Model of intersecting bands for interaction of closely approaching atomic particles

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(Submitted April 10, 1973; resubmitted January 17, 1974)
Zh. Eksp. Teor. Fiz. **66**, 1933–1944 (June 1974)

The interaction between two many-electron atomic particles is considered for strong collisions, when the inner electron shells overlap. Owing to the pronounced nonadiabaticity of the collision, the system cannot be described by separated terms, and a large number of states are involved in the interaction. It is suggested that the behavior of the system at small internuclear distances be described by a small number of energy bands. Each band corresponds to a certain state of the inner shells and possesses a certain width, since the state of the outer shell is not fixed and may vary. This description is justified since the energy change following transitions of the inner electron is much greater than both the bandwidth and the nonadiabatic perturbation. Transitions between bands are therefore possible only if they are close to each other or intersect. Such transitions are analyzed by solving a model problem in which the bands are represented as a set of discrete terms. Transitions between terms of different bands in the intersection region, and also transitions between terms of a given band resulting from nonadiabatic coupling, are considered. Transition probabilities are obtained for a single traversal of the band-intersection region. The behavior of the bands for Kr–Kr and Ar–Ar systems is determined on the basis of the experimental data and by employing the model. The model explains the high probability of formation of inner vacancies, the singularities in the differential scattering cross sections, and the satisfactory applicability of adiabatic interaction potentials for the description of scattering in deep collisions of atomic particles.

I. FORMULATION OF PROBLEM

The interaction of multielectron atoms and ions in deep collisions is connected with overlap of the internal electron shells; the characteristic approach distances of the nuclei are 0.1—1 A. Collision energies on the order of tens of keV are considered, when the relative velocity of the nuclei is lower than the velocity of the external electrons. Experimental study of these collisions has revealed, for complex atomic particles, a discrete structure in the spectra of the inelastic energy losses Q[1]. The loss spectra consist in most cases of well resolved lines Q_l with energies of tens and hundreds of eV. There is every reason for assuming that the presence of several lines in the loss spectrum is due to the formation of vacancies in the internal shells of the colliding particles (see, e.g.,[2]).

A structure was observed earlier[3] in the total differential scattering cross sections $\sigma(\vartheta)$ (summed over all channels). Singularities in the form of maxima were observed on the $\sigma(\vartheta)$ curves, which decreased smoothly with increasing scattering angle ϑ. This phenomenon was investigated in detail for a large number of collision partners[4-6]. In terms of the universal coordinate $\rho = \sigma(\vartheta) \sin \vartheta$ and $\tau = T_0\vartheta$, all the results, regardless of the initial kinetic energy T_0 of the particles, fit approximately one curve (see Fig. 1a), thus indicating a rather weak dependence of the interaction forces on the relative particle velocity. The singularity in the scattering becomes manifest at a constant value of τ, i.e., it is connected with reaching of a definite closest-approach distance R_0.

An analysis of the scattering data for different pairs of particles shows that the characteristic approach distances at which the singularities appear coincide with the distance at which internal vacancies begin to be produced in the colliding particles. The data shown in Fig. 1 for Kr^+-Kr collisions illustrate this connection. As shown in[2], in the case Kr^+-Kr the line Q_I corresponds to excitation of the outer shells of the colliding particles, while the lines Q_{II} and Q_{III} correspond to excitation of the outer shells and to the simultaneous formation of one or two 3d vacancies. The existence of a well localized region of inter-nuclear distances, the reaching of which is accompanied by formation of internal vacancies, shows that the probable excitation mechanism is the crossing of the terms. Fano and Lichten[7,8] attribute, within the framework of the molecular orbitals, the crossing of the terms to the "advancement" of the orbital corresponding to the internal electrons.

Under the considered conditions, a complete description of the system requires that account be taken of a large number of states, since each of the lines in the loss spectrum is connected with participation of several electrons in the interaction, and with a multiplicity of transitions for each of the electrons. Estimates show that the value of the non-adiabatic perturbation due to the motion of the nuclei greatly exceeds the distance between neighboring terms corresponding to different configurations of the external shells, i.e., the region of the interaction of these terms is not localized. The presence of a sufficiently tight binding between the electronic and nuclear subsystems signifies that the electron energy, at a certain internuclear distance, is

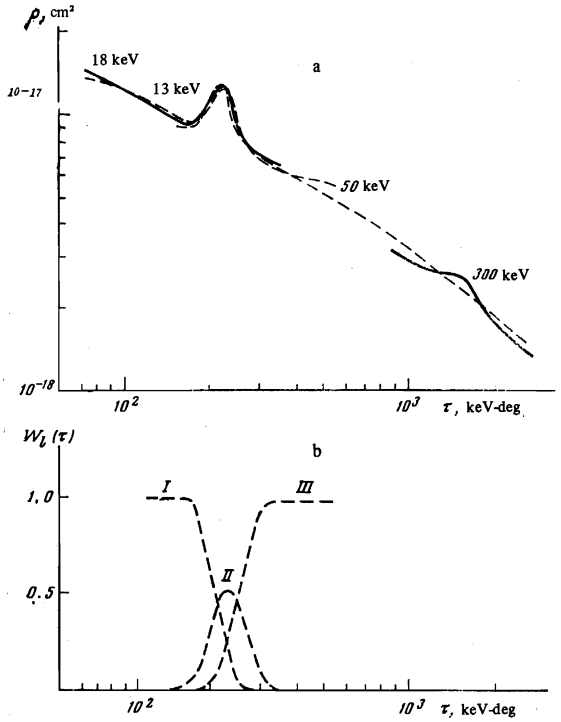

FIG. 1. Angular dependences of the scattering cross sections (a) and of the relative probabilities for the excitation of different inelastic-loss lines: Q_I, Q_{II}, and Q_{III} (b), for Kr^+-Kr collisions. Dashed curves–data of [3,4,6], solid curves–data of [5].

no longer fixed, i.e., the concept of an individual term becomes meaningless. At the same time, the change of the system energy in transitions of internal electrons greatly exceeds the nonadiabatic perturbation. Therefore only the states that differ in the configuration of the internal electrons can be regarded as different states of the system. Thus, a system of two atomic particles in the case of deep collision can be described with the aid of several energy bands, each of which corresponds to a definite state of the internal shells.

For a simplified analysis it is useful to introduce the concept of effective terms, each of which describes on the average the behavior of a corresponding band. The scattering singularities were qualitatively explained[6] as being the result of the crossing of two effective terms: in the case of crossing there exist trajectories that correspond to scattering by a potential with a break, and this leads to the appearance of peaks of the "rainbow" type in the corresponding cross sections.

As applied to individual terms, the crossing model makes it possible, as is well known, to solve the inverse scattering problem, i.e., to reconstruct the course of the terms from the experimental data. In final analysis, this is caused by the fact that the probability of the transition between the ground $1-1'$ and excited $2-2'$ terms in the case of forward and backward passage through the intersection point R_C are equal, $P_{12'} = P_{2'1}$. As a result the probability of excitation of the system after the collision is expressed by the known formula $W = 2P_{12'}(1 - P_{12'})$, which enables us to determine $P_{12'}$ from the experimental data on W, and the behavior of the system is thus known at all $R > R_0$.

The maximum inelastic transition probability W for crossing of individual terms is 0.5. Experiments[1,2] have shown, on the other hand, that in deep collisions the probability of the transition of the system to an excited effective term approaches unity. The only possible reason is that the condition $P_{12'} = P_{2'1}$ is not satisfied is the crossing of the effective terms. Experiment makes it possible to find the probability of the transition of the system to various final states W, but the probabilities of the transition between the terms for a single passage through the intersection point remain unknown in this case, i.e., the behavior of the system in the region $R_0 < R < R_C$ turns out to be unknown. To go from a qualitative explanation to a quantitative description, and in particular to a reconstruction of the course of the effective terms, it is necessary to construct a model that makes it possible to determine the transition probability for a single passage through the region of intersection of the effective terms.

II. APPROXIMATION OF INTERSECTING BANDS OF TERMS

1. Transitions in Intersection of Bands

For convenience in calculation, we represent the energy bands corresponding to the effective terms in the form of bands of individual terms (Fig. 2). We consider the probability of the transition of a system from the states $1-1'$ to the states $2-2'$ in the first passage of the intersection region. Let r be the number of terms in the band $1-1'$ corresponding as $R \to \infty$ to the effective term of the ground state, let s be the number of terms in the band $2-2'$ corresponding to the effective term of the excited state, and let p be the probability of the transition on going through one intersection of the individual terms. We assume for simplicity that p is the same for all the intersections. The number of channels that differ in the combinations of the final charges of the particles, say in K^+-Kr collisions, is approximately 40 (particles with charges from 1 to 7 are observed)[3]. Inasmuch as the particles in each of these channels can be in different excited states, the number of terms in the bands will be much larger. We note that under the considered conditions we not only have a large number of terms in the bands r and s, but also $s \gg r$, since an internal vacancy can be produced in a large number of ways as a result of the transition of an internal electron to free discrete levels or to the continuous spectrum.

Demkov and Osherov[9] considered the case of intersection of one term with a band of parallel terms and have shown that an arbitrary ratio of the magnitude of the interaction and of the distance between the terms, the probability of the transition from the initial state to

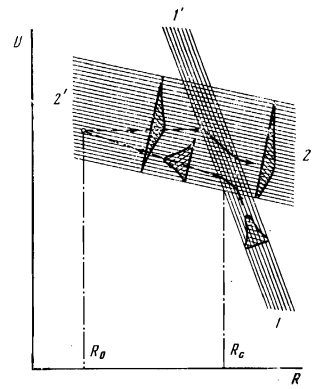

FIG. 2. Intersection of bands of terms. Thick line–most probable trajectory of motion of the system in the intersection region. The cross-hatched areas near the bands are the initial and final distributions of the term populations. R_C–intersection region, R_0–turning point. The dashed line shows the displacement of the center of the population distribution as a result of the nonadiabatic interaction.

any final state can be calculated as the product of the probabilities of the corresponding transitions.

In the case of intersection of two bands of terms, a contribution to the population of any level of the band $2-2'$ is made by many different trajectories of the representative point (in the coordinates U and R), so that interference terms must appear in the calculation of the probability of the transition from the k-th term of band $1-1'$ to the l-th level of band $2-2'$. However, recognizing that in real collisions the phase differences accumulated on passing over different interfering trajectories can be arbitrary, and that the number of such trajectories is large, we can neglect the contribution of the interference terms. Using the deductions of Demkov and Osherov, we shall assume that in the case of the intersection of two bands of terms the probabilities of the transitions from any initial state to any final state can be calculated as a product of the probabilities of the corresponding transitions in the intersection of the individual terms, naturally, by summing over all possible trajectories.

Let us consider a situation wherein the system experiences many transitions on going through the intersection region, and let us ascertain the conditions for the realization of this situation. The average number of intersections that the system passes through prior to the first transition is

$$M=p+2p(1-p)+3p(1-p)^2+\ldots+np(1-p)^{n-1}+\ldots \qquad (1)$$

Summing, we obtain $M = 1/p$. Thus, the condition of interest to us is

$$s>r\gg 1/p. \qquad (2)$$

Since the system makes an approximately equal number of crossings with the terms of each of the bands when this condition is satisfied, the center of the population distribution of the terms of band $1-1'$ will shift in the intersection region along the "diagonal" (see Fig. 2).

Detailed computer calculations have shown that indeed at $sp > rp \geq 3$ the initial distribution of the populations of the term of band $1-1'$ is projected along the "diagonal" on the terms of the band $2-2'$ with a certain broadening that depends on the value of p (Fig. 2). If (2) is satisfied, the probability $P_{12'}$ of the transition between the bands depends mainly on the ratio r/s, and at $s > 3r \geq 9/p$ we have $P_{12'} \approx 1$ and $P_{11'} \approx 0$ regardless of the initial distribution of the populations of the terms of band $1-1'$.

If no significant change in the populations of the terms of the band $2-2'$ takes place during the time between two passages through the intersection region, then it is easily seen that if condition (2) is satisfied an inverse "diagonal projection" on the terms of the band $1-1'$ occurs, and, depending on the initial population of the terms and the value of the broadening, the transition probability will assume values in the interval $\frac{1}{2} < P_{2'1} < 1$.

This result is in sharp contrast to the experimental data[1,2], according to which the probability of the transition to the final state $1-1'$ after collision is equal to zero. This means that account must be taken of the possible change in the population of the terms of the band $2-2'$ during the time between two successive passages through the intersection region. The reason for this redistribution of the population may be nonadiabatic transitions between terms of one band.

2. Transitions Between Terms of One Band

The system of equations for the expansion coefficients of the wave function of the system in the complete set of adiabatic functions for an infinitely discrete equidistant spectrum was considered by Presnyakov and Urnov[10].

$$i\hbar\frac{\partial a_m}{\partial t}=-\sum_n a_n(t)C_{mn}\exp[-i\omega_0(n-m)t], \qquad (3)$$

where $C_{mn} = \langle m | i\hbar\partial/\partial t | n \rangle$ and $\hbar\omega_0$ is the distance between neighboring terms.

In our case, the need for considering a strongly excited multielectron system makes the exact calculation of C_{mn} exceedingly difficult, and we confine ourselves to a model solution. Let λ be the characteristic distance over which an appreciable change takes place in the wave function, and then the nonadiabatic interaction is of the order of $\hbar v/\lambda$, where v is the velocity of the incident particle. When measured in the scale of the characteristic internuclear distance, the matrix elements C_{mn} are slowly varying functions, so that it is natural to assume in the model calculation that they do not depend on the time. Assuming that direct transitions are possible between the terms separated by a distance $\hbar\omega_0|m-n|$ and does not exceed $\hbar v/\lambda$, and assuming an exponential decrease of the matrix elements with increasing $\hbar\omega_0|m-n|$, we chose C_{mn} in the form

$$C_{mn}=\frac{\hbar v}{\lambda}\exp\left(-\frac{\omega_0\lambda}{v}|m-n|\right)\exp\left(i\varphi_0\frac{m-n}{|m-n|}\right), \qquad (4)$$

where the last phase factor takes into account the Hermitian character of the operator $\hat{C}$.

Making in (3) the substitutions

$$b_m=a_m\exp(-i\omega_0 mt), \quad t'=vt/\lambda,$$

we obtain a system of differential equations with constants coefficients, which is convenient for calculations:

$$\frac{\partial b_m}{\partial t'}=i\sum_{n=1}^{\infty} b_n\exp\left\{-\gamma|m-n|+i\varphi_0\frac{m-n}{|m-n|}\right\}-i\gamma m b_m, \qquad (5)$$

where $\gamma = \omega_0\lambda/v$.

In the case of large γ ($\gamma \gg 1$), perturbation theory can be used and the redistribution of the term populations is negligible. At small γ, the strong-coupling approximation can be used, and in the scale $t' = vt/\lambda$ the solution does not depend on γ. Numerical calculations have shown that at $\gamma^2 < 0.1$ during the time $t' \approx \gamma$ the distribution center shifts by $\gamma/2$ (it is assumed that at the initial instant of time only the lower levels of the band are populated). In order to satisfy the condition $P_{2'1} \approx 0$ as the particles move apart after passing through the intersection region, it is necessary that during the time t_0' between two passages through the intersection region the center of the population distribution shifts by an amount

$$t_0'/2\gamma^2>3r \qquad (6)$$

(it is understood that $s \gg 3r$).

For the situation of interest to us (e.g., Kr^+-Kr, 25 keV), depending on the impact parameter, we have $t' \lesssim 2$ and $\hbar v/\lambda \sim 6$ eV, while the distance between neighboring terms is $\hbar\omega_0 = \Delta Q/s$, where $\Delta Q \sim 40$ eV is the linewidth in the spectrum of the inelastic energy losses[2]. Then $\gamma = \Delta Q\lambda/s\hbar v \approx 7/s$, and the conditions (6) and $\gamma^2 < 0.1$ will be satisfied at $s > 22$ ($s > 3r$).

This requirement is easily satisfied in the collisions

in question, meaning that the redistribution of the term population during the time t_0' can be very large. In this case, taking the relation $s \gg r$ into account, the calculation of the transition probabilities for the backward passage through the intersection region yields the values $P_{2'2} \approx 1$ and $P_{2'1} \approx 0$. We recall that in the absence of population redistribution we had $\frac{1}{2} < P_{2'1} < 1$.

In the case when one term intersects a band we can no longer speak of "diagonal projection" of the initial distribution of the populations, since (2) is not satisfied, but at $sp > 3$ and in the presence of strong population redistribution during the time t_0' the transition probabilities will be the same as in the case of the intersection of two bands of terms, i.e., $P_{12'} = 1$ and $P_{2'2} \approx 1$.

III. APPLICATION OF THE INTERSECTING-BAND MODEL

1. Effective Interaction Potential

The obtained transition probabilities enable us to describe the behavior of the system at all distances R. The approach at $R > R_c$ occurs via the effective term $1-1'$. A transition to the terms of the band $2-2'$ takes place in the intersection region. When the particles move apart, the system is in the state 2. This model explains in natural fashion the high probability of formation of internal vacancies close to 100%, which was observed in experiment. Thus, the trajectory $1-2'-2$ is the fundamental one at $R_0 < R_c$ (Fig. 2).

We note that at $R < R_c$ the term $2-2'$ is the adiabatic term of the ground state. This means that as the particles approach each other the system moves all the time along the adiabatic term of the ground state, passes along the same term from the turning point R_0 to the intersection point R_c, and only at $R > R_c$ does the separation of the system follow the adiabatic term of the excited state. The scattering is determined principally by the course of the potential near the turning point. It is therefore clear that in our case, even in the presence of intersections, the scattering will be close to that described with the aid of the adiabatic potential. The influence of the separation along the excited terms will be noticeable only in those cases when the turning point is close to the corresponding intersection point.

With decreasing R_0 and on passing through the succeeding intersection points, owing to a more rapid Coulomb repulsion of the nuclei in comparison with the inelastic losses, the role of this effect should decrease. This conclusion agrees well with the results of experiment[3-6], according to which only the formation of the first vacancies in the internal shells correlates with the noticeable singularities in the scattering, while the formation of the succeeding vacancies with decreasing R_0 causes only very weak deviations from the smooth course of the $\sigma(\vartheta)$ curves.

Since it is now clear why the main course of the cross sections can be successfully described with the aid of an adiabatic potential, it is useful, in the comparison with experiment, to choose the best theoretical model. Such a comparison is shown in Fig. 3. Here U_{exp} is the potential reconstructed by us from the experimental data using the Firsov procedure. To calibrate the cross sections we used the results of Loftager's absolute measurement[5].

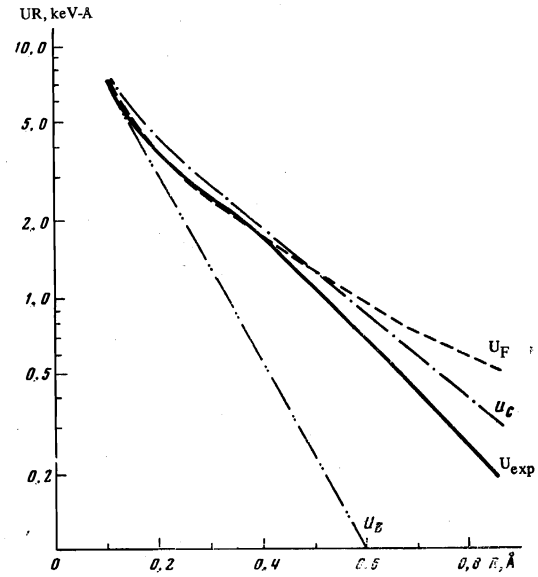

FIG. 3. Comparison of the Kr-Kr interaction potential obtained from the experimental data (U_{exp}) with the theoretical models (U_B–Bohr potential [11], U_F–Firsov potential [12], U_C–Czavinszky potential [14]).

It is seen from the figure that the Bohr potential frequently used in the calculations[11]

$$U_B = \frac{Z_1 Z_2 e^2}{R} \exp\left(-\frac{R}{a_B}\right), \quad a_B = \frac{a_0}{(Z_1^{2/3}+Z_2^{2/3})^{1/2}}, \quad a_0 = 0.529\ \text{Å}, \tag{7}$$

is in good agreement with experiment only at very small distances. In much better with experiment is the potential obtained by Firsov[12] in the form

$$U_F = \frac{Z_1 Z_2 e^2}{R} \varphi\left(\frac{R}{a_F}\right), \quad a_F = \frac{0{,}8853 a_0}{(Z_1^{1/2}+Z_2^{1/2})^{2/3}}, \tag{8}$$

where φ is the Thomas-Fermi screening function.

Nikulin[13] has calculated the potential within the framework of the statistical theory, using quantum-mechanical electron densities; his potential agrees well with the Csavinszky potential[14]:

$$U_C = \frac{Z_1 Z_2 e^2}{R}\left[a \exp\left(-\frac{\alpha}{a_F} R\right) + b \exp\left(-\frac{\beta}{a_F} R\right)\right]^2, \tag{9}$$

$$a+b=1; \quad a=0.7111; \quad \alpha=0.175; \quad \beta=9.5\alpha.$$

This potential describes the scattering most accurately.

2. Reconstruction of the Effective Terms

Knowing the transition probabilities for single passage through the intersection region, we can reconstruct from experiment the course of the effective terms of the system. Since, as already established in[1,2], three lines are distinctly represented in the energy-loss spectrum, it is natural to consider a model of three intersecting terms. The model of intersecting terms makes it possible to distinguish in each separation term the most important trajectory (see Fig. 4):

$$\begin{aligned} &\text{I)}\ 1-2'-1, \\ &\text{II)}\ 1-2'-2, \\ &\text{III)}\ 1-2'-3'-3. \end{aligned} \tag{10}$$

We note that no scattering by the terms $1-1'$ and $2-2'$ takes place at $R < R_{c1}$ and $R < R_{c2}$, respectively, meaning that their behavior in these regions can be obtained only by extrapolating the corresponding sections at $R > R_c$. It is well known that to reconstruct the potential on the section $R > R_i$ it is necessary to know the

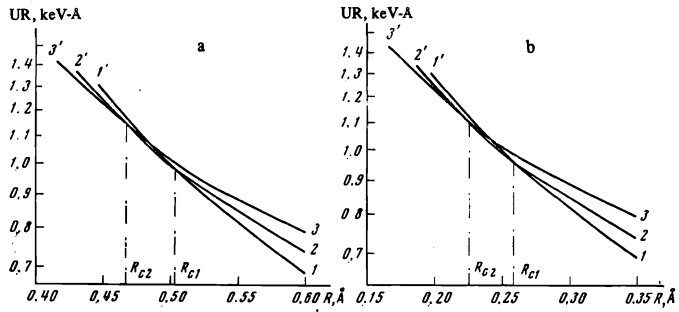

FIG. 4. Effective terms for different internal-shell configurations: a) Kr-Kr: $1-1'$ ($3d^{10}-3d^{10}$), $2-2'$ ($3d^{10}-3d^{9}$), $3-3'$ ($3d^{10}-3d^{8}$, $3d^{9}-3d^{9}$); b) Ar-Ar: $1-1'$ ($2p^{6}-2p^{6}$), $2-2'$ ($2p^{6}-2p^{5}$), $3-3'$ ($2p^{6}-2p^{4}$, $2p^{5}-2p^{5}$). R_C–intersection points.

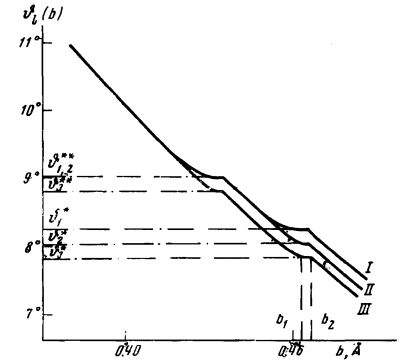

FIG. 5. Scattering angle vs. the impact parameter for Kr^{+}-Kr collisions, T_0 = 25 keV. I–scattering via channel $1-2'-3'-2'-1$, II–scattering via channel $1-2'-3'-2'-2$. III–scattering via channel $1-2'-3'-3'$. ϑ^* and ϑ^{**} are the limits of the ambiguous $\vartheta_l(b)$ dependence.

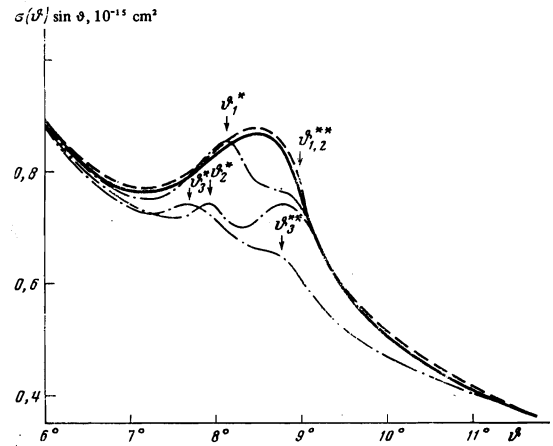

FIG. 6. Differential scattering cross sections for Kr^{+}-Kr collisions, T_0 = 25 keV. Solid curve–total cross section, experiment; dash-dot curve–cross sections for scattering via different channels, calculated from the deviation functions, dashed–calculated total cross section.

deviation function $\vartheta(R)$ at $\vartheta \le \vartheta(R_i)$, so that the course of the term $1-1'$ at $R \ge R_{C1}$ can be reconstructed immediately by using Firsov's procedure. The threshold angle of the excitation of the line Q_{II} in the energy-loss spectrum is used to determine the coordinates of the first point of intersection $U(R_{C1})$ and R_{C1}. We then determine the course of the term $2-2'$ at $R > R_{C1}$, in the form

$$U_{2-2'}(R)=\frac{U(R_{c1})-Q_{II}}{U(R_{c1})-Q_I}[U_{1-1'}(R)-Q_I]+Q_{II}, \qquad (11)$$

and, calculating on the basis of (11) the missing section of the deviation function of the trajectory II (at $\vartheta < \vartheta_2(R_{C1})$), we reconstruct the course of the term $2-2'$ at $R_{C1} > R_{C2}$. We next obtain, in similar fashion, the course of the term $3-3'$. The need for a parametrization of the type (11) leads to corresponding errors when it comes to reconstruct the course of the effective terms in the region $R > R_C$, but the farther the turning point from R_C the more accurate the calculation.

Similar calculations were carried out for the systems Kr-Kr and Ar-Ar, inasmuch as it is precisely in this case that a large (~100%) probability of scattering via the most inelastic channel is observed, and consequently the model of intersecting bands is applicable. Figure 4 shows the experimentally obtained effective terms of the quasimolecular systems Kr-Kr and Ar-Ar.

Since appreciable errors can accumulate in the calculation process, to verify the calculation accuracy we solved the direct scattering problem, i.e., we calculated, on the basis of the obtained terms, the deviation functions $\vartheta_l(b)$, where b is the impact parameter (Fig. 5), and the corresponding cross sections (Fig. 6). The calculations were performed for each of the three indicated channels in the entire investigated interval of approach distances. In the calculation of the deviation functions for the channels II and III in the regions $R_0 > R_{C1}$ and $R_0 > R_{C2}$ respectively (Fig. 4) it was assumed that the approach is along the lowest term, and that a transition to the corresponding excited term from which the scattering takes place occurs at the turning point.

In view of the strong redistribution of the excitation probabilities of the energy loss lines (Fig. 1b), it was assumed in the calculation of the total cross section $\sigma_\Sigma(\vartheta)$ that the scattering is only via channel I in the region $R_0 > R_{C1}$, via channel II in the region $R_{C2} < R_0 < R_{C1}$, and via channel III in the region $R_0 < R_{C2}$. It turns out that although each value of R_0 the scattering is assumed to be single-channel, in some angle regions a mutual superposition takes place of the cross sections for scattering via various channels. For example, it is seen from Fig. 5 that near the point $b_2(R_{C1})$, the particles are deflected through a smaller angle for scattering via channel II than for scattering via channel I. Consequently, the cross sections $\sigma_I(\vartheta)$ and $\sigma_{II}(\vartheta)$ will add up in the calculation of the total cross section $\sigma_\Sigma(\vartheta)$ in the angle interval $\vartheta_2^* < \vartheta < \vartheta_1^*$, and the resultant contribution to the singularity in $\sigma_\Sigma(\vartheta)$ is

$$\sigma_c \approx \sigma_{I,II}(\vartheta_{1,2}^*)\sin\vartheta_{1,2}^*(\vartheta_1^{*\prime}-\vartheta_2^{*\prime}) \approx 4.3\cdot 10^{-20}\ \text{cm}^2. \qquad (12)$$

This effect is due to the multichannel character of the scattering and can be called the effect of "inelastic shift" of the cross section.

The presence of minima in the deviation functions leads to the appearance of singularities of the rainbow type in the differential scattering cross section $\sigma_l(\vartheta)$. This effect was discussed earlier [6]. The regions of the minimum in the functions $\vartheta_l(b)$ (Fig. 5) turn out to be narrow in comparison with the region of angles in which a singularity is observed in $\sigma(\vartheta)$. This difference is due to the length of the band-intersection region, to the presence of three intersecting bands, and to the superposition of the contribution of several channels. Taking into account such a natural "smearing," one can get away in the comparison with experiment without an exact calculation of the rainbow peaks in the cross sections, and confine oneself to a determination of integral

contribution of the rainbow effect to the singularity in the differential scattering cross section

$$\sigma_R=\pi(b_2^2-b_1^2)\approx 4.1\cdot 10^{-20}\ \text{cm}^2 \qquad (13)$$

(see Fig. 5).

When constructing the calculated summary cross section $\sigma_\Sigma(\vartheta)$ (Fig. 6), both cross sections σ_R and σ_C were "smeared out" over an angle range ~2°, with the area maintained constant, so as to make the comparison with experiment more illustrative. The calculated and experimental cross sections agree well in their general behavior, in the position of the singularity, and in magnitude, thus indicating that the calculation is of sufficient accuracy.

Thus, the model of intersecting bands, by providing the missing information concerning the transition probabilities, describes adequately multichannel scattering of atomic particles in deep collisions, and makes it possible to obtain, on the basis of the experimental data, the course of the effective terms of the system.

Preliminary results obtained with the model of intersecting bands were reported in[15].

In conclusion, the authors are grateful to Yu. M. Demkov, G. F. Drukarev, A. M. Polyanskiĭ, and A. P. Shergin for a useful discussion of the present results.

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Translated by J. G. Adashko
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