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Scattering of slow electrons by polar molecules

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The scattering of electrons by polar molecules is considered for the energy range in which, on the one hand, the molecule may be considered as immobile, and on the other, the electron wavelength is large in comparison with the radius of short-range forces. The existence of dipole resonances is discussed. The results of the theory are compared with the experimental data and calculations are carried out by the close-coupling method.

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1. INTRODUCTION

The fundamental contribution to the scattering of slow electrons by polar molecules is made by the long-range electron-dipole interaction. Therefore, only this part of the interaction between electron and molecule has been taken into account in a number of researches on the calculation of the scattering cross section. Scattering has been considered by an immobile[1] and by a rotating[2] dipole in the Born approximation. In the first case, the total cross section diverges, owing to the long-range character of the interaction,[3] while in the second case, if the molecule is regarded as a rigid rotator, we get1)

$$\sigma(j\to j\pm1)=\frac{8\pi}{3k_i^2}D^2\frac{j_>}{2j+1}\ln\left|\frac{k_i+k_f}{k_i-k_f}\right|, \qquad (1)$$

where j is the rotational quantum number of the rotator, $j_>=\max(j, j\pm1)$, D is the dipole moment, while k_i and k_f are the initial and final wave numbers of the electron and are connected by the relation

$$k_i^2+j(j+1)/I=k_f^2+(j\pm1)(j\pm1+1)/I, \qquad (2)$$

where I is the moment of inertia of the rotator.

Mittleman and von Holdt[4] have given an exact solution of the problem of scattering by an immobile point dipole. Because of the singularity of the potential $D\cos\theta/r^2$ at zero, such an approach is limited to values of $D<D_{cr}=0.639$. At $D\geqslant D_{cr}$, collapse to the center takes place. Therefore a more realistic approach is the consideration of scattering by a finite dipole. This problem has been solved both numerically[5] and analytically.[6]

Simultaneous account of strong interaction and rotation of the molecule has been carried out by the method of strong coupling,[7] used in the consideration of scattering by a whole series of molecules.

In all these researches, the short-range part of the interaction has not been computed from first principles, but introduced in the form of a model potential, which introduces some ambiguity in the interpretation of the results. On the one hand, it is well known that the behavior of the cross sections at low energies is determined by the long-range part of the interaction. Therefore, in some electron energy region, without using complicated calculations of the type of the strong coupling method and without making assumptions on the specific form of the short-range forces, we can obtain for the cross sections simple expressions of the type of the formulas of the effective radius theory. This is in fact the aim of the present work.

2. SCATTERING AMPLITUDE

We regard the molecule as an immobile dipole. We introduce a sphere of radius r_0, the center of which is identical with the center of gravity of the molecule. Let the interaction be described by the potential

$$U(\mathbf{r})=\begin{cases} V(\mathbf{r}), & r<r_0, \\ \mathbf{Dr}/r^3, & r>r_0, \end{cases} \tag{3}$$

where $V(\mathbf{r})$ is an arbitrary function, such that it does not collapse onto the center.

At $r>r_0$, the particular solution of the Schrödinger equation in the set of coordinates in which the polar axis is directed along D, has the form

$$\begin{aligned} &\psi_\nu{}^m=u_\nu{}^m(r)r^{-1}Z_\nu{}^m(\theta,\varphi), \\ &Z_\nu{}^m(\theta,\varphi)=Q_\nu{}^m(\cos\theta)e^{im\varphi}, \end{aligned} \tag{4}$$

where m is the conserved projection of the angular momentum of the electron on the axis of the molecule, and u_ν^m and Z_ν^m are the solutions of the equations

$$\left[\frac{d^2}{dr^2}+k^2-\frac{\lambda_\nu{}^m(\lambda_\nu{}^m+1)}{r^2}\right]u_\nu{}^m(r)=0, \tag{5}$$

$$[\Delta_{\theta\varphi}+2D\cos\theta+\lambda_\nu{}^m(\lambda_\nu{}^m+1)]Z_\nu{}^m(\theta,\varphi)=0, \quad \nu=0,1,\ldots. \tag{6}$$

The eigenvalues λ_ν^m and the eigenfunctions of Eq. (6) can be sought in the form of the expansion

$$Q_\nu{}^m(\cos\theta)=\sum_{n=0}^{\infty}a_{\nu n}{}^m\bar{P}_{n+|m|}^{|m|}(\cos\theta), \tag{7}$$

where $\bar{P}_{n+|m|}^{|m|}$ are the normalized associated Legendre functions. Then $a_{\nu n}^m$ and λ_ν^m are found numerically by the variational method.

We construct solutions of Eq. (5) in the form of linear combinations of the functions

$$\varphi_{\nu m}{}^{\pm}(kr)=\pm i(\pi kr/2)^{1/2}H_{\lambda+1/2}^{(1,2)}(kr), \quad \lambda=\lambda_\nu{}^m, \tag{8}$$

where $H_{\lambda+1/2}^{(1,2)}$ are Hankel functions. We write out the general solution of the Schrödinger equation in the form

$$\begin{aligned} \psi&=\frac{1}{r}\sum_{\nu m}u_\nu{}^m(r)Z_\nu{}^m(\theta,\varphi) \\ &=\frac{1}{r}\sum_{\nu m}A_{\nu m}[\varphi_{\nu m}^{(-)}(kr)-s_\nu{}^m\varphi_{\nu m}^{(+)}(kr)]Q_\nu{}^m(\cos\theta)e^{im\varphi}. \end{aligned} \tag{9}$$

From the condition at ∞, where there should be a plane plus a diverging wave, we determine the coefficients $A_{\nu m}$ and the scattering amplitude f:

$$\begin{aligned} &A_{\nu m}=i\exp[i\pi(m-\lambda_\nu{}^m/2)]Q_\nu{}^m(-\cos\xi), \\ &f(\xi,\theta,\varphi) \\ &=\frac{i}{k}\sum_{\nu m}\{Q_\nu{}^m(\cos\xi)-\exp[i\pi(m-\lambda_\nu{}^m)]s_\nu{}^mQ_\nu{}^m(-\cos\xi)\}Q_\nu{}^m(\cos\theta)e^{im\varphi}, \end{aligned} \tag{10}$$

where ξ is the angle between the direction of the incident electron beam and the axis of the molecule.

Thus, for given m, the scattering is completely determined by the choice of the numbers s_ν^m, $\nu=0,1,\ldots$, which satisfy the unitarity condition

$$|s_\nu{}^m|=\exp(-\operatorname{Im}\lambda_\nu{}^m). \tag{11}$$

In the approximation of a point dipole $s_\nu^m=1$ and (10) gives the amplitude of scattering obtained by Mittleman and von Holdt.[4] In the general case, the amplitude (10) agrees with that given by Abramov and Komarov,[6] the only difference being that in place of the functions Q_ν^m we have the eigenfunctions of the operator $\Delta_\eta+D\eta$, where η is the angular variable in prolate spheroidal coordinates and Δ_η is the corresponding part of the Laplace operator. The diagonal elements of the scattering operator correspond to the numbers $s_\nu^m\exp(-i\pi\lambda_\nu^m)$ in the paper of Abramov and Komarov.[6] In our case, the scattering operator is diagonal only when λ is conserved. However, the condition of conservation of λ leads to a singular behavior of the potential at zero (as in the case of a point dipole). Therefore, the S matrix in the λ representation should be nondiagonal. Nevertheless the elements s_ν^m contain all the information on the scattering and the S matrix can be established from them.

For the determination of s_ν^m, we match the function (9) to the solution Ψ of the Schrödinger equation in the region $r<r_0$. For given m, Ψ can be expanded in the functions Z_ν^m in the form

$$\Psi^m(\mathbf{r})=\frac{1}{r}\sum_\nu v_\nu{}^m(r)Z_\nu{}^m(\theta,\varphi),$$

and the Wigner R matrix

$$R^m=v^m\left(\frac{dv^m}{dr}\right)^{-1}\Bigg|_{r=r_0},$$

can be constructed from the functions v_ν^m. Here v^m is the matrix of solutions v_ν^m, in which the rows correspond to different ν and the columns to different, linearly independent solutions. Then the matching conditions are written in the form[8]

$$u^m(r_0)=R^m\frac{du^m}{dr}\Bigg|_{r=r_0}, \tag{12}$$

where u^m is the column with elements $u_{\nu m}$.

From (9), we get

$$u^m=A^m(\varphi_m{}^-I-\varphi_m{}^+s^m), \tag{13}$$

where A^m and $\varphi_m^\pm$ are diagonal matrices with elements

$A_{\nu m}$ and $\varphi^{\pm}_{\nu m}$; s^m is a column with elements s^m_ν and I is a column of unit values.

$$s^m=(A^m)^{-1}\left[\left(R^m\frac{d}{dr}-1\right)\varphi_m^+\right]^{-1}\left(R^m\frac{d}{dr}-1\right)\varphi_m^-A^mI\Big|_{r=r_0}. \tag{14}$$

If none of the poles of the R matrix is close to zero (i.e., there are no resonances produced by the potential $V(\mathbf{r})$ in (3) near $k^2=0$), then it is possible to expand in powers of k^2 and limit ourselves at first to the zeroth term. The functions $\varphi^{\pm}_{\nu m}$ can be represented in the form

$$\varphi^{\pm}_{\nu m}=B_{\nu m}k^{-\lambda_\nu^m}-\exp[\mp i\pi(\lambda_\nu^m+{}^1/_2)]C_{\nu m}k^{\lambda_\nu^m+1}, \tag{15}$$

where $B_{\nu m}$ and $C_{\nu m}$ are integral functions of k^2 and can be assumed to be independent of k in the zeroth approximation.

We further distinguish between two cases: 1) for given ν, m, the value of λ^m_ν is real; 2) λ^m_ν is complex. In the second case,

$$\lambda_\nu^m=-{}^1/_2+i\mu_\nu^m, \tag{16}$$

where μ^m_ν are real.

In case 1), $B_{\nu m}$ and $C_{\nu m}$ are real, and in case 2) they are complex but connected by the relation

$$C_{\nu m}=-B^*_{\nu m}. \tag{17}$$

Substituting (15) in (14), we obtain a formula similar to that introduced by Gailitis and Damburg in Ref. 9 in the study of the threshold behavior of the cross section for electron scattering from a hydrogen atom,

$$\begin{aligned} s^m=I+2i(A^m)^{-1}k^{\lambda^m}(M^m+\exp[-i\pi(\lambda^m+{}^1/_2)]\\ \times k^{2\lambda^m+1})^{-1}\sin[\pi(\lambda^m+{}^1/_2)]k^{\lambda^m+1}A^mI, \end{aligned} \tag{18}$$

$$M^m=-\left[\left(R^m\frac{d}{dr}-1\right)C^m\right]^{-1}\left(R^m\frac{d}{dr}-1\right)B^m\Big|_{r=r_0}, \tag{19}$$

where λ^m, B^m, C^m are diagonal matrices. The M matrix (19) possesses the same analytic properties as the R matrix.

The behavior of s^m_ν at small k^2 depends on the properties of the λ^m_ν. If none of the λ^m_ν is complex, then, in the zeroth approximation, $s^m=I$. In the next approximation (and if there are complex λ, then immediately), one must take into account the second term in (18). For most molecules, D is such that account only of $\lambda^0_0=\lambda$ makes a significant contribution to (18). In this case,

$$\begin{aligned} s_0^0&=1+\frac{2i\sin\pi(\lambda+{}^1/_2)k^{2\lambda+1}}{\eta+\exp[-i\pi(\lambda+{}^1/_2)]k^{2\lambda+1}},\\ s_\nu^m&=1+O(k^{\lambda+\lambda_\nu^m+1}),\quad (\nu,\ m)\neq(0,\ 0), \end{aligned} \tag{20}$$

where $\eta=1/(N^{-1})_{00}$ and N is the zeroth term of the expansion of the M matrix in k^2. If $D>3.79$, then λ^1_0 becomes complex and s^1_0 must be taken in the form (20).

If λ is real, then η is also real. In the case of complex λ (which corresponds to $D>D_{\text{cr}}$), we have from (17), (19) that $|\eta|=1$ and we can write (20) in the form

$$s_0^0=\frac{1+e^{-\pi\mu+i\alpha}k^{2i\mu}}{1+e^{\pi\mu+i\alpha}k^{2i\mu}},\qquad \alpha=\arg\eta. \tag{21}$$

If $\lambda=-\frac{1}{2}(D=D_{\text{cr}})$, then $\eta=-1$ and

$$s_0^0=1+\frac{2\pi i}{\zeta-\pi i+2\ln k},\qquad \zeta=\lim_{\lambda\to-1/2}\frac{d\eta}{d\lambda}. \tag{22}$$

The expression obtained for s^0_0 coincides (after multiplication by $e^{-i\pi\lambda}$) with the first diagonal element of the scattering operator for a finite dipole, calculated by Abramov and Komarov[6] with the help of the technique developed by them[10] if we set

$$-\frac{1}{\eta}=\left(\frac{R}{8}\right)^{2\lambda+1}\frac{\Gamma^2({}^1/_2-\lambda)\Gamma(\lambda+1)}{\Gamma^2({}^3/_2+\lambda)\Gamma(-\lambda)},$$

where R is the length of the dipole. Such an identity will exist in the case $m\neq0$, $\nu=0$. At $\nu\neq0$ the terms in s^m_ν become significant that are connected with the mixing of different λ_ν, and there is no similar coincidence. Thus, for each m, the results of our model are identical to the results of the model of the finite dipole in the zeroth approximation, as $k\to0$.

The scattering amplitude (10) in the case of a single isolated λ can be written in the form

$$f(\xi,\theta,\varphi)=\frac{i}{k}\{a_0(\xi,\theta,\varphi)-e^{-i\pi\lambda}s_0^0Q_0^0(-\cos\xi)Q_0^0(\cos\theta)\}, \tag{23}$$

$$a_0(\xi,\theta,\varphi)={\sum_{\nu m}}'[Q_\nu^m(\cos\xi)-\exp[i\pi(m-\lambda_\nu^m)]Q_\nu^m(-\cos\xi)]Q_\nu^m(\cos\theta)e^{im\varphi}. \tag{24}$$

The prime on the summation sign denotes that at $\nu=0$ and $m=0$, the second term in the square brackets is omitted.

3. CROSS SECTIONS

We now average the scattering cross sections obtained from (23) over the orientations of the molecule. Such an approach is equivalent to consideration of the scattering from a rotator with subsequent transition to the limit as $I\to\infty$.[11] Then the diffusion cross section is determined by the expression

$$\begin{aligned} \sigma_d&=\frac{1}{k^2}\{b-\operatorname{Re}(ce^{-i\pi\lambda}s_0^0(k))\},\\ b&=\frac{1}{2}\int(1-\cos\vartheta)\{|a_0(\xi,\theta,\varphi)|^2\\ &\quad+[Q_0^0(-\cos\xi)Q_0^0(\cos\theta)]^2\}\,d\cos\xi\,d\cos\theta\,d\varphi,\\ c&=\int(1-\cos\vartheta)a_0^*(\xi,\theta,\varphi)Q_0^0(-\cos\xi)Q_0^0(\cos\theta)\,d\cos\xi\,d\cos\theta\,d\varphi, \end{aligned} \tag{25}$$

where ϑ is the scattering angle:

$$\cos\vartheta=\cos\theta\cos\xi+\sin\theta\sin\xi\cos\varphi.$$

For the average total cross section we have, formally,

$$\begin{aligned} \sigma&=\frac{2\pi}{k}\int\operatorname{Im}f(\xi,\xi,0)\,d\cos\xi=\sum_{m=-\infty}^{\infty}\sigma^{(m)}\\ &=\frac{2\pi}{k^2}\left\{-\beta_{00}\operatorname{Re}(e^{-i\pi\lambda}s_0^0(k))+{\sum_{\nu m}}'[1-\beta_{\nu m}e^{i\pi(m-\lambda_\nu^m)}]\right\}, \end{aligned} \tag{26}$$

where

$$\beta_{\nu m}=\int Q_\nu{}^m(-\cos\xi)Q_\nu{}^m(\cos\xi)\,d\cos\xi.$$

Since we are considering a fixed dipole, σ diverges. In (26), this is due to the slow decrease of the series $\sigma^{(m)}$ (like $1/|m|$). On the other hand, at large $|m|$, the scattering takes place on the periphery and favorable conditions exist for the application of the Born approximation. Therefore, the difference

$$\sigma_B(I)-\sum_m \sigma_B^{(m)}(\infty)$$

represents a reasonable correction to (26). Here $\sigma(I)$ denotes the cross section for scattering from a molecule with moment of inertia I, and the index B denotes the Born approximation.

The following formula is obtained for the total cross section:

$$\sigma(I)=\sum_m [\sigma^{(m)}(\infty)-\sigma_B^{(m)}(\infty)]+\sigma_B(I), \tag{27}$$

and the series in m no longer diverges. $\sigma^{(m)}(\infty)$ is determined from (26), and $\sigma_B^{(m)}(\infty)$ is simply obtained as the first term of the expansion of $\sigma^{(m)}(\infty)$ in D^2:

$$\sigma_B^{(m)}(\infty)=\frac{4\pi D^2}{k^2}[2m^2\psi'(|m|)-2|m|-1], \tag{28}$$

where ψ' is the derivative of the digamma function.

From (1) and (2) we have for the Born cross section of scattering from a molecule with rotational quantum number j:

$$\sigma_B{}^j=\frac{8\pi D^2}{3k^2}\left[\ln 2Ik^2-\frac{(j+1)\ln(j+1)+j\ln j}{2j+1}\right], \tag{29}$$

where we have assumed that $k^2 \gg 2j/I$ (see below for more on this condition).

Equation (29), strictly speaking, is applicable for scattering from a diatomic molecule in a state with definite Λ (then I is the principal moment of inertia about the axis perpendicular to the axis of the molecule). However, since σ depends on I weakly, (29) can be used for an arbitrary molecule by introducing some mean moment of inertia I.

All the quantities entering in (25) and (26), with the exception of s_0^0, depend only on D, and only a single real parameter enters into s_0^0, which is dependent on the short-range forces (and does not depend on the energy). We can find it from the solution of the total problem by the method of strong coupling for one energy. If it is difficult to do this, then the parameter can be regarded as semi-empirical.

4. REGION OF APPLICABILITY OF THE THEORY

For the estimate of the region of applicability of the immobile-dipole approximation (adiabatic approximation), we use classical considerations. Adiabaticity is satisfied if the time of collisions t is much smaller than the period τ of rotation of the molecule. The characteristic dimension ρ of the collision region is determined from the equation

$$D/\rho^2\sim k^2,$$

whence we find the collision time

$$t\sim D^{1/2}/k^2.$$

For the period of rotation of a molecule with rotational quantum number j we have

$$\tau\sim I/j \tag{30}$$

and it follows from $\tau \gg t$ that2)

$$k^2\gg D^{1/2}j/I. \tag{31}$$

If $j=0$, then the classical estimate (30) does not hold and in place of the period of rotation τ we must calculate the characteristic time of change of the rotator wave function at a specified initial condition. We then obtain the inequality (31) with $j\sim 1$.

The second assumption is connected with the retention of only the zeroth term in the expansion of the R matrix and of the Bessel functions of argument kr_0, which holds at $(kr_0)^2 \ll 1$. Thus, the region of applicability of the theory is determined by the relations

$$D^{1/2}j/I\ll k^2\ll r_0{}^{-2}. \tag{32}$$

The value of r_0 in order of magnitude can be taken to be equal to one-half the distance between the farthest nuclei of the molecule. Then, for most molecules with distribution over j corresponding to $T\sim 10^2$–10^3 °K, the region (32) lies between 0.001–0.01 and 0.5–1 eV, i.e., right where the experiments of the type of Refs. 12 and 13 were carried out to determine the drift velocity of electrons in gases.

The limited nature of the theory is connected also with the neglect of the quadrupole and polarization interactions. These should be taken into account if the molecule has a small dipole moment (for example, CO).

5. BOUND STATES AND RESONANCES

It is known (see, for example, Ref. 14), that at given ν and m there exists such a state $D=D_{\text{cr}}^{\nu m}$ (the D_{cr} introduced above is identical with D_{cr}^{00}), for which there should appear, in the field of a fixed dipole, an infinite number of bound states with a condensation point at zero, similar to the states in the field $-\alpha/r^2$.[3] This circumstance has given rise to a set of speculative opinions3) regarding the sharp jump in the cross section near D_{cr}. It was later shown that these suppositions were incorrect. First, when account is taken of rotation, the number of bound states becomes finite, and the value of D at which even a single bound state appears increases strongly even for rather large moments of inertia.[16] Second, numerical calculations[17,18] have shown that the cross sections vary continuously in the transition through D_{cr}.

In the work of Crawford, Dalgarno and Hays,[19] and Bottcher[20] an incorrect conclusion was drawn that any theory in which an infinite number of bound states appears is unsatisfactory and leads to discontinuities as,

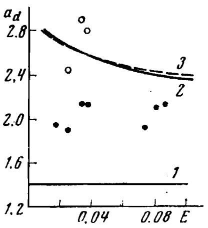

FIG. 1. Scattering by the water molecule. The dependences of the dimensionless quantity (34) on the energy of the electron (in eV) is shown in the figure. Curve 1—Born approximation; 2—experiment[12]; 3—calculation according to Eq. (35); the points are calculated according to the method of strong coupling[27] in the case of a different choice of the range of short-range action, r_0; ○—$r_0=0125$ Å; ●—$r_0=1$ Å.

for example, the theory of Mittleman and von Holdt.[4] However, the inapplicability of their theory[4] upon approach of D to D_{cr} is in no way due to the appearance of bound states (i.e., not to the long-range character of the potential), but to the singular behavior of the potential at zero. It follows from the results of our present work that the regularization of the potential leads to an absence of discontinuities even upon consideration of a fixed dipole. Actually, Eq. (20) (and, consequently, (23)), actually has a root discontinuity at $D=D_{cr}$, but it is continuous.

The factor $k^{2i\mu}$ in (21) leads to oscillations of the cross section as a function of D at $D>D_{cr}$, while the locations of the maxima depend on the energy and the short-range interaction (the parameter α). Thus there exists no universal maximum in the dependence of σ on D. This same conclusion was reached on the basis of numerical calculations by Garrett,[17] where the conclusion of Takayanagi and Itikawa[5] that a universal discontinuity exists was subjected to valid criticism.

The possibility of oscillations of the cross section as a function of k also follows from (21), similar to the oscillations which are observed in the scattering of electrons by hydrogen atoms[9] (dipole resonances). However, in order that there be even a single period in the range of applicability of the theory (32), it is necessary that the dipole moment be sufficiently large and satisfy the condition

$$E_1/E_2 \gg e^{2\pi/\mu}, \qquad (33)$$

where E_1 and E_2 are the limits of applicability of the theory.

The relation (33) begins to be satisfied at $D \approx 3$ a.u. But for such large D, the relative contribution of the oscillating part to the cross sections (25) and (26) becomes very small and experimental observation of these oscillations is scarcely possible. The hydrogen atom in this sense is favorably distinguished by the smallness of E_2, which is brought about by the small distance between the 2s and the 2p levels. Thus, the rotation of the molecule leads (for not too large D) to the vanishing of the dipole resonances in the region of the continuous spectrum.4) Oscillations in the functions $\sigma(D)$ and $\sigma(k)$ were obtained earlier in the finite-dipole model.[6]

6. COMPARISON WITH EXPERIMENT AND THE STRONG-COUPLING METHOD

In view of the presence of an adjustment parameter in the theory, which we shall consider as semi-empirical, we shall touch on principally only those experiments in which the energy dependence of the cross sections was determined, and we shall not be concerned with the numerous data on σ_d, averaged according to Maxwell.[13] In comparison, we shall frequently operate with the quantity,

$$a_d=\sigma_d k^2/\pi. \qquad (34)$$

The NH$_3$ molecule (D=0.579)

Calculation according to Eqs. (20) and (25) leads to the following expression for a_d:

$$a_d = 1.45 + \frac{2.06z^2 + 1.63z\eta}{\eta^2 + z^2 + 1.60z\eta},$$

where $z=k^{0.410}$. The Born approximation gives $a_d = 0.893$. The constant 1.45 was obtained in Ref. 4.5)

It follows from the experimental work of Pack *et al.*[12] that, in the energy range from 0.01 to 0.1 eV, the value of a_d is close to 1.45. However, further improvement of accuracy is difficult in view of the scatter of the curves obtained from different approximations of the temperature dependence of the drift velocity.

The molecule H$_2$O (D=0.729)

It follows from (21) and (25) that

$$a_d = \frac{2.70 + 1.95\cos\beta - 1.09\sin\beta}{1 + 0.74\cos\beta}, \qquad (35)$$

$$\beta=\alpha+2\mu\ln k. \qquad (36)$$

In our case, $\mu=0.261$. Choosing $\alpha=1.70$, we obtain very good agreement with experiment[12] (see Fig. 1). Such excellent agreement is connected, of

TABLE I. Total scattering cross sections of electrons by molecules with large dipole moments, in Å^2, at $E=1$ eV. Data on the dipole moments are taken from Refs. 23–25.

		Theory			
Molecule	Dipole moment	Born approximation	Method of strong coupling	Eq. 27	Experiment (Refs. 23–25)
CsF	3.11	2359	2003	2017 ± 4	1100 ± 100
CsCl	4.15	4970	—	4180 ± 20	1640 ± 200
KI	4.26	5670	—	4820 ± 20	2170 ± 380

course, with the adjustment character of the calculation; however, it is not accidental that the theory gives the correct energy dependence for the slowly changing quantity a_d. The cross section (35), averaged over the velocities of the electrons for the case $T = 300$ °K, is equal to 2750 Å^2. In the Born approximation, $\langle \sigma_d \rangle = 1300$ Å^2.

Molecules with large dipole moments.

For the molecule CsF, theory gives

$$a_d = 9.10 + 0.72 \sin(\beta - 0.975), \tag{37}$$

$$\sigma = \sigma_B^j - (28.6 + 0.3 \sin\beta)\pi/k^2. \tag{38}$$

β is determined by Eq. (36) with $\mu = 1.722$. The cross section σ_B^j is found from (29). Since the contribution, which depends on the short-range interaction, is small in Eqs. (37), (38) we can, without making the value of the parameter α more accurate, obtain excellent estimates for σ_d and σ. For example, in the case of $E = 1$ eV,

$$100\ \text{Å}^2 \leqslant \sigma_d \leqslant 117\ \text{Å}^2. \tag{39}$$

The Born approximation and the strong-coupling method[22] at $j = 41$ (the most probable j at $T = 1000$ °K) give 308 and 103 Å^2, respectively. The experimental value[23] at $R = 1000$ °K is 35 Å^2. The total cross sections are shown in Table I. The complete scattering cross sections are given there for CsCl and KI. It is seen that the exact allowance for the dipole interaction leads to a significant reduction in the diffusion cross sections in comparison with the Born cross sections, but the complete cross sections change very little. The latter is due to the fact that the principal contributions to the total cross section are made by the higher partial waves.[19]

Similar results are obtained in the consideration of the excitation of atoms of the akali metals in the Seaton model.[26] The basic contributions to the total cross section there are also made by the higher partial waves, which are considered in the Born approximation, and a model with degenerate atomic levels is used for the calculation of the lower partial waves. However, for the scattering by atoms, this model is less accurate, since the separation of the low-lying atomic terms is much greater than the separation of the rotational molecular levels.

The agreement of the results of the present work with the calculations by the method of strong coupling indicates that the approximations made above, such as the neglect of the rotation and of the energy dependence of the R matrix, are justified, while the divergence of the theory from experiment can be explained by other reasons, especially by our not taking into account the molecular vibrations, since the separation of the vibrational levels is comparable with the considered energies of the electrons. We note that any modification of the model of short-range forces (including the introduction of exchange interaction) does not lead in the strong coupling method for the CsF molecule to significant change in the results by virtue of the inequalities of the type (39). One of the merits of this theory is the fact that it allows us to estimate the accuracy of the result connected with the specific choice of the short-range interaction. For H_2O, for example, as is seen from (35), the correct account of the short-range interaction is very important, which also follows from the work of Crawford.[27]

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[1)] Atomic units are used in this paper.

[2)] This condition is equivalent to neglect of the energy differences between channels with different rotational quantum numbers.

[3)] For example, Ref. 15. There exists a broad literature on the problem of the existence of bound states in the field of a fixed dipole and their effect on scattering, citations to which can be found in Refs. 16 and 17.

[4)] Resonances having another mechanism of appearance are possible, however.[23] This question is not discussed here.

[5)] The value of a_d for NH_3 in Ref. 4 was incorrectly cited in the case of D = 0.579/2.

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