particular rotational states for certain types of molecules (quadrupole lenses, etc.).[5] The crossed-beam technique has become generally available. Finally, as we shall see below, we can discuss experiments of this type in which the incident particles and both final detected particles are charged. Such experiments are technically very simple.

2. GENERAL THEORY OF QUASIELASTIC KNOCKOUT OF ATOMS

The expression for the cross section for quasielastic knockout of a particle B from a compound system (BC) by an incident particle A has the form[1]

$$\frac{d^3\sigma}{dE_A d\Omega_A d\Omega_B}=\frac{p_A p_B}{p_0}\frac{(m_A+m_B)^2}{m_B}\left(\frac{d\sigma_{AB}}{d\Omega}\right)_{\mathrm{fr}}|M_{0f}(\mathbf{q})|^2. \tag{1}$$

Here we are discussing the process

$$A+(BC)\rightarrow A+B+C, \tag{2}$$

which reduces in the impulse approximation to quasifree scattering of particle A by atom B, with the radical C being a spectator. It is assumed that the emitted particles A and B are detected in coincidence and that their momenta p_A and p_B are measured. The experimental geometry must be chosen so that p_A and p_B are comparable with the incident-particle momentum p_0 and the radical C obtains a momentum $\mathbf{q}=\mathbf{p}_0-\mathbf{p}_A-\mathbf{p}_B$ small in comparison with p_0, p_A, and p_B. In Eq. (1)

$$M_{0f}(\mathbf{q})=n_B^{1/2}\int e^{-i\mathbf{q}\mathbf{R}_B}\Psi^*_{C,f}(\mathbf{r}_C)\Psi_{(B,C),0}(\mathbf{r}_C,\mathbf{R}_B)\,d\mathbf{r}_C\,d\mathbf{R}_B, \tag{3}$$

and n_B is the number of equivalent atoms of type B in the molecule (BC). All coordinates are given in the laboratory system. It is contemplated that the energy E_0 of the bombarding particles A is several hundred electron volts. Here the velocities of atoms A and B in the final state are rather large in comparison with the velocities of vibrational motion of the nuclei in the molecule, which permis use of the impulse approximation for description of this process. At the same time they are small in comparison with the velocities of the electrons in the molecule, so that it is possible to use the adiabatic approximation and thereby exclude electronic degrees of freedom from the discussion.[6]

Equation (3) corresponds to the transition between definite states $(0)=(\nu JK)$ of the initial molecule (BC) and $(f)=(\nu_C J_C K_C)$ of the final radical C. Consequently we have

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$$|M_{0f}(\mathbf{q})|^2=(2J+1)^{-1}\sum_{MM_C}|M_{0f}^{MM_C}(\mathbf{q})|^2, \tag{4}$$

$$M_{0f}^{MM_C}(\mathbf{q})=\sum_{\Lambda}D^{J_C}_{\Lambda K_C}(\Omega_C)\int d\Omega\langle J_C\Lambda M_C|\Omega\rangle M^{\text{in}}_{vv_C}(\Omega^{-1}\mathbf{q})\langle\Omega|JKM\rangle, \tag{5}$$

$$M^{\text{in}}_{vv_C}(\Omega^{-1}\mathbf{q})=M^{\text{in}}_{vv_C}(\mathbf{q}^{\text{in}})=\int\exp(-i\mathbf{q}^{\text{in}}R_B)\varphi^{*}_{v_C}(\Omega_C^{-1}\mathbf{y})\Phi_v(\mathbf{y},\mathbf{R}_B)\,d\mathbf{y}\,d\mathbf{R}_B. \tag{6}$$

Here $\mathbf{R}_B$ is the coordinate of the nucleus of atom B relative to the center of mass of the molecule (BC), and the set of vectors $\mathbf{y}$ are the vibrational variables of the radical C. All of these variables and also the momentum $\mathbf{q}^{\text{in}}=\Omega^{-1}\mathbf{q}$ in Eq. (6) are taken in the internal coordinate system of the molecule (BC), which is related to its principal axes of inertia. The transition from it to the laboratory system is carried out by rotation of Ω; $\langle\Omega|JKM\rangle$ and $\langle\Omega|J_CK_CM_C\rangle$ are the rotational wave functions respectively of the molecule and the radical; M and M_C are the magnetic quantum numbers. If the orientations of the principal axes of inertia of the molecule (BC) and the radical C do not coincide, it is necessary to carry out, as is done in Eqs. (5) and (6), a rotation of Ω_C from the axes of inertia of the molecule (BC) to the axes of inertia of the radical C.

Using the Boltzmann distribution $W_{JK}(T)$ for the target molecules and assuming that the vibrational degree of freedom for them is frozen, we can write the final formula:

$$|M_{vv_C}(\mathbf{q})|^2=\sum_{JKJ_CK_C}W_{JK}(T)|M_{0f}(\mathbf{q})|^2. \tag{7}$$

Here there arises the very interesting problem of the correct transition from the rotational and vibrational variables Ω, Q of the initial molecule (BC) to the rotational and vibrational variables Ω', Q' of the residual radical C and the coordinate $\boldsymbol{\rho}$ of the knocked out atom B relative to the radical C. Here it is necessary to take into account that the system of principal axes of inertia of the molecule (BC) and of the residue C do not coincide. The approach to solution of this nontrivial problem has been noted in the work of Davydov and Filippov[7] (at least for triatomic molecules), but we shall not immerse ourselves in this question, which is important when we are considering a transition from a fixed rotational level of the molecule to a specified rotational state of the radical. The fact is that in the early stages the level of the energy resolution ΔE will probably be too crude to separate individual rotational states of the radical, and the measured cross section will include practically the entire rotational band. Therefore it is desirable to make use of the completeness relation for the rotational functions of the radical and to simplify Eq. (7), reducing it to the form (the details of the procedure of this simplification can be found in our 1975 article[1])

$$|M_{vv_C}(q)|^2=\int\frac{d\Omega}{8\pi^2}|M^{\text{in}}_{vv_C}(\Omega^{-1}\mathbf{q})|^2=\int\frac{\sin\theta\,d\theta\,d\varphi}{4\pi}|M^{\text{in}}_{vv_C}(\mathbf{q}^{\text{in}})|^2, \tag{8}$$

where θ and φ are angles specifying the orientation of the vector $\mathbf{q}^{\text{in}}$ in the internal system of the molecule (BC).

In the earlier publication[2] Matthies and Neudachin did not use this folding and obtained the distribution of intensities of excitation of the final radical OH in various rotational and vibrational states, but only for $q=0$. The question of form factors was not raised in that work.

3. QUASIELASTIC KNOCKOUT OF A HYDROGEN ATOM FROM THE MOLECULES H_2O and H_2

These specific examples permit a good demonstration, in essence, of the general method of calculation of the integrals (6). We introduce the following designations for the variables of the vibrational wave functions of the H_2O molecule ρ^H is the relative coordinate of the nucleus of the knocked out hydrogen atom $H_{(1)}$ and the center of mass of the residual nucleus, and ρ_0^H is the equilibrium value of this coordinate, so that $\rho^H=\rho_0^H+\Delta\rho^H$. We shall designate by y_1 and y_2 the components of the displacement vector $\Delta\rho^H$ relative to the equilibrium position ρ_0^H respectively parallel and perpendicular to ρ_0^H. Finally, r_1, r_2, and r_3 will specify the distances $H_{(1)}-H_{(2)}$, H_1-O, and $H_{(2)}-O$ in the H_2O molecule, and s_1, s_2, and s_3 are their departures from the equilibrium values:

$$r_1=r_{HH}+s_1,\quad r_2=r_{OH}+s_2,\quad r_3=r_{OH}+s_3.$$

Assuming that the vibrations relative to the equilibrium distances are small, we obtain

$$\begin{gathered}s_1=k_1y_1+k_2y_2+k_3y_3,\\ s_2=k_4y_1+k_5y_2+k_6y_3,\quad s_3=y_3,\end{gathered} \tag{9}$$

where

$$\begin{gathered}k_1=-\frac{16}{17}\frac{r_{OH}}{r_{HH}}\sin\varphi_0,\quad k_2=\frac{\rho_0^H}{r_{HH}}+\frac{16}{17}\frac{r_{OH}}{r_{HH}}\cos\varphi_0,\\ k_3=\frac{16^2}{17^2}\frac{r_{OH}}{r_{HH}}+\frac{16}{17}\frac{\rho_0^H}{r_{HH}}\cos\varphi_0,\quad k_4=\frac{1}{17}\sin\varphi_0,\\ k_5=\frac{\rho_0^H}{r_{OH}}-\frac{1}{17}\cos\varphi_0,\quad k_6=\frac{1}{17^2}-\frac{1}{17}\frac{\rho_0^H}{r_{OH}}\cos\varphi_0.\end{gathered} \tag{10}$$

Here φ_0 is the equilibrium angle between the vector $\boldsymbol{\rho}_0^H$ and the bond $H_{(2)}-0$.

We now can express the normal coordinates Q_1, Q_2, and Q_3 of the H_2O molecule in terms of the displacements y_1, y_2, and y_3:

$$\begin{gathered}Q_1=a_1s_1+a_2(s_2+s_3)=d_1y_1+d_2y_2+d_3y_3,\\ Q_2=a_3s_1+a_4(s_2+s_3)=d_4y_1+d_5y_2+d_6y_3,\\ Q_3=a_5(s_2-s_3)=d_7y_1+d_8y_2+d_9y_3.\end{gathered} \tag{11}$$

The quantities a_1, a_2, ..., a_5 are known from study of the vibrational spectra of the H_2O molecule, and therefore the coefficients d_i can easily be computed by means of Eqs. (9) and (10). We finally obtain for the vibrational wave function of the ground state of the H_2O molecule the following expression:

$$\begin{aligned}\Phi_0(\mathbf{y},\mathbf{R}_B)&=N_Q^0\exp\left\{-\frac{1}{2\hbar}\sum_i\omega_iQ_i^2\right\}\\ &=N_y^0\exp\left\{-{}^1/{}_2(f_{11}y_1^2+f_{22}y_2^2+f_{33}y_3^2+f_{12}y_1y_2\right.\\ &\qquad\left.+f_{13}y_1y_3+f_{23}y_2y_3)\right\},\end{aligned} \tag{12}$$

where

$$\begin{aligned}
f_{11}&=(\omega_1 d_1^2+\omega_2 d_4^2+\omega_3 d_7^2)/\hbar=0.139\cdot 10^{18}\ \mathrm{cm}^{-2},\\
f_{22}&=(\omega_1 d_2^2+\omega_2 d_5^2+\omega_3 d_8^2)/\hbar=1.995\cdot 10^{18}\ \mathrm{cm}^{-2},\\
f_{33}&=(\omega_1 d_3^2+\omega_2 d_6^2+\omega_3 d_9^2)/\hbar=1.893\cdot 10^{18}\ \mathrm{cm}^{-2},\\
f_{12}&=2(\omega_1 d_1 d_2+\omega_2 d_4 d_5+\omega_3 d_7 d_8)/\hbar=-0.528\cdot 10^{18}\ \mathrm{cm}^{-2},\\
f_{13}&=2(\omega_1 d_1 d_3+\omega_2 d_4 d_6+\omega_3 d_7 d_9)/\hbar=-0.602\cdot 10^{18}\ \mathrm{cm}^{-2},\\
f_{23}&=2(\omega_1 d_2 d_3+\omega_2 d_5 d_6+\omega_3 d_8 d_9)/\hbar=1.778\cdot 10^{18}\ \mathrm{cm}^{-2},
\end{aligned} \tag{13}$$

and the normalization is

$$(N_y^0)^2=\left|\frac{\partial Q}{\partial y}\right|(N_Q^0)^2=0.887\cdot 10^{26}\ \mathrm{cm}^{-3},$$

$$\frac{\partial Q}{\partial y}=\det\begin{vmatrix} d_1 & d_2 & d_3\\ d_4 & d_5 & d_6\\ d_7 & d_8 & d_9\end{vmatrix}. \tag{14}$$

Introducing the variables y_1, y_2, and y_3 into Eq. (6), it is easy to carry out in it integration over y_1 and y_2 and to arrive at the result

$$\begin{aligned}
M_{0\nu_C}^{\mathrm{in}}(\mathbf{q})&=\int_{-\infty}^{\infty} dy_1\,dy_2\,dy_3 \exp\{-i(q_1 y_1+q_2 y_2)\}\varphi_{\nu_C}^{*}(y_3-\Delta r_{\mathrm{OH}})\\
\Phi_0(y_1 y_2 y_3)&=\int dy_3\,\varphi_{\nu_C}(y_3-\Delta r_{\mathrm{OH}})F_0(q_1,q_2;y_3),
\end{aligned} \tag{15}$$

where

$$\begin{aligned}
&F_0(q_1,q_2;y_3)=4\pi N_y^0 a^{-1/2}\exp\{-{}^1\!/\!_2(\alpha q_1^2+\beta q_2^2\\
&\qquad+\gamma q_1 q_2)\}\exp\{i(c_1 q_1+c_2 q_2)y_3-{}^1\!/\!_2 b y_3^2\},\\
&a=4f_{11}f_{22}-f_{12}^2,\quad b=f_{33}-a^{-1}(f_{22}f_{13}^2+f_{11}f_{23}^2-f_{12}f_{13}f_{23}),\\
&c_1=a^{-1}(2f_{22}f_{13}-f_{12}f_{23}),\quad c_2=a^{-1}(2f_{11}f_{23}-f_{12}f_{13}),\\
&\alpha=4f_{22}/a,\quad \beta=4f_{11}/a,\quad \gamma=-4f_{12}/a,\\
&(\mathbf{q}^{\mathrm{in}}\Delta\boldsymbol{\rho}^{\mathrm{II}})=q_1 y_1+q_2 y_2,\quad \Delta r_{\mathrm{OH}}=r_{\mathrm{OH}}(\mathrm{OH})-r_{\mathrm{OH}}(\mathrm{H_2O}).
\end{aligned} \tag{16}$$

Substituting this result into Eq. (8), we eventually obtain the form factor

$$\begin{aligned}
|M_{0\nu_C}(q)|^2&=A_1 K_{\nu_C}\int_0^1 dt\\
&\times\int_0^{2\pi} d\varphi\exp\{-q^2(1-t^2)(\bar{\alpha}\cos^2\varphi+\bar{\beta}\sin^2\varphi+\bar{\gamma}\sin\varphi\cos\varphi)\}\,|H_{\nu_C}(e+ig(\mathbf{q}^{\mathrm{in}}))|^2,
\end{aligned} \tag{17}$$

in which

$$\begin{aligned}
&A_1=2^5\pi^{5/2}|N_y^0|^2 f_0^{1/2}a^{-1}(b+f_0)^{-1}\exp\{-f_0 b\Delta r_{\mathrm{OH}}^2/(b+f_0)\},\\
&K_\nu=(2\pi 2^\nu \nu!)^{-1}[(b-f_0)/(b+f_0)]^\nu,\quad t=\cos\theta,\\
&\bar{\alpha}=\alpha+c_1^2(b+f_0)^{-1},\quad \bar{\beta}=\beta+c_2^2(b+f_0)^{-1},\\
&\bar{\gamma}=\gamma+2c_1c_2(b+f_0)^{-1},\quad e=-b\Delta r_{\mathrm{OH}}f_0^{1/2}(b^2-f_0^2)^{-1/2},\\
&g(\mathbf{q}^{\mathrm{in}})=(c_1q_1+c_2q_2)f_0^{1/2}(b^2-f_0^2)^{-1/2},\quad f_0=\hbar^{-1}\mu_{\mathrm{OH}}\omega_{\mathrm{OH}},
\end{aligned}$$

μ_{OH} is the reduced mass of the OH radical and $H_\nu(x)$ is a Hermite polynomial.

The result (17) is greatly simplified if we sum the contributions from all vibrational states φ_{ν_C} of the OH radical. Indeed, the completeness relation

$$\sum_{\nu_C}\langle \mathbf{y}|\varphi_{\nu_C}\rangle\langle\varphi_{\nu_C}|\mathbf{y}'\rangle=\delta(\mathbf{y}-\mathbf{y}')$$

leads to the following expression for the complete form factor of H_2O molecule:

$$\begin{aligned}
|M_0(q)|^2&\equiv\sum_{\nu_C}|M_{0\nu_C}(q)|^2=\int_0^{2\pi} d\varphi\int_0^{\pi}\frac{\sin\theta\,d\theta}{4\pi}\int_{-\infty}^{\infty} dy_3|F_0(q_1,q_2;y_3)|^2\\
&=A_2\exp\left(-\frac{1}{2}\beta' q^2\right)\int_0^1 dt\exp\left\{-\left(\alpha'-\frac{1}{2}\beta'\right)q^2t^2\right\}I_0\left\{\frac{1}{2}\beta' q^2(1-t^2)\right\},
\end{aligned} \tag{18}$$

where

$$\begin{aligned}
A_2&=16\pi^{5/2}a^{-1}b^{-1/2}|N_y^0|^2,\quad \alpha'=\frac{1}{2}[\alpha+\beta+((\alpha-\beta)^2+\gamma^2)^{1/2}],\\
\beta'&=\frac{1}{2}[\alpha+\beta-((\alpha-\beta)^2+\gamma^2)^{1/2}],
\end{aligned} \tag{19}$$

and $I_0(x)$ is a Bessel function of imaginary argument.

In Fig. 1 we have shown the result of calculation of the form factors (17) and (18) for knockout of a hydrogen atom from H_2O, and also the complete form factor (18) for knockout of an oxygen atom. It is evident that in knockout of an H atom only the several lowest vibrational states of the OH radical are excited. This is explained by the small change Δr_{OH} of the equilibrium distance r_{OH} in the transition from the H_2O molecule to the OH radical. In contrast to this, in knockout of an oxygen atom from the H_2O molecule the distance r_{HH} decreases by 50% in the transition to the H_2 residue, and states of the H_2 molecule with high vibrational quantum numbers are mainly excited. Therefore, we *shall limit* ourselves to illustration of the complete form factor for this case.

Our adiabatic discussion assumes that as R_B approaches infinity there is no crossing of terms and the final radical C is formed in the ground state. It is obvious that by knocking out various atoms from a molecule it is possible to study very diverse radicals, including short-lived ones.

If we now turn to knockout of a hydrogen atom from the H_2 molecule, we obtain for the corresponding form factor

$$\begin{aligned}
M_{LM}(\mathbf{q})&=\int e^{-i\mathbf{q}\mathbf{R}}\Phi_0(R)Y_{LM}(\Omega_R)\,d\mathbf{R},\\
M_L^2(q)&=\frac{1}{2L+1}\sum_M|M_{LM}(\mathbf{q})|^2=4\pi\left|\int_0^{\infty} j_L(qR)\Phi_0(R)R^2dR\right|^2\\
&=4\pi^{1/2}\alpha_0\left|\int_{-\infty}^{\infty} j_L(qR_0+qx)\exp\left(-\frac{\alpha_0^2x^2}{2}\right)(R_0+x)\,dx\right|^2,
\end{aligned} \tag{20}$$

where $\alpha_0^2=\mu\omega_0/\hbar$, and R_0 is the is the equilibrium distance between the nuclei in this molecule.

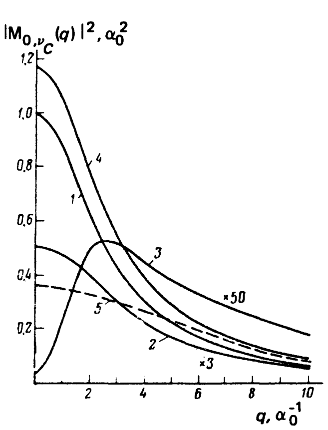

FIG. 1. Form factors for quasielastic knockout of a hydrogen atom from the H_2O molecule with transition to various vibrational states $|\nu_C\rangle$ of the OH radical. Curves 1, 2, and 3 correspond to $\nu_C=0$, 1, and 2. Curves 4 and 5 show complete form factors for knockout from H_2O of an H atom and an O atom, respectively.

The last integral can be calculated approximately in analytical form if we take into account that the main contribution to it is from the region $\Delta x \sim \alpha_0^{-1} \ll R_0$. For this purpose we use the well known expression for the spherical Bessel function

$$j_L(z)=(-1)^L z^L \left(\frac{d}{z\,dz}\right)^L \left(\frac{\sin z}{z}\right),$$

which can be reduced to the form

$$j_L(z)=U_{L+1}(z^{-1})\sin z+U_L(z^{-1})\cos z. \tag{21}$$

Here U_L is some polynomial of degree L, and $z=q(R_0+x)$.

It is clear that U_L and U_{L+1} in Eq. (21) for not too large L vary slowly in the indicated interval Δx in comparison with the oscillating functions $\sin(qR_0+qx)$ and $\cos(qR_0+qx)$. This permits us approximately to take U_L and U_{L+1} out from under the integral sign. Calculating the remaining integral, we obtain

$$M_L^2(q)\approx\frac{8\pi^{3/2}R_0^2}{\alpha_0}j_L^2(qR_0)\exp\left(-\frac{q^2}{\alpha_0^2}\right). \tag{22}$$

If we are interested in the result for some final temperature T of the gas target, it is necessary to take in accordance with Eq. (7) the appropriate combination of form factors (22).

In Fig. 2 we have shown the results of calculation of the form factor (in relative units) for knockout of a hydrogen atom from the H_2 molecule at various temperatrues. It can be seen that with increase of T the width of the form factor increases. The narrowest form factor is at $T=0$, when the contribution to the cross section is only from the state with $L=0$. On increase of T, states with higher angular momenta begin to play a part, but the number of such states which contribute substantially to the cross section is comparatively small. Thus, for $T=300$ K it is sufficient to take into account states with $L \leqslant 4$. We note that with increase of T the absolute value of the maximum of the form factor decreases.

The cross section $(d\sigma_{AB}/d\Omega)_{f\,r}$ which determines the cross section (1) of the quasielastic knockout process is rather large, of the order of 10^{-19} cm^2/sr. Therefore the achievement of such an experiment in gaseous targets similar to those used in Weigold's group[1] is quite realistic, including also measurement of the angular correlations of the final products. The energy resolution $\Delta E \sim 0.1-0.01$ eV desired in such experiments at bombarding-particle energies $E_0=p_0^2/2m_A=300-500$ eV is not very far removed from the resolution already used by experimenters at the present time[1] and appears quite achievable.

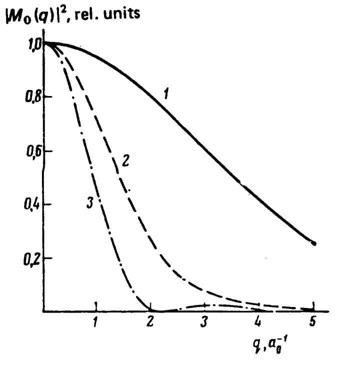

FIG. 2. Form factors for knockout of a hydrogen atom from the H_2 molecule at different temperatures: curve 1) $T \gg {}^{\mathrm{rot}}_{C} = 85.4$ K; curve 2) $T = 300$ K; curve 3) $T \ll T_C^{\mathrm{rot}}$.

Considering briefly more complicated molecules, we note that there can be both cases in which the radical C in its electronic ground state is a slightly changed fragment of the (BC) molecule (for example, the transition $NH_3 \to NH_2$), and cases where the radical will be substantially rearranged in shape (in the transition $CH_4 \to$ CH3 this last radical in its electronic ground state is planar, and only one of the lowest electronically excited states is a pyramidal fragment of the tetrahedron; the behavior of the shape of radicals is discussed in Herzberg's book[8]). In the first case naturally only the lowest vibrational levels of the radical will be excited, and in the second case—higher levels. The question of the relative probabilities of excitation of various electronic states of the final radicals requires special consideration. The approximation of adiabaticity does not exclude electronic excitation of the final radical as the result of possible crossing of levels. This question is closely related to another interesting problem—the physics of the process of quasielastic knockout of an atom by a doubly charged ion A^{++} (for example, an α particle) with pickup of an electron, where we finally detect singly charged ions A^+ and B^+. This is apparently a technically very simple experiment, but the ions will exert a strong perturbing influence on the electronic configurations (since we are discussing in the present work especially stable atoms of noble gases such as He or even neutrons as bombarding particles, we shall everywhere neglect this effect). Therefore the information obtained will be greatly complicated—it will be characterized by vibrational and electronic degrees of freedom simultaneously.

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Hydrodynamic instability and spontaneous magnetic fields in a spherical laser plasma

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We consider the magnetic fields generated in a spherical laser target by the appearance of thermoelectric currents in the region between the thermal-wave front and the surface on which the hydrodynamic velocity is equal to the local velocity of sound (the Jouguet point). Noncollinear temperature and density gradients are produced by small perturbations and by the development of a Rayleigh-Taylor instability. For targets in the form of glass shells, which are being studied in contemporary experiments, these fields amount to $\sim 10^6$ G at laser-irradiation energies $\sim 10^2$ J [N. G. Basov *et al.*, JETP Lett. 23, 428 (1976)] and are capable of magnetizing the plasma in the indicated region ($\omega_e \tau_e \sim 1$). Outside the target, the fields decrease rapidly to less than one gauss at a distance ~ 1 mm.

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1. Magnetic fields of appreciable magnitude (up to 10^6 G) have been observed in experiments on the interaction of laser radiation with the matter in the produced plasma.[1-5] Although many experiments have not been uniquely interpreted, the possibility of formation of strong magnetic fields in a laser produced plasma is subject to no doubt. The presence of a field of $\sim 10^6$ G can significantly alter the transport coefficients of the plasma, influence the transport of "fast electrons" from the "corona" of the target, deform the profile of the electron density in the corona, and change the character of the evolution of the hydrodynamic perturbations. The strongest effect can be exerted on the target compression by the plasma magnetization in the region between the zone where the laser radiation is absorbed and the front of the thermal wave, since this region is responsible for the formation of the pressure pulse.

The present paper deals with the generation of the fields in this region. The field generation can be the result of a number of mechanisms: a) resonant absorption of plane-polarized light[5] and anisotropy of the light pressure[7]; b) magneto-thermal instability[8,9]; thermoelectric power in inhomogeneous plasma.[3] We shall show that at radiation fluxes $\sim 10^{14}$ W/cm² and at the plasma parameters in the indicated zone ($N_e \sim 10^{21-22}$ cm^{-3}, $T_e \sim 1$, eV) the main contribution to the generation of the field is made by a mechanism connected with the thermoelectric power in the inhomogeneous plasma.
Let us estimate the fields for the aforementioned mechansims.

a) In the general case, the magnetic-field generation is connected with the anisotropy of the energy-momentum tensor T^{ik} of the electromagnetic field[5,7]:

$$\frac{\partial \mathbf{B}}{\partial t} = \frac{c}{e} \operatorname{rot} \frac{\mathbf{f}}{N_e},$$
$$f^i = \frac{\partial T^{ik}}{\partial x^k}.$$

In particular, magnetic fields can result from an increase in the longitudinal component of the electric field in the incident wave as the critical density is approached.

Let us estimate the magnetic field in the case when the presence of the longitudinal component is due to oblique incidence of the wave on the critical surface,[10] while the saturation mechanism is connected with the fact that the electrons carry the field out of the generation region[5]:

$$B \leqslant \frac{c}{JL_0} \left(\frac{\omega}{\nu}\right)^2 \frac{E_0^2}{8\pi} \sin\theta \cos\theta \exp\left[-\frac{4}{3} k_0 L_0 \sin^3\theta - 2k_0 L_0 \left(\frac{\nu}{\omega}\right)^2 \right],$$

where $J = eN_e v_e$, $L \sim 3\lambda_0$, $\nu \sim 0.1\omega_p$ ($\omega_p = (4\pi N_e e^2/m_e)^{1/2}$ is the plasma frequency), and $\theta = 10°$. For the specified parameters we obtain

$$B \leqslant 3 \cdot 10^4 \text{ G}.$$

b) The magneto-thermal instability mechanism causes the field to increase in the case when the direc-