Application of zero range potentials in the theory of collisions of electrons with molecules

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The collision of a light particle 1 with a bound system of two heavy particles (2,3) ($m_1 \ll m_{23}$) is considered under the assumption that the energy of particle 1 appreciably exceeds the binding energy of the system (2,3), and that the attraction of 1 to 2 and 3 can be replaced by a zero range potential. An approximate solution of the Faddeev equations is obtained and on its basis expressions are derived for the effective cross sections for elastic and inelastic collisions and for the rearrangement process $1+(2,3)\rightarrow(1,2)+3$. It is suggested that the expressions obtained may be used for calculating the excitation of rotation and oscillations of molecules by electron impact, and also the process of dissociative attachment at electron energies of several eV.

1. INTRODUCTION

In this paper we consider the excitation of rotational and vibrational states of a molecule by electron impact, and also the process of dissociative attachment (i.e., a reaction of the type $AB + e \rightarrow A^- + B$) under the following assumptions: 1) the electron energy is significantly greater than the dissociation energy of the molecule in its ground electron state; 2) the attraction of the electron to each of the atoms forming the molecule is replaced by a zero-range potential (or, what amounts to the same thing, by the assignment of a logarithmic derivative of the wave function at the places where the nuclei of the atoms are located). The condition for applicability of the zero-range potentials limits the energy of the electron from above. The range of energies defined by these assumptions amounts to several electron volts. Just this range of energies is of interest in connection with the existence of broad resonance maxima of the effective cross sections of the processes mentioned.[1]

The adiabatic approximation is used for calculation of the excitation of rotations and vibrations in the range considered, its starting point being the electron-scattering pattern in the case of a constant distribution of the coordinates of the nuclei, characterized by the initial wave function $\varphi_0(r \ldots r_n)$. The amplitude of the transition to the state $\varphi_n(r_1 \ldots r_n)$ is calculated by perturbation theory and turns out to be proportional to the matrix element

$$M_{no} = \int \varphi_n^* A(r_1 \ldots r_n) \varphi_0 dr_1 \ldots dr_n, \qquad (1.1)$$

where $A(r_1 \ldots r_n)$ is the scattering amplitude of the electron for the fixed positions of the nuclei.

The value of A is not equal to the sum of the scattering amplitudes from each of the atoms separately, because of the existence of multiple scattering of the electron inside the molecule. In specific calculations of the amplitude A, various models have been used (see the review article [2], in which an extensive bibliography is included).

However, the model of zero-range potentials has not been used to date for calculation of the matrix element M_{no}, although the expression $A(r_1 r_2)$ is well known in the simplest case of two centers and a general method has been worked out for the construction of $A(r_1 \ldots r_n)$.[3]

This model obviously does not take into account the long-range interactions brought about by the existence of an electric quadrupole moment at the molecule, or by the electric dipole moment induced by the incident electron. In addition, the effects of other channels with possible excitation of electron states are not taken into account. But in return, this model allows us to take the multiple scattering into account in explicit fashion, as well as the resonances connected with it, for arbitrary number and location of the centers.[3] Under conditions in which such resonances play a dominant role, by determining the order of magnitude of the cross sections of the processes in which we are interested, the use of the zero range potential allows us to obtain a simple and effective estimate of the cross section.

At the same time, the model of several zero range potentials has specific features that require special consideration before we use it for calculation of M_{no}. The fact is that in a system of three particles 1, 2, 3 of which two, say, 2 and 3, interact with 1 by means of zero-range potentials, an attraction $-c/r^2$ arises between particles 2 and 3; here the coefficient c depends on the ratio of the masses. This attraction causes the particle to fall into the center.[4] The indeterminacy of the solution of the integral equation describing the scattering in such a system is closely connected with this fact, inasmuch as a nontrivial solution of the corresponding homogeneous equation is found to exist [5]. It is rather evident that none of these features appears within the framework of the adiabatic approximation. However, it is nevertheless important to obtain a formal proof of the possibility of application of the zero range potential within this framework.

Besides consideration of admissibility problems, it is also desirable to broaden the range of application of the zero range potentials beyond the limits of the problem of elastic and inelastic scattering, and to consider dissociative attachment also. With this purpose, we shall systematically investigate the interaction of a light particle with a bound system of two heavy particles, with the help of the Faddeev equations.

It is shown how the adiabatic approximation arises as the ratio of the mass of the light particle to the reduced mass of the heavy particles approaches zero. It is found that the transition to the zero range potential in this limiting case is entirely correct from the mathematical viewpoint. An expression is obtained for the amplitudes of the elastic and inelastic scattering and dissociative attachment.

2. THE FADDEEV EQUATIONS AND THEIR TRANSFORMATION

The Faddeev equations [6] are formulated for three parts into which the wave function is split:

$$\psi = \psi_{12} + \psi_{13} + \psi_{23} \qquad (2.1)$$

and have the form

$$\psi_{12} = -G_0(Z) T_{12}(\psi_{13} + \psi_{23}),$$
$$\psi_{13} = -G_0(Z) T_{13}(\psi_{12} + \psi_{23}), \qquad (2.2)$$
$$\psi_{23} = \Phi - G_0(Z) T_{23}(\psi_{12} + \psi_{13}).$$

The function Φ describes the free motion of particle 1 and the bound state of the system (2, 3);

$$G_0(Z) = (H_0 - Z)^{-1}, \qquad (2.3)$$

H_0 is the operator of the energy of free motion of all three particles;

$$Z = E + i0; \qquad (2.4)$$

E is the total energy of the system, equal to the sum of the binding energy of particles 2, 3 and the kinetic energy of particle 1; $T_{\alpha\beta}$ is the transition operator of the pair (α, β) in the absence of interaction with the particle γ.

For our purposes, it is convenient to transform Eqs. (2.2) to a more suitable form. We set

$$\psi_{12} = -G_0 F_3, \quad \psi_{13} = -G_0 F_2. \qquad (2.5)$$

We then get the following set of equations for F_2 and F_3:

$$[1 - T_{13} G_0 T_{23} G_0] F_2 + [T_{13} G_0 - T_{13} G_0 T_{23} G_0] F_3 = T_{13} \Phi,$$
$$\qquad (2.6)$$
$$[T_{12} G_0 - T_{12} G_0 T_{23} G_0] F_2 + [1 - T_{12} G_0 T_{23} G_0] F_3 = T_{12} \Phi,$$

and the equation for ψ is given below in terms of F_2 and F_3:

$$\psi = (1 - G_0 T_{12} - G_0 T_{13}) \Phi - G_0 T_{23} G_0 (F_2 + F_3) - G_0 T_{12} G_0 F_2$$
$$- G_0 T_{13} G_0 F_3 - G_0 (T_{12} + T_{13}) G_0 T_{23} G_0 (F_2 + F_3). \qquad (2.7)$$

This expression appears at first glance to be cumbersome and difficult to understand. Actually, the structure of (2.7) and the meaning of the individual terms become clear if we take into account that the residue of an expression of the type $G_0 T_{\alpha\beta} G_0 F$ at the poles of $T_{\alpha\beta}$ represents (accurate to within a coefficient) the amplitude of one of the possible processes of excitation or redistribution, and the residue at the pole of G_0 gives the amplitude of the disintegration. [7,8]

Leaving aside for a time from the last term in (2.7), the second term in (2.7) gives the elastic-scattering amplitude or the excitation of the system (2, 3), and the third and fourth terms give the amplitudes of the reactions $1 + (2, 3) \rightarrow (1, 2) + 3$ and $1 + (2, 3) \rightarrow (1, 3) + 2$, respectively. The last term gives contributions to all amplitudes and at the same time takes into account the mutual effect of these processes on one another.

In what follows, we shall consider (2.6) and (2.7) in the momentum representation. We shall denote the momenta of the particles by k_α and assume that the center of inertia of all three particles is at rest:

$$\sum_\alpha k_\alpha = 0. \qquad (2.8)$$

Then the wave functions depend on the two vector variables $k_{\alpha\beta}$, k_γ, where

$$k_{\alpha\beta} = (m_\beta k_\alpha - m_\alpha k_\beta)/(m_\alpha + m_\beta) \qquad (2.9)$$

$\alpha, \beta, \gamma = (1, 2, 3), (3, 2, 1), (2, 3, 1)$. We can use any

sequence (α, β, γ) as the arguments of the wave functions, but the combinations

$$\psi_{\alpha\beta}(k_{\alpha\beta}, k_\gamma).$$

turn out to be the most convenient.

The connection of the momentum and coordinate representations is given by the relation

$$\psi(r_{\alpha\beta}, \rho_\gamma) = \frac{1}{(2\pi)^3} \int \exp i (k_{\alpha\beta} r_{\alpha\beta} + k_\gamma \rho_\gamma) \psi(k_{\alpha\beta}, k_\gamma) dk_{\alpha\beta} dk_\gamma, \qquad (2.10)$$

where

$$r_{\alpha\beta} = r_\alpha - r_\beta,$$
$$\rho_\gamma = r_\gamma - (m_\alpha r_\alpha + m_\beta r_\beta)/(m_\alpha + m_\beta). \qquad (2.11)$$

In order not to encumber the formulas, we shall not write out Planck's constant, i.e., we shall assume $\hbar = 1$ (in the final formulas, it is an easy matter to restore the necessary power of $\hbar$). The function Φ is given by the expression

$$\Phi = \varphi_0(k_{23}) \delta(k_1 - p_0), \qquad (2.12)$$

where $\varphi_0(k_{23})$ is the wave function of the initial state of the system (2, 3).

We represent the energy level of the system (2, 3) in the form

$$E_n = -\varkappa_n^2 / 2m_{23}.$$

the quantity $\varkappa_n$ characterizes the scale of momentum distribution in the state φ_n. Thus, Z in Eqs. (2.2) is represented in the form

$$Z = p_0^2 / 2n_1 + \varkappa_0^2 / 2m_{23} + i0. \qquad (2.13)$$

The operators G_0 and $T_{\alpha\beta}$ are integral operators in momentum space, and their kernels have the form

$$G_0(k_{23}, k_1, k_{23}', k_1', Z) = \frac{\delta(k_{23} - k_{23}') \delta(k_1 - k_1')}{k_{23}^2 / 2m_{23} + k_1^2 / 2n_1 - Z}, \qquad (2.14)$$

where

$$m_{\alpha\beta} = \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}, \qquad n_\gamma = \frac{m_\gamma (m_\beta + m_\alpha)}{m_\alpha + m_\beta + m_\gamma}, \qquad (2.15)$$

$$T_{\alpha\beta} = t_{\alpha\beta} \left(k_{\alpha\beta}, k_{\alpha\beta}', Z - \frac{k_\gamma^2}{2n_\gamma} \right) \delta(k_\gamma - k_\gamma'). \qquad (2.16)$$

In the zero range potential approximation, the $t_{\alpha\beta}$ do not depend on the $k_{\alpha\beta}$ and have the form [6]

$$t_{\alpha\beta}(Z) = [(2\pi)^2 m_{\alpha\beta}(\alpha_{\alpha\beta} + i\sqrt{2m_{\alpha\beta}Z})]^{-1}, \qquad (2.17)$$

where the quantities $\alpha_{\alpha\beta}$ represent the inverse scattering lengths:

$$\alpha_{\alpha\beta} = a_{\alpha\beta}^{-1}. \qquad (2.18)$$

3. TRANSITION TO THE ADIABATIC APPROXIMATION AND THE ZERO RANGE POTENTIALS

We shall consider the operator $G_0 T_{23} G_0$ which enters into (2.6) and show that the result of its action on an arbitrary, sufficiently smooth function $F(k_{23}, k_1)$ vanishes in the limit $n_1/m_{23} \rightarrow 0$ under the condition that the $\varkappa_n$ are fixed (i.e., that the form of the functions φ_n remains unchanged). Inasmuch as the function F can be expanded in a series in the eigenfunctions

$$F = \sum_n \varphi_n(k_{23}) f_n(k_1),$$

it is sufficient to consider the effect of the operator on the function $\varphi_n f_n$.

Taking into account that

$$G_0 T_{23} G_0 = G_0 - G,$$

where

$$G = (H_0 + V_{23} - Z)^{-1},$$

and also that φ_n is the eigenfunction of the operator $k_{23}^2/2m_{23} + V_{23}$ with the eigenvalue $-\kappa_n^2/2m_{23}$, we get

$$(G_0 T_{23} G_0)\varphi_n f_n = \left[\left(k_1^2 + \frac{n_1}{m_{23}}k_{23}^2 - Z\right)^{-1} - \left(k_1^2 - \frac{n_1}{m_{23}}\kappa_n^2 - Z\right)^{-1}\right] 2n_1 \varphi_n f_n. \tag{3.1}$$

It is evident from this expression that as $n_1/m_{23} \to 0$ and for κ_n fixed, the right side vanishes. Thus, Eqs. (2.6) in the limit $n_1/m_{23} \to 0$ take the form

$$F_2 + T_{13}G_0 F_3 = T_{13}\Phi, \quad T_{12}G_0 F_2 + F_3 = T_{12}\Phi. \tag{3.2}$$

Our approximation is that for finite but small values of n_1/m_{23} we determine F_2 and F_3 from the system (3.2), in which $n_1/m_{23} = 0$.

We draw attention to the fact that for fixed κ_n and $m_{23} \to \infty$, all the energy levels of the system (2, 3) tend to zero. For finite m_{23}, however, the binding energy is different from zero. Therefore, use of (3.2) will be a reasonable approximation only if the presence of coupling in the system (2, 3) does not play a significant role in elastic scattering of particle 1. But this only can be the case when the energy of the incident particle appreciably exceeds the value of the binding energy.

Formally, all this can be seen from Eq. (3.1). To be precise, if we assume that $p_0^2/n_1 \gg \kappa_0^2/m_{23}$, we get

$$(G_0 T_{23} G_0)\varphi_n f_n = \left[\left(k_1^2 - p_0^2 + \frac{n_1}{m_{23}}k_{23}^2\right)^{-1} - (k_1^2 - p_0^2)^{-1}\right] 2n_1 \varphi_n f_n.$$

Through the entire important range of variation of k_{23} (which is determined by the rate of decay of the function φ_n as $k_{23} \to \infty$)

$$(G_0 T_{23} G_0)\varphi_n f_n \sim \frac{n_1^2}{m_{23}} \frac{k_{23}^2}{(k_1^2 - p_0^2)^2} \varphi_n f_n,$$

i.e., it is a small quantity, the order of smallness of which is determined by the parameter n_1/m_{23}. An exception is the region close to the poles, the width of which in the momentum scale $\sim (n_1/m_{23})k_{23}^2$.

Inasmuch as the width of the interval is small, it does not play a significant role in the equations (but for calculation of the amplitudes, it is precisely the behavior of $G_0 T_{23} G_0$ that is important near the poles; therefore we keep the term $G_0 T_{23} G_0$ in the expression for ψ).

Neglect of the operator $G_0 T_{23} G_0$ is equivalent to replacement of ψ_{23} by Φ in Eqs. (2.2). Hence it follows that the set of Eqs. (3.2) describes the scattering of particle 1, just as if the distribution of the momenta of particles 2 and 3 were to keep its initial value φ_0 in the scattering process.

Such an approximate description of the scattering process lies at the base of the well-known momentum approximation. Thus, in the problem considered, the scattering of a light particle by a system of heavy particles, the terms "adiabatic approximation" and "momentum approximation" are related to one another as the Fourier transform and its original.

We now write down the system (3.2) in the momentum representation, taking into account all the assumptions that have been made:

$$F_3(k_1, k) + 2m_1 \int dk' \frac{t_{12}(k_1, k-k', Z)F_2(k-k', k')}{(k-k')^2 - p_0^2 - i0}$$
$$= t_{12}(k_1, p_0, Z)\varphi_0\left(k - \frac{m_3}{m_2 + m_3}p_0\right),$$

$$F_2(k_1, k) + 2m_1 \int dk' \frac{t_{13}(k_1, k-k', Z)F_3(k-k', k')}{(k-k')^2 - p_0^2 - i0} \tag{3.3}$$
$$= t_{13}(k_1, p_0, Z)\varphi_0\left(k + \frac{m_2}{m_2 + m_3}p_0\right),$$

We now make the transition to the zero range potential. Inasmuch as t_{12} and t_{13} do not depend on k_{12}, k_{23}, the functions F_2, F_3 will depend not on two but on a single vector variable.

The limiting expressions for t_{12}, t_{13} as $n_1/m_{23} \to 0$, which should be substituted in (3.3), have the form

$$t_{12} = [(2\pi)^2 m_1(\alpha_{12} + ip_0)]^{-1},$$
$$t_{13} = [(2\pi)^2 m_1(\alpha_{13} + ip_0)]^{-1}.$$

The following set of equations is obtained:

$$F_3(k) + 2t_{12}m_1 \int \frac{dk' F_2(k')}{(k-k')^2 - p_0^2 - i0} = t_{12}\varphi_0\left(k - \frac{m_3}{m_2 + m_3}p_0\right),$$
$$F_2(k) + 2t_{13}m_1 \int \frac{dk' F_3(k')}{(k-k')^2 - p_0^2 - i0} = t_{13}\varphi_0\left(k + \frac{m_2}{m_2 + m_3}p_0\right). \tag{3.4}$$

The homogeneous equations which are obtained by discarding the right-hand sides do not have nonvanishing solutions, since t_{12}, t_{23} are complex numbers.

Equations (3.4) are solved exactly by means of the Fourier transform, i.e., by transition to the coordinate representation. After a simple calculation we get

$$F_3(r) = \frac{(\alpha_{13} + ip_0)\exp\left(-i\frac{m_3}{m_2 + m_3}p_0 r\right) - r^{-1}\exp i\left(\frac{m_2}{m_2 + m_3}p_0 r + p_0 r\right)}{(2\pi)^2 m_1[(\alpha_{12} + ip_0)(\alpha_{13} + ip_0) - r^{-2}\exp(2ip_0 r)]}\varphi_0(r),$$

$$F_2(r) = \frac{(\alpha_{12} + ip_0)\exp\left(i\frac{m_2}{m_2 + m_3}p_0 r\right) - r^{-1}\exp i\left(p_0 r - \frac{m_3}{m_2 + m_3}p_0 r\right)}{(2\pi)^2 m_1[(\alpha_{12} + ip_0)(\alpha_{13} + ip_0) - r^{-2}\exp(2ip_0 r)]}\varphi_0(r). \tag{3.5}$$

4. AMPLITUDES AND EFFECTIVE CROSS SECTIONS

The amplitudes of the processes of interest to us are determined from expression (2.7) for the wave function. In the approximation used here, the last term can be neglected (which means neglect of the mutual effects of the scattering processes and dissociative attachment).

Then the amplitude of each of the processes is determined from an expression of the form $G_0 T_{\alpha\beta} G_0 F$; we shall not assume $n_1/m_{23} = 0$ in the operators T_{12} and T_{13}, but shall use the exact expressions (2.17).

The determination of the amplitudes is carried out according to the following scheme.[7,8] Near the pole which corresponds to the bound state of the system (α, β), we have

$$t_{\alpha\beta}(k_{\alpha\beta}, k_{\alpha\beta}', Z - k_\gamma^2/2n_\gamma) = \frac{(k_{\alpha\beta}^2/2m_{\alpha\beta} - \varepsilon_n)(k_{\alpha\beta}'^2/2m_{\alpha\beta} - \varepsilon_n)}{Z - k_\gamma^2/2n_\gamma - \varepsilon_n}$$
$$\times \varphi_n(k_{\alpha\beta})\varphi_n^*(k_{\alpha\beta}') + (\text{smooth part}) \tag{4.1}$$

where φ_n is the wave function of the bound state and ε_n the energy of the system (α, β).

Therefore the expression $G_0 T_{\alpha\beta} G_0 F$ can be represented as the product of three factors:

$$G_0 T_{\alpha\beta} G_0 F = \varphi_n(k_{\alpha\beta})\left[\frac{1}{2n_\gamma}k_\gamma^2 + \varepsilon_n - Z\right]^{-1} M. \tag{4.2}$$

The middle factor describes the free motion of the particle γ relative to the system (α, β) (this corresponds to a diverging wave in the coordinate represen-

tation). It is then clear that the factor M (which is expressed in terms of an integral of the product of the function φ_n^* and F) represents the amplitude.

In addition, there also is the amplitude connected with the pole of G_0. It corresponds to dissociation of the molecule, and all the particles are found to be in the continuous spectrum. All three operators contribute to this amplitude.

In view of the fact that all the necessary calculations were carried out in detail in [8], we give only the final result here, with account of the fact that the energies of all the bound states are small in comparison with the energy of the incident particle.

The amplitude of the excitation in state n is equal to

$$M_{n0} = (2\pi)^2 m_1 \int \left[\varphi_n^* \left(\mathbf{p}' - \frac{m_3}{m_2+m_3} \mathbf{p} \right) F_3(\mathbf{p}') \right.$$
$$\left. + \varphi_n^* \left(\mathbf{p}' + \frac{m_2}{m_2+m_3} \mathbf{p} \right) F_2(\mathbf{p}') \right] d\mathbf{p}', \qquad (4.3)$$

and $\mathbf{p} = \mathbf{p}_0$ accurate to the discarded terms $\sim |E_n/E|$.

Transforming to the coordinate representation, we get

$$M_{n0} = (2\pi)^2 m_1 \int \varphi_n^*(\mathbf{r}) \left[\exp \left(i \frac{m_3}{m_2+m_3} \mathbf{p}\mathbf{r} \right) F_3(\mathbf{r}) \right.$$
$$\left. + \exp \left(-i \frac{m_2}{m_2+m_3} \mathbf{p}\mathbf{r} \right) F_2(\mathbf{r}) \right] d\mathbf{r}. \qquad (4.4)$$

In particular, for the case of identical particles 2 and 3, we have

$$M_{n0} = 2 \int \varphi_n^*(\mathbf{r}) \left[\frac{\cos(\mathbf{p}\mathbf{r}/2)\cos(p_0 r/2)}{\alpha + i p_0 + r^{-1} \exp i p_0 r} + \frac{\sin(\mathbf{p}\mathbf{r}/2)\sin(p_0 r/2)}{\alpha + i p_0 - r^{-1} \exp i p_0 r} \right] \varphi_0(\mathbf{r}) d\mathbf{r}. \qquad (4.5)$$

The effective cross section is

$$d\sigma/d\Omega = |M_{n0}|^2. \qquad (4.6)$$

The amplitude of the redistribution process $1 + (2, 3) \rightarrow (1, 2) + 3$ is equal to

$$M_D = (2\pi)^2 m_{23} \int \varphi_{12}^* \left(\mathbf{p}' - \sqrt{\frac{m_{23}}{m_1}} \mathbf{p} \right) F_2(\mathbf{p}') d\mathbf{p}' \qquad (4.7)$$

$(\mathbf{p} \approx \mathbf{p}_0)$. Transforming to the coordinate representation, we have

$$M_D = (2\pi)^2 m_{23} \int \varphi_{12}^*(\mathbf{r}) \exp \left(i \sqrt{\frac{m_{23}}{m_1}} \mathbf{p}\mathbf{r} \right) F_2(\mathbf{r}) d\mathbf{r}, \qquad (4.8)$$

where φ_{12} is the wave function of the system (1, 2) in the zero range potential approximation:

$$\varphi_{12}(r) = \sqrt{\frac{\alpha}{2\pi}} \frac{1}{r} \exp(-\alpha r). \qquad (4.9)$$

The effective cross section is

$$d\sigma_D/d\Omega = (m_1/m_{23})^{1/2} |M_D|^2. \qquad (4.10)$$

Using the optical theorem, we get the total cross section σ_t of all processes (including dissociation and dissociative attachment). If the system (2, 3) does not have spherical symmetry in the ground state, then we must average σ_t over all possible directions of the initial momentum $\mathbf{p}_0$. In particular, for the case of identical particles 2 and 3, we have

$$\langle \sigma_t \rangle = \frac{4\pi}{p_0^2} \int d\mathbf{r} |\varphi_0|^2 \left\{ \left[1 + \left(\frac{\alpha r + \cos p_0 r}{p_0 r + \sin p_0 r} \right)^2 \right]^{-1} \right.$$
$$\left. + \left[1 + \left(\frac{\alpha r - \cos p_0 r}{p_0 r - \sin p_0 r} \right)^2 \right]^{-1} \right\}. \qquad (4.11)$$

The expression in braces, together with the factor $4\pi/p_0^2$, is identical with the averaged cross section of

scattering by fixed centers as calculated by Demkov and Rudakov.[3]

5. DISCUSSION

The expressions given in Sec. 4 for the effective cross sections reproduce the principal characteristic features observed in the interaction of electrons with molecules at energies of several eV.[1] We shall demonstrate this with the simplest example of molecules consisting of identical atoms.

Let us consider the expression

$$J_{\pm}(p_0) = \alpha + i p_0 \pm r^{-1} \exp(i p_0 r), \qquad (5.1)$$

which enters into the denominators of the functions F_2 and F_3 of (3.5).

For fixed values of r and varying p_0, cases in which the real part of $J_{\pm}$ vanishes are possible, i.e.,

$$r\alpha \pm \cos p_0 r = 0. \qquad (5.2)$$

These points correspond to resonance maxima of the functions F_2 and F_3, and this leads to resonance maxima in the cross sections of all the processes, and also in the total cross section $\langle \sigma_t \rangle$. Integration over r, which is provided for in the corresponding formulas, will spread out these maxima.

Furthermore, the presence of $\sqrt{m_{23}}$ in the exponent in the formula (4.7) for the amplitude of dissociative attachment leads to the appearance of a significant isotope effect in the cross section of this process, which is also observed experimentally.

In the present paper all these features have been expressed in terms of the multiple-scattering picture, the effect of which is characterized by the term $r^{-1} \exp(i p_0 r)$ in the functions F_2 and F_3.

The traditional interpretation of resonance phenomena in the interaction of electrons with molecules is based on the picture of quasistationary terms of the negative molecular ion AB^-.[1] In particular, the isotope effect in the process of dissociative attachment was predicted by Demkov[9] in just such an approach.

A connection can be established between these two pictures of the phenomenon if it is noted that the imaginary zeroes of the expression for $J_{\pm}(p_0)$ give the terms of the system A_2^- in the Firsov-Smirnov model, while the complex zeroes correspond to the continuation of the terms into the region of quasistationary states.[10]

The problem of the quantitative agreement between the measured absolute values of the cross sections and those computed from the equations of Sec. 4, can be solved only as we accumulate specific numerical calculations. The problem of the choice of values of α should be discussed in this connection.

It would be simplest to take quantities that correspond to the scattering of atoms that are not free. Here, if the atoms have nonvanishing spins (which, as a rule, is the case in molecules), it is necessary to take into account that the scattering length depends on the total spin of the electron and atom, and to carry out the appropriate averaging over the spin variables. One can obtain a more flexible model by considering the α as empirical parameters.

The model of the zero range potential can be generalized within the framework of the adiabatic approximation

to any polyatomic molecule. The expression for $\langle \sigma_t \rangle$ is generalized most directly and simple, viz.,

$$\langle \sigma_t \rangle = \int d\mathbf{r}_1 \ldots d\mathbf{r}_n |\varphi_0|^2 \bar{\sigma} (\mathbf{r}_1 \ldots \mathbf{r}_n), \qquad (5.3)$$

where $\bar{\sigma}(\mathbf{r}_1 \ldots \mathbf{r}_n)$ is the scattering cross section for a system of fixed centers, averaged over all directions of the momentum of the incident electron. The general method for calculation of $\bar{\sigma}$ is developed in [3]; φ_0 is the wave function which describes the motion of the nuclei in the polyatomic molecule in the ground electron state.

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