CALCULATION OF THE COLLISION CROSS SECTIONS FOR SLOW EXCITED ATOMS AND MOLECULES

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Submitted February 28, 1972

Zh. Eksp. Teor. Fiz. 63, 63–74 (July, 1972)

The dependence of the elastic cross section, overexcitation cross section, and diffusion cross section on resonance defect is calculated. The difficulties that arise as a result of the restricted applicability of the quasiclassical description of the motion given by a set of two second-order differential equations are set forth. It is shown that the well-known Stuekelberg result for the overexcitation cross section is correct only for sufficiently large resonance defects.

1. We consider processes of the form

$$A^* + B \to A^* + B, \qquad (1.1a)$$

$$A^* + B \to A + B^*, \qquad (1.1b)$$

which describes slow elastic (1.1a) and inelastic (1.1b) collisions of an excited atom A* with an unexcited atom B. If the initial states of the atoms are connected by a resonance-allowed dipole transition, the collision cross sections in both channels (1.1a) and (1.1b) can significantly exceed the gas kinetic cross section.[1]

We are interested in the dependence of the elastic scattering cross section σ_s, the excitation transfer cross section σ_t, and the transport (diffusion) cross section σ_D on the value of the resonance defect $\Delta\epsilon$.

Existing data in the literature on excitation transfer cross sections refer primarily to the case of exact resonance ($\Delta\epsilon = 0$) and are based on the calculation of σ_t in the impact-parameter approximation.[2-4] The excitation transfer cross sections for small resonance defects in the straight flight approximation was carried out in[5]. This research deals with the collision of alkali metal atoms excited to one of the doublet levels with atoms in the ground state (Galitskiĭ, Vdovin, Dobrodeev). Calculation of the excitation transfer cross section for collisions of slow atoms in the case $\Delta\epsilon \neq 0$ was performed by Stuekelberg,[6] who used a combination of the quasiclassical method with the Born approximation. For values of the orbital momentum l less than some value j, he calculated the partial cross sections quasiclassically, and for $l > j$ he used the Born approximation. The energy of interaction was written in the form

$$u = b/r^s, \qquad (1.2)$$

which includes the case s = 3 of interest to us (the dipole-dipole interaction). As will be shown below, the results of Stuekelberg describe correctly only the asymptotic behavior of the excitation transfer cross section at large resonance defects. As to the intermediate values of $\Delta\epsilon$, the contribution to σ_t of the region $l \sim$ J turns out to be important, where the results of Stuekelberg (and also of Novikov[7]) are incorrect.

The calculation of the cross section in the case $\Delta\epsilon \neq 0$ presents difficulties due to the restricted applicability of the quasiclassical description of the motion prescribed by a set of two coupled second order equations. The region where both the classical and the Born approximations lead to incorrect results turns out to be important in the problem.

We have attempted a correct calculation of the elastic scattering cross section σ_s, the excitation transfer cross section σ_t, and also the transport cross section σ_r over a wide range of resonance defects $\Delta\epsilon$. In addition to the problem of the total cross sections, definite interest attaches to the dependence of the phase shift of the scattering on l and on the value of the resonance defect, and also the partial cross sections of the atomic collisions in channels (1a) and (1b). These quantities are calculated in the given case and in the case of exact resonance ($\Delta\epsilon = 0$).

2. In the two-state approximation,[1] the wave function describing the collision can be written in the form

$$\psi = \chi_1(\mathbf{r}_a, \mathbf{r}_b)\psi_1(\mathbf{r}) + \chi_2(\mathbf{r}_a, \mathbf{r}_b)\psi_2(\mathbf{r}). \qquad (2.1)$$

Here $\mathbf{r}_a$ and $\mathbf{r}_b$ are the coordinates of the electrons in atoms A and B relative to the corresponding nucleus, $\mathbf{r}$ the vector joining the centers of the masses A and B, χ_1 and χ_2 the wave functions which describe the initial and final states of these atoms.

The functions ψ_1 and ψ_2 satisfy the set of equations

$$(\nabla^2 + k_1^2)\psi_1 = u_{12}\psi_2, \quad (\nabla^2 + k_2^2)\psi_2 = u_{21}\psi_1, \qquad (2.2)$$

where

$$u_{ij} = \frac{2M}{\hbar^2}\iint V(\mathbf{r}_a, \mathbf{r}_b, r)\psi_i\psi_j^* \, d\mathbf{r}_a \, d\mathbf{r}_b,$$

$V(\mathbf{r}_a, \mathbf{r}_b, \mathbf{r})$ is the interaction operator of atoms A and B, k_1 and k_2 are the wave numbers of the relative motion of the atoms before and after collision.

Expanding ψ_j in Legendre polynomials,

$$\psi_j = \sum_l (2l+1) f_{lj} P_l(\cos\theta),$$

we obtain the following set of equations for the functions f_{lj}:

$$\left(\frac{d^2}{dr^2} + k_1^2 - \frac{l(l+1)}{r^2}\right) f_{l,1} = u_{12} f_{l,2},$$
$$\left(\frac{d^2}{dr^2} + k_2^2 - \frac{l(l+1)}{r^2}\right) f_{l,2} = u_{21} f_{l,1}, \qquad (2.3)$$

where $u_{12} = u_{21} = b/r^3$.

From considerations of convenience, we chose a model description of the dipole-dipole interaction, corresponding to the "rotating model approximation," according to which the dipole moments of the atoms follow one another in the time of collisions, i.e.,

$$b = -2\langle d_{1z} d_{2z}\rangle M/\hbar^2,$$

where d_i are the projections of the dipole moments of the atoms on the axis connecting them. Such a notation simplifies the calculation and leads only to an inconsequential error in a numerical factor of the order of unity in the final expression for the cross sections.[3]

If the energies of the relative motion of the atoms before and after scattering are the same (exact resonance), the characteristic value of the orbital quantum number is the value $l = l_0$ for which the kinetic energy and the interaction energy of the atoms are equal at the classical turning point, i.e.,

$$l_0 = (bk)^{1/3}. \tag{2.4}$$

We shall further assume that $l_0 \gg 1$. (For example, at room temperature, $l_0 \sim 30$ for hydrogen and $l_0 \sim 100$ for mercury.)

The set of equations (2.4) must satisfy boundary conditions of the form

$$f_{l,1}(r=0) = f_{l,2}(r=0) = 0,$$
$$f_{l,1}|_{r\to\infty} \sim i^l \sin(k_1 r - \pi l/2) + \alpha_l e^{ik_1 r}, \tag{2.5}$$
$$f_{l,2}|_{r\to\infty} \sim \beta_l e^{ik_2 r}.$$

The asymptotic expressions (2.5) describe the behavior of the wave functions at infinity, both in the elastic and the inelastic scattering channels. It is natural that the incident wave is absent from the inelastic channel. The coefficients α_l and β_l are subject to determination. The cross sections of interest to us, expressed in terms of the quantities α_l and β_l, have the following form:[1] excitation transfer cross section

$$\sigma_t = \frac{4\pi k_2}{k_1^3}\sum (2l+1)|\beta_l|^2, \tag{2.6}$$

elastic scattering cross section

$$\sigma_e = \frac{4\pi}{k_1^2}\sum_l (2l+1)|\alpha_l|^2, \tag{2.7}$$

total scattering cross section

$$\sigma = \frac{4\pi}{k_1^2}\sum_l (2l+1)\left[|\alpha_l|^2 + \frac{k_2}{k}|\beta_l|^2\right] \tag{2.8}$$

and, finally, the cross section σ_D describing the diffusion is equal to

$$\sigma_D = \sigma_D^\alpha + \sigma_D^\beta,$$
$$\sigma_D^\alpha = \frac{2\pi}{k^2}\sum_l (l+1)|\alpha_l - \alpha_{l+1}|^2,$$
$$\sigma_D^\beta = \frac{2\pi}{k^2}\sum_l (l+1)|\beta_l - \beta_{l+1}|^2. \tag{2.9}$$

The solution of the set (2.3) will be sought in the form

$$f_{l,1} = C_{11} j_{l+1/2}(k_1 r) + C_{12} n_{l+1/2}(k_1 r),$$
$$f_{l,2} = C_{21} j_{l+1/2}(k_2 r) + C_{22} n_{l+1/2}(k_2 r), \tag{2.10}$$

where

$$j_{l+1/2}(kr) = (\pi kr/2)^{1/2} J_{l+1/2}(kr),$$
$$n_{l+1/2}(kr) = -(\pi kr/2)^{1/2} N_{l+1/2}(kr),$$

and $J_\nu(x)$, $N_\nu(x)$ are Bessel and Neumann functions, respectively. Conditions describing the behavior of the waves functions at zero and at infinity must be imposed on the coefficients C_{ij}.

$$C_{12}(r=0) = C_{22}(r=0) = 0,$$
$$C_{11}(r\to\infty) \to i^l(1+i\alpha), \quad C_{21}(r\to\infty) \to i^{l+1}\beta, \tag{2.11}$$
$$C_{12}(r\to\infty) \to i^l\alpha, \quad C_{22}(r\to\infty) \to i^l\beta.$$

We also impose on C_{ik} additional conditions of the form

$$\frac{dC_{11}}{dr} j_{l+1/2}(k_1 r) + \frac{dC_{12}}{dr} n_{l+1/2}(k_1 r) = 0,$$
$$\frac{dC_{21}}{dr} j_{l+1/2}(k_2 r) + \frac{dC_{22}}{dr} n_{l+1/2}(k_2 r) = 0.$$

Then the functions C_{ik} satisfy the following equations:

$$C_{11}' = (b/k_1 r^3) n_{l+1/2}(k_1 r) f_{l,2}(k_2 r),$$
$$C_{12}' = -(b/k_1 r^3) j_{l+1/2}(k_1 r) f_{l,2}(k_2 r),$$
$$C_{21}' = (b/k_2 r^3) n_{l+1/2}(k_2 r) f_{l,1}(k_1 r), \tag{2.12}$$
$$C_{22}' = -(b/k_2 r^3) j_{l+1/2}(k_2 r) f_{l,1}(k_1 r).$$

Here it is taken into account that the Wronskian is

$$j'_{l+1/2}(kr) n_{l+1/2}(kr) - j_{l+1/2}(kr) n'_{l+1/2}(kr) = k.$$

3. We first consider the case of exact resonance ($\Delta\epsilon = 0$), i.e., we assume that $k_1 = k_2 = k$. We investigate the solution of the set (2.12) in various ranges of change of r. For $r - l/k \gg l^{1/3}/k$, we have

$$J_\nu(\nu\sec\gamma) \approx \left(\frac{2}{\pi\nu\,\mathrm{tg}\,\gamma}\right)^{1/2} \sin\left(\nu\,\mathrm{tg}\,\gamma - \nu\gamma + \frac{\pi}{4}\right),$$
$$N_\nu(\nu\sec\gamma) \approx -\left(\frac{2}{\pi\nu\,\mathrm{tg}\,\gamma}\right)^{1/2} \cos\left(\nu\,\mathrm{tg}\,\gamma - \nu\gamma + \frac{\pi}{4}\right). \tag{3.1}$$

Noting that the product of the functions n and j oscillates, and those of nn and jj do not, and averaging over the interval $(r - \pi/2k, r + \pi/2k)$, we get the following set of equations as the zeroth approximation:

$$\frac{dC_{11}}{d\xi} = C_{22}; \quad \frac{dC_{12}}{d\xi} = -C_{21}; \quad \frac{dC_{21}}{d\xi} = C_{12}; \quad \frac{dC_{22}}{d\xi} = -C_{11}. \tag{3.2}$$

Here

$$\xi = -\int_r^\infty \frac{b}{2x^2}\frac{dx}{(x^2 - l^2)^{1/2}}.$$

The solution of the set (3.2) satisfying the conditions at infinity (2.11) is

$$C_{11} = i^l[(1+i\alpha_l)\cos\xi - \beta_l\sin\xi],$$
$$C_{12} = i^l(\alpha_l\cos\xi + i\beta_l\sin\xi],$$
$$C_{21} = i^l[i\beta_l\cos\xi - \alpha_l\sin\xi], \tag{3.3}$$
$$C_{22} = i^l[\beta_l\cos\xi + (1+i\alpha_l)\sin\xi].$$

For the determination of α_l and β_l it is necessary to use the conditions of the vanishing of the functions C_{12} and C_{22} for r = 0. With the help of the second and fourth equations of the set (2.12), these conditions can be written in the following form:

$$i^l\alpha_l + \int_0^\infty \frac{b}{r^3 k} j_{l+1/2}(kr) f_{l,2}(r)\,dr = 0,$$
$$i^l\beta_l + \int_0^\infty \frac{b}{r^3 k} j_{l+1/2}(kr) f_{l,1}(r)\,dr = 0. \tag{3.4}$$

We consider the range $r - l/k \ll l^{1/3}/k$. The functions $f_{l,1}$ and $f_{l,2}$ are exponentially small in this region with account of the condition that $b/r^3 \ll k^2$ for $r = l/k$; therefore the boundary conditions for C_{12} and C_{22} can refer to the point $r = r^*$, where $r^* = l/k \sim l^{1/3}/k$. In the region $|r - l/k| \lesssim l^{1/3}/k$, the relative change in the coefficients C_{ij} does not exceed $|\Delta C_{ij}/C_{ij}| \lesssim l_0^3/l^{7/3}$. Therefore, if $l_0^3/l^{7/3} \ll 1$, i.e.,

$$l \gg l_0^{9/7}, \qquad (3.5)$$

then in the range $|r - l/k| \lesssim l^{1/3}/k$, the coefficients C_{ij} change only slightly. In view of this, the conditions of the vanishing of C_{12} and C_{22} can be imposed for $r_0 = l/k$. Then

$$\beta_l \cos \xi_0 + (1 + i\alpha_l) \sin \xi_0 = 0,$$
$$\alpha_l \cos \xi_0 + i\beta_l \sin \xi_0 = 0, \qquad (3.6)$$

$$\xi_0 = \int_{l/k}^{\infty} \frac{b}{2r^2} \frac{dr}{(1 - l^2/r^2)^{1/2}} = \frac{l_0^3}{2l^2}. \qquad (3.7)$$

Solving the set (3.6), we obtain

$$\alpha_l = i \sin^2 \xi_0, \quad \beta_l = -{}^1\!/_2 \sin 2\xi_0. \qquad (3.8)$$

We recall that the expression (3.8) is valid only under the condition (3.5).

We now compute the excitation transfer cross section σ_t. With account of (2.6), (3.8) and (3.5), we have

$$\sigma_t = \sigma_t^{(1)} + \sigma_t^{(2)},$$

$$\sigma_t^{(1)} = \frac{4\pi}{k^2} \sum_{l=1}^{l_0^{9/7}} (2l + 1) |\beta_l|^2 \leqslant \frac{4\pi}{k^2} l_0^{18/7},$$

$$\sigma_t^{(2)} = \frac{4\pi}{k^2} \sum_{l=l_0^{9/7}}^{\infty} (2l + 1) |\beta_l|^2 = \frac{\pi^2 l_0^3}{2k^2} [1 + O(l_0^{-3/7})]. \qquad (3.9)$$

Consequently, for sufficiently large l_0,

$$\sigma_n = \pi^2 l_0^3 / 2k^2. \qquad (3.10)$$

Similarly, for the case of elastic scattering, we get

$$\sigma_s = \sigma_s^{(1)} + \sigma_s^{(2)};$$

$$\sigma_s^{(1)} = \frac{4\pi}{k^2} \sum_{l=1}^{l_0^{9/7}} (2l + 1) |\alpha_l|^2 \leqslant \frac{4\pi}{k^2} l_0^{18/7},$$

$$\sigma_s^{(2)} = \frac{4\pi}{k^2} \sum_{l=l_0^{9/7}} (2l + 1) |\alpha_l|^2 = \frac{\pi^2 l_0^3}{2k^2} [1 + O(l_0^{-3/7})], \qquad (3.11)$$

i.e., for $l_0 \gg 1$,

$$\sigma_s = \pi^2 l_0^3 / 2k^2. \qquad (3.12)$$

It is interesting to note that in the case of exact resonance, the values of the cross sections in the elastic and inelastic scattering channels are identical with accuracy to terms of order of the cross section multiplied by a small quantity $O(l_0^{-3/7})$.

It follows from Eqs. (3.10)—(3.14) that the excitation transfer cross section and the scattering cross section are determined by the large values $l \sim l_0^{3/2}$, and therefore knowledge of α_l and β_l for small l is not required.

We now compute the diffusion cross section σ_D. If we assume that the expressions (3.8) for α_l and β_l are valid for any l, and compute the diffusion cross section, it is then seen that the cross section is determined by $l \sim l_0$. For such l, the quantities α_l and β_l cannot be determined by Eqs. (3.8). Using Eqs. (3.3), we can see that the error in the differences $\alpha_l - \alpha_{l+1}$ and $\beta_l - \beta_{l+1}$, produced by the imposition of the boundary conditions at the point $r = l/k$ rather than at zero, can be determined in the following way:

$$\Delta |\alpha_l - \alpha_{l+1}| \sim \frac{b}{r^3} j_{l+1/2}(kr) \frac{\partial j_{l+1/2}(kr)}{\partial l} \Delta r |_{\Delta r \sim l^{1/3}/k} \sim \frac{l_0^3}{l^3},$$

$$\Delta |\alpha_l - \alpha_{l+1}| \sim \Delta |\beta_l - \beta_{l+1}|.$$

Therefore, for the estimate of the diffusion cross section, we can use the expressions (3.8) for α_l and β_l. Then

$$\sigma_D^\alpha \approx \pi \Gamma(1/3) l_0^2 / 2^{4/3} k^2, \quad \sigma_D^\beta = \sigma_D^\alpha.$$

Consequently,

$$\sigma_D = 2^{-1/3} \pi \Gamma(1/3) l_0^2 / k^2, \qquad (3.13)$$

where $\Gamma(x)$ is the gamma function.

4. We now consider the more interesting case of inexact resonance: $\Delta k = k_1 - k_2 \neq 0$. It must be expected that the scattering and overexcitation cross sections change if even for $l \sim l_0^{3/2}$ the turning points in the first and second channels are separated sufficiently, i.e., if

$$x = \left| \frac{\Delta k}{k} \right| l_0^{3/2} \gg 1, \quad k = \frac{k_1 + k_2}{2}. \qquad (4.1)$$

We first investigate the vicinity of the resonance, i.e., the region

$$x \ll 1. \qquad (4.2)$$

If $x \ll 1$, we can solve the set (2.12) by perturbation theory. Here we obtain for the coefficients α_l and β_l, with accuracy to x^2,

$$\alpha_l = {}^1\!/_4 i \{2 - \exp[-2\xi i][w_1 - iw_4]^2 - \exp[2\xi i][w_3 + iw_4]^2\},$$
$$\beta_l = {}^1\!/_4 i \{-(w_4^2 + w_3^2) \exp[2\xi i] + [w_1^2 + w_2^2] \exp[-2\xi i]\}, \qquad (4.3)$$

where

$$\xi = -\int_{l/k}^{\infty} dr \frac{\cos \Delta kr}{2(k^2 - l^2/r^2)^{1/2}} \frac{b}{r^3},$$

$$w_1 = -\int_{l/k}^{\infty} \frac{b}{2x^3} \frac{\sin \Delta kx \, dx}{(k^2 - l^2/x^2)^{1/2}} e^{2i\xi(x)} \int_x^{\infty} dy \frac{b}{2y^3} \frac{\sin \Delta ky}{(k^2 - l^2/y^2)^{1/2}} e^{-2i\xi(y)},$$

$$w_2 = i \int_{l/k}^{\infty} \frac{b}{2x^3} \frac{\sin \Delta kx}{(k^2 - l^2/x^2)^{1/2}} e^{2i\xi(x)} dx;$$

$$w_3 = w_1^*; \quad w_4 = -w_2^*.$$

It follows from the expressions (4.3) that at small x the cross sections depend on the resonance defect in the following way:

$$\sigma_s(x) = \sigma_s(\Delta k = 0) \left[1 - \frac{\ln 2}{4\pi} x^2 \ln \frac{1}{|x|}\right], \qquad (4.4)$$

$$\sigma_t(x) = \sigma_t(\Delta k = 0) \left[1 - \frac{x^2}{\pi} \ln^2 \frac{1}{|x|}\right]. \qquad (4.5)$$

According to (2.9),

$$\sigma_D^\alpha = \sigma_D^\alpha(\Delta k = 0)[1 - x^2(\pi/2)^{1/2}] = \sigma_D^\beta. \qquad (4.6)$$

5. We consider now the case of "large" resonance defects ($x \gg 1$). For the calculation of the coefficients α_l and β_l, it suffices to know only $C_{11}(r)$ and $C_{12}(r)$. Actually, the coefficient β_l can be computed from the formula

$$\beta_l = i^{-l} \int_0^{\infty} \frac{b \, dr}{kr^3} j_{l+1/2}(k_2 r) f_{l,1}(k_1 r),$$

and for α_l we have the expression

$$\alpha_l = i^{-l} \int_0^{\infty} \frac{b \, dr}{kr^3} j_{l+1/2}(k_1 r) f_{l,2}(k_2 r),$$

which, using (2.12), can be transformed into

$$\alpha_l = C_{21}(\infty) \int_0^{\infty} \frac{b \, dr}{kr^3} j_{l+1/2}(k_1 r) j_{l+1/2}(k_2 r)$$

$$+ C_{22}(\infty) \int_0^{\infty} \frac{b \, dr}{k(r + a)^3} j_{l+1/2}(k_1 r) n_{l+1/2}(k_2 r)$$

$$+\int_0^\infty dr\left\{-\frac{b}{r^3}n_{l+1/2}(k_2r)f_{l,1}(k_1r)\int_0^r\frac{b\,dr}{r^3}j_{l+1/2}(k_1r)j_{l+1/2}(k_2r)\right\}$$
$$+\int_0^\infty dr\left\{\frac{b}{r^3}j_{l+1/2}(k_2r)f_{l,1}(k_1r)\int_0^r\frac{b\,dr}{(r+a)^3}j_{l+1/2}(k_1r)n_{l+1/2}(k_1r)\right\}. \tag{5.1}$$

We have introduced the parameter a in the potential in order to avoid the divergence that arises with formal use of the potential b/r^3 at small r.

In order to find C_{11} and C_{12}, we eliminate C_{21} and C_{22} from the equations of (2.12). Then

$$C_{21}=-\int_0^\infty\frac{b\,dr}{r^3}n_{l+1/2}(k_2r)f_{l,1}(k_1r),$$
$$C_{22}=\int_0^\infty\frac{b\,dr}{r^3}j_{l+1/2}(k_2r)f_{l,1}(k_1r). \tag{5.1'}$$

Substituting (5.1) in Eq. (2.12) for C_{11} and C_{12}, we get

$$\frac{dC_{11}}{dr}=\frac{b}{r^3k}n_{l+1/2}(k_1r)\left\{-j_{l+1/2}(k_2r)\int_r^\infty\frac{b\,dr}{r^3}n_{l+1/2}(k_2r)f_{l,1}(k_1r)+n_{l+1/2}(k_2r)\int_r^\infty\frac{b\,dr}{r^3}j_{l+1/2}(k_2r)f_{l,1}(k_1r)\right\},$$
$$\frac{dC_{12}}{dr}=-\frac{b}{r^3k}j_{l+1/2}(k_1r)\left\{-j_{l+1/2}(k_2r)\int_r^\infty\frac{b\,dr}{r^3}n_{l+1/2}(k_2r)f_{l,1}(k_1r)+n_{l+1/2}(k_2r)\int_r^\infty\frac{b\,dr}{r^3}j_{l+1/2}(k_2r)f_{l,1}(k_1r)\right\}. \tag{5.2}$$

We find the solution of the set (5.2) for $r \gg l/k$. For definiteness, we shall assume that $k_1 > k_2$. We use the representations of the functions $j_{l+1/2}(kr)$ and $n_{l+1/2}(kr)$ in the form

$$j_{l+1/2}(x)=\mathrm{Re}\,h^{(1)}_{l+1/2}(x),\quad n_{l+1/2}(x)=\mathrm{Im}\,h^{(1)}_{l+1/2}(x),$$

where

$$h_l^{(1)}(x)=(\pi x/2)^{1/2}H_l^{(1)}(x),$$

and $H_l^{(1)}(x)$ in a Hankel function of the first kind.

To calculate the integrals in (5.2), we replace the integration over the interval $[r, \infty)$ by integration over the interval $[r, r + i\infty)$. This can be done since the integral over the arc of infinite radius is zero and the singularities of the functions C_{ij}, if they are inside the contour formed by the interval of the real axis $[r, \infty)$, the arc of infinite radius and the interval $[r, r + i\infty)$, make a contribution of the order $|\beta_l| \ll 1$ to the integral. The advantage of the substitution given above is that along straight lines parallel to the imaginary axis, $h_l^{(1)}(x)$ has an asymptote of the type of a damped exponential. Using the asymptotic representations of the Bessel function (3.1) for $r \gg l/k$, and expanding the product $bz^{-3}C_{ij}(z)$ under the integral in a series about the point z = r, we replace the set (5.2) by

$$\frac{dC_{11}}{dr}\left[1+\left(\frac{b}{2r^3k\Delta k}\right)^2\right]=\frac{3b^2}{4r^7(k\Delta k)^2}C_{11}+\frac{1}{4}\frac{b^2k}{r^6(k\Delta k)^2}C_{12},$$
$$\frac{dC_{12}}{dr}\left[1+\left(\frac{b}{2r^3k\Delta k}\right)^2\right]=\frac{3b^2}{4r^7(k\Delta k)^2}C_{12}-\frac{1}{4}\frac{b^2k}{r^6(k\Delta k)^2}C_{11}. \tag{5.3}$$

If we seek a solution of the set (5.3) in the form

$$C_{ij}=\left[1+\frac{b^2}{4r^6(k\Delta k)^2}\right]^{-1/2}F_{ij},$$

then we get the following system of equations for F_{ij}:

$$\frac{dF_{11}}{dr}=\frac{F_{12}}{4k^2\Delta k}\frac{b^2}{r^6}\left[1+\left(\frac{b}{2r^3k\Delta k}\right)^2\right]^{-1};$$
$$\frac{dF_{12}}{dr}=-\frac{F_{11}b^2}{4k^2\Delta kr^6}\left[1+\left(\frac{b}{2r^3k\Delta k}\right)^2\right]^{-1}. \tag{5.4}$$

The solution of the set (5.4), which takes into account the boundary conditions (2.11), is

$$F_{11}=i^l\cos\Delta k\xi(1+i\alpha_l)+i^l\alpha_l\sin\Delta k\xi,$$
$$F_{12}=i^l\cos\Delta k\xi\alpha_l-i^l(1+i\alpha_l)\sin\Delta k\xi, \tag{5.5}$$

where

$$\xi(r)=\int_r^\infty dr\left[1+\frac{b^2}{4(k\Delta k)^2r^6}\right]^{-1}\frac{b^2}{4r^6(\Delta kk)^2}$$
$$=r_0\left\{\frac{\sqrt{3}}{12}\ln\frac{1+\sqrt{3}\,r/r_0+(r/r_0)^2}{1-\sqrt{3}r/r_0+(r/r_0)^2}+\frac{1}{6}\,\mathrm{arctg}\,2\left(\frac{r}{r_0}-\frac{\sqrt{3}}{2}\right)+\frac{1}{3}\,\mathrm{arctg}\,2\left(\frac{r}{r_0}+\frac{\sqrt{3}}{2}\right)-\frac{\pi}{3}\right\}.$$

Here

$$r_0=l_0/k(2\Delta k/k)^{1/3}.$$

We now calculate α_l and β_l. We first note the following. When Eqs. (5.3)–(5.5) are used we have three branch points in the upper half-plane

$$r_1=r_0e^{i\pi/6};\quad r_2=r_0e^{i\pi/2};\quad r_3=r_0e^{5i\pi/6}. \tag{5.6}$$

The solutions (5.3)–(5.5) are valid for $r \gg l/k$ and also in the case $r_0\Delta k \gg 1$. Since $x^2 \gg 1$, the solutions (5.3)–(5.5) make it possible to determine α_l and β_l for values of l, such that $l \ll J$, where

$$J=l_0\Big/\left(\frac{\Delta k}{k}\right)^{1/3}. \tag{5.7}$$

substituting the expressions for C_{ij} in Eq. (5.1), we obtain

$$\beta_l=-\mathrm{Re}\,I_1+\mathrm{Im}\,I_2,$$

where

$$I_1=\int_0^\infty\frac{bdr}{(r^6+r_0^6)^{1/2}}j_{l+1/2}(k_2r)\left[j_{l+1/2}(k_1r)+in_{l+1/2}(k_1r)\right]e^{i\xi\Delta k},$$
$$I_2=\int_0^\infty\frac{bdr}{(r^6+r_0^6)^{1/2}}j_{l+1/2}(k_2r)\left[j_{l+1/2}(k_1r)+in_{l+1/2}(k_1r)\right]e^{-i\xi\Delta k}.$$

The function $e^{i\xi\Delta k}$ can be written in the more convenient form

$$e^{i\xi\Delta k}=\left[\frac{1+\sqrt{3}\,r/r_0+(r/r_0)^2}{1-\sqrt{3}\,r/r_0+(r/r_0)^2}\right]^{ir_0\Delta k/4\sqrt{3}}\left(\frac{1+ir/r_0}{1-ir/r_0}\right)^{r_0\Delta k/12}$$
$$\times e^{-i\pi r_0\Delta k/3}\left[\frac{1+2i(r/r_0+\sqrt{3}/2)}{1-2i(r/r_0+\sqrt{3}/2)}\right]^{r_0\Delta k/24}\left[\frac{1+2i(r/r_0-\sqrt{3}/2)}{1-2i(r/r_0-\sqrt{3}/2)}\right]^{r_0\Delta k/24}$$

Transforming to the upper half-plane, we can calculate the integral approximately along the real axis in terms of an integral over the vertical cut $[r_0, r_0 + i\infty)$. Consequently,

$$I_1\approx\int_{r_1}\frac{bdr}{(r^6+r_0^6)^{1/2}}j_{l+1/2}(k_2r)\left[j_{l+1/2}(k_1r)+in_{l+1/2}(k_1r)\right]\exp(i\xi\Delta k),$$

whence

$$I_1\approx\frac{br_0}{r_0^3}j_{l+1/2}(k_2r_0)\left[j_{l+1/2}(k_1r_0)+in_{l+1/2}(k_1r_0)\right]\exp\left(-i\frac{\pi}{3}r_0\Delta k\right)$$

for $(\Delta k/k)J \gg 1$, we get $I_1 \sim \exp\left(-\frac{\Delta k}{k}J\right)$.

Similarly, we find that $I_2 \sim I_1$. Therefore, for $l \ll J$,

$$\beta_l\sim\exp\left(-\frac{\Delta k}{2k}J\right). \tag{5.8}$$

We note the following. We have found the functions C_{11} and C_{12}, taking it into account that the Bessel functions change much more rapidly than C_{ij} and the potential, and using the asymptotic representations for the functions n_ν and j_ν. For $l \gtrsim J$, the calculations can be carried out in similar fashion if we seek a solution in the complex plane (in the upper half-plane). We can use here asymptotic expressions of the type (3.1) for large l, without limitation on the value of r. Therefore, the calculations for $l \gtrsim J$ are similar. The complication of the calculations lies in the fact that the singularities of the solution (previously for $l \ll J$), located at the points r_1, r_2 and r_3, are determined now by the more complicated condition of the form

$$b^2/4r^6 + (k\Delta k)^2(1 - l^2/r^2) = 0.$$

For β_l we have here

$$\beta_l \sim \mathrm{Re}\int_{r_1}^{r_1+i\infty} \frac{b\,dr}{kr^3} j_{l+1/2}(k_2 r) n_{l+1/2}(k_1 r).$$

Then, in the case $l \sim J^{9/8}$, we have $r_1 \approx l - l^{1/3}$. For $(\Delta k/k) l^{1/3} < 1$, we have $j_{l+1/2}(k_2 r) n_{l+1/2}(k_1 r) \sim J^{9/8}$, i.e., in the region $(\Delta k/k) J^{3/8} < 1$ the dependence of Δl on the resonance defect takes on a power-law character. The width of this region Δl is determined by the condition $\Delta l \sim l^{1/3} \approx J^{3/8}$.

Consequently, for $l \sim J^{9/8}$ and $\Delta k/k < l_0^{-3/7}$ we get

$$\beta_l \approx \left(\frac{\Delta k}{k}\right)^{-1} J^{-9/8}. \qquad (5.9)$$

We recall that this expression is valid if the resonance defect is such that

$$(\Delta k/k) l_0^{3/7} < 1. \qquad (5.10)$$

For large l ($l \gg 1$), we get the result that $r_0 \ll l/k$. Here β_l falls off with increase in the resonance defect in exponential fashion (similar to[6]):

$$\beta_l \sim \exp(-\Delta k l/k). \qquad (5.11)$$

We write out the contributions to the value of the excitation transfer cross section for $l \sim J^{9/8}$, $l \ll J^{9/8}$, $l \gg J^{9/8}$:

$$\text{a) } l \sim J^{9/8},\ \frac{\Delta k}{k} l_0^{3/7} \ll 1, \quad \Delta\sigma_t^J \approx \frac{4\pi}{k^2}\left(\frac{\Delta k}{k} J^{9/8}\right)^{-2}; \qquad (5.12)$$

$$\text{b) } l \gg J^{9/8}, \quad \Delta\sigma_t^> \approx \frac{4\pi}{k^2}\exp\left(-\frac{2\Delta k}{k}\right)\left(\frac{\Delta k}{k} J\right)^2;$$

$$\text{c) } l \ll J^{9/8}, \quad \Delta\sigma_t^< \approx \frac{4\pi}{k^2}\exp\left(-\frac{\Delta k}{k} J\right).$$

It is of interest to note that for sufficiently large l_0 the contribution of the region $l \sim J^{9/8}$ determines the value of the cross section. Thus, for example, for $l_0 \sim 100$ and $\Delta k/k \sim 5 \times 10^{-3}$, we get

$$\Delta\sigma_t^J \approx 3\cdot 10^2 4\pi/k^2; \quad \Delta\sigma_t^> \approx 5\cdot 10^{-2} 4\pi/k^2;$$
$$\Delta\sigma_t^< \approx 10^{-2} 4\pi/k^2.$$

Up to the values of the resonance defect $(\Delta k/k) l_0^{3/7} \sim 1$, the excitation transfer cross section falls off according to a power law:

$$\sigma_t \approx \frac{4\pi}{k^2} l_0^{-3/4}\left(\frac{\Delta k}{k}\right)^{-7/4}. \qquad (5.13)$$

If $\Delta k/k > l_0^{-3/7}$, then in the region $|l - J^{9/8}| < J^{1/3}$,

$$\beta_l \sim e^{-kJ} J^{-9/8}. \qquad (5.14)$$

Therefore, for such Δk, the region of intermediate values of l does not give a large contribution to the excitation transfer cross section. For the cross section in this case, we get a result which is identical with the result of Stuekelberg:[6]

$$\sigma_t \approx \frac{4\pi}{k^2}\exp\left(-\frac{\Delta k}{k} J\right).$$

We now calculate the elastic scattering cross section. The contribution to the elastic scattering cross section from the region $l \lesssim J^{9/8}$ does not exceed $4\pi k^{-2} J^{9/4}$. As will be seen below, the region $l \gg J^{9/8}$ gives a contribution which greatly exceeds this value. Therefore, for calculation of the elastic scattering cross section, we can limit ourselves to the calculation of α_l for $l \gg J$. Here, all the integrations in the expression (5.1) can be made not from zero but from the point l/k. Then

$$\alpha_l = e^{i\xi_l \Delta k}\sin \Delta k \xi_l,$$

$$\xi_l = \int_{l/k}^{\infty} \frac{b^2 dr}{k^2(\Delta k)^2 r^6} j_{l+1/2}^2(kr) \approx \frac{1}{5}\frac{J^6}{l^5},$$

and the elastic scattering cross section is equal to

$$\sigma_s \approx \frac{15\pi}{k^2} l_0^3\left(\frac{\Delta k}{k} l_0^{3/2}\right)^{-2/5} \qquad (5.15)$$

For the determination of the diffusion cross section, knowledge of α_l for $l \gg J^{9/8}$ is not sufficient. For $l \ll J$, the singularity of the solution satisfies the condition $|r_0| \gg l$. Consequently, α_l is virtually independent of l in this region:

$$\alpha_l = e^{i\xi_0 \Delta k}\sin \Delta k \xi_0, \qquad (5.16)$$

where

$$\xi_0 = \frac{b^2}{k^2(\Delta k)^2 r_0^5}\left(1 + O\left(\frac{l}{r_0}\right)\right).$$

Therefore, the moments $l \ll J$ make a contribution to the diffusion cross section of the order

$$\sigma_D^< \sim \frac{4\pi}{k^2} J^2\left(\frac{b^2}{k^2(\Delta k)^2 r_0^6}\right)^2 \sim \frac{4\pi}{k^2}\left(\frac{\Delta k}{k} J\right)^2 l_0^2\left(\frac{\Delta k}{k}\right)^{4/5} \qquad (5.17)$$

In the region $l \sim J$, but $|l - J| \lesssim J^{1/3}$, the values of α_l change rapidly with change in l. This is primarily associated with the strong dependence of r_0 on l. In the given case, α_l has the form (5.16) as before, but here

$$|\alpha_l - \alpha_{l+1}| \sim 1, \quad \xi_0 \approx l_0^3/l^2.$$

Therefore, in the considered region of change of l, we have $|\alpha_l - \alpha_{l+1}| \sim 1$, and the contribution to the diffusion cross section is determined by the expression

$$\sigma_D^J \approx \frac{4\pi}{k^2} J^{4/3} = \sigma_D(\Delta k = 0)\left(\frac{\Delta k}{k} l_0^{3/2}\right)^{-4/9}. \qquad (5.18)$$

Consequently, in the case of sufficiently large resonance defects, such that $x^2 \gg 1$, the diffusion cross section for $l_0 \gg 1$ is much less than its own value for a resonance defect equal to zero. We note that for $x^2 \gg 1$, the contribution of the inelastic scattering channel to the diffusion cross section is negligibly small, i.e., $\sigma_D^\beta \ll \sigma_D^\alpha$ (see (2.8)).

The given results show that the calculation of the diffusion cross section should be more accurate than was the case in[7], avoiding large errors.

The authors thank Ya. A. Smorodinskiĭ for interest in the research.

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Translated by R. T. Beyer
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