Dynamic symmetry of charge-dipole interaction in scattering and relaxation

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A quasiclassical realization of the irreducible tensor operators in the basis of spin coherent states is proposed. The dynamic symmetry of charge-dipole interactions is considered and the classical Bloch equations of motion of the angular momentum of the state of the perturbing particle in the collision is obtained. The exact M-exchange matrix is obtained on this basis. The scattering-problem data are used to analyze the anisotropy of the collisions in the relaxation and in the spectral structures. An increase of the relaxation rate with increasing multipole moment of the state in isotropic collisions is predicted. It is observed that the anisotropic part of the relaxation rates, due to the "wind effect," amounts to 1/8 to 1/5 of the isotropic part. As a result of this effect, the line contour can comprise a superposition of an abrupt component and a broad one.

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1. INTRODUCTION

This paper is devoted to the disorientation produced in collisions of atomic particles with charge-dipole interaction (CDI)

 $V = e(\mathrm{d}\mathbf{r})/\mathbf{r}^3. \tag{1.1}$

Scattering with CDI was investigated earlier by Lisitsa, Sholin, and Strekalov.^{1,2} Lisitsa and Sholin¹ solved the particular problem of the broadening of hydrogen spectral lines in a plasma on account of collisions with electrons. They used in their calculations a special quantity connected with the additional O(4) symmetry of the states in a Coulomb field. Strekalov² considered the CDI within the framework of an exponential approximation that is applicable only under nonadiabatic conditions. In the case of close flyby, strong disorientation takes place and this approximation cannot be used here.

We propose below an exact solution of the problem of elastic M-exchange with CDI both in the adiabatic and the nonadiabatic collision regions; this solution is not connected with the presence of additional symmetry of the states and of the conserved quantities.

The approach developed is also of independent interest in quantum theory of systems whose dynamics is determined by an interaction characterized by irreducible tensor operators (ITO).

For the ITO responsible for the quantum transitions between states, we develop quasiclassical representation that is at the same time also an exact quantum representation. In this representation it is easy to go over in standard fashion to a quasiclassical description of the internal quantum degrees of freedom and obtain the corresponding classical equations of motion.

We shall consider rotation states that are degenerate in the projections M of the angular momentum J of the system, in the representation of the spin coherent states of the rotation group. The coherent states (CS) of the rotation group began to be discussed in the physics literature intensively about 10 years ago.^{3,4} A complete review of the dynamic symmetries (DS) of the most important groups in physics, and of the corresponding CS, can be found in Perelomov's paper.⁴ Such constructions have been known in group theory and their representation for a long time.⁵ The idea of realization of ITO of general form in a CS basis is discussed here apparently for the first time.

The JM-exchange matrix in scattering is determined by the dynamic-symmetry group and its representations. The quasiclassical approximation mentioned above assures asymptotically correct expressions of the representations of the DS group. In the case of elastic scattering with CDI, however, the quasiclassical approach leads to an exact solution. This is no accident and is due to the fact that the DS group of the interaction coincides with the SU(2) group of quantization of directions on a sphere.

The concept of the DS is necessary also in the analysis of the observed structures of spectral lines. We recall that as a result of the anisotropy of the collisions (the "wind effect") the impact contour of a spectral line broadens and splits into several components.⁶ The diagonal elements of the relaxation matrix determine the relaxation rate of the states, while the off-diagonal elements determine the mixing in this process.

If the collisions are isotropic, the irreducible multipole moments of the states relax but can become mixed, because of the wind effect. The mixing structure is determined by the space-time properties of the symmetry of the states in the scattering and by the DS interaction group. In anisotropic collisions, the mixing of the states is significant to the extent of the resultant collisional disorientation. If the region corresponding to strong disorientation is important (the interaction is not long-range), then, besides the quasiclassical approximation, it is possible to use in individual cases a numerical solution of the scattering problem.⁷⁻¹¹ Of great interest to us are analytic methods not restricted by specific values of the moments of the states.

The content of this paper is the following. We consider first elastic *M*-exchange in collisions of charged particles and molecules with an intrinsic or induced dipole moment. We obtain the dynamic symmetry of the CDI and the equation of motion of the classical angular momentum. Next, on the basis of the concept of coherent states and complex realization of the ITO we introduce the disorientation current. A generalized power-law model is analyzed. Next, the consequences of the DS of the CDI in the structure of the matrix relaxation and in the spectral-line contours are discussed. Methodological aspects of the complex realization of ITO and of the Hamiltonian approach are relegated to the Appendix, where the polarization relaxation rates also given in the case of different perturbations on the combining levels.

2. COLLISIONAL DISORIENTATION IN CDI

We consider disorientation, due to collisions with charged particles, of states that are degenerate in Mand have no inversion center. In the coordinate system (see Fig. 1) whose z axis is parallel to the direction of the relative velocity u of the colliding particles (the *u*-system), the dynamics of elastic M exchange is described by the following equation for the scattering matrix:

$$i\frac{\partial S_{MM'}^{J}}{\partial \alpha} = C\left(\frac{4\pi}{3}\right)^{J_{2}} \sum_{mM_{1}} Y_{im}^{*}(\alpha,0) \hat{T}_{im}^{J}(MM_{1}) S_{M,M'}^{J}.$$
(2.1)

For simplicity we assume that the scattering orbit is a linear trajectory $r^2 = \rho^2 + (ut)^2$ with an impact parameter ρ . We introduce on this trajectory an angular time $\alpha = \pi/2 + \arctan(ut/2)$, which ranges from 0 to π during a collision time from $t = -\infty$ to $t = \infty$. The parameter C is the product of the energy difference of the neighboring M-sublevels in the potential (1.1) during the time of flight ρ/u (i.e., C is the Massey parameter):

$$C = e(nJ ||d|| nJ) / \hbar \rho u [J(J+1)(2J+1)]^{\frac{1}{2}}$$

Here e is the charge, (nJ||d||nJ) is the reduced matrix element of the dipole moment of the level nJ.

The *M*-exchange dynamics proper is specified by a first-rank tensor operator with components

$$\hat{T}_{im}^{JJ} = [J(J+1)(2J+1)]^{\frac{1}{3}-\frac{1}{2}} \sum_{MM_{i}} |JM\rangle(-1)^{J-M_{i}} \langle JMJ-M_{i}|1m\rangle \langle JM_{i}|.(2.2)$$

The operators (2.2) form a closed algebra of the SU(2) group:

$$[\hat{T}_{i\pm i}^{JJ}, \hat{T}_{i0}^{JJ}] = \mp \hat{T}_{i\pm i}^{JJ}, \quad [\hat{T}_{i+1}^{JJ}, \hat{T}_{i-1}^{JJ}] = -\hat{T}_{i0}^{JJ}.$$
(2.3)

Since the Hamiltonian of Eq. (2.1) is linear in the generators of the SU(2) group, it follows that the scattering operator is the Wigner rotation operator.⁴ We have thus established the analytic structure of the scattering matrix.

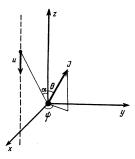


FIG. 1. The u-coordinate system.

We tie to the molecule a coordinate system whose z axis coincides with the direction of the average angular momentum J (the M system). The rotation of the M system upon collision will be described by the Euler angles ψ, θ, φ between the M and u systems. The scattering operator then takes the form

$$\hat{D}^{J}(\psi, \theta, \varphi) = \exp\left(-i\psi\hat{T}_{iz}^{JJ}\right) \exp\left(-i\theta\hat{T}_{iy}^{JJ}\right) \exp\left(-i\varphi\hat{T}_{iz}^{JJ}\right),$$

$$S_{MM'}^{J} = \langle JM|\hat{S}|JM'\rangle = D_{MM'}^{J}(\psi, \theta, \varphi).$$

$$(2.4)$$

Here \hat{T}_{1a}^{JJ} (a = x, y, z) are the Cartesian components of the tensor \hat{T}_{1m}^{JJ} .

In the moving M system, the initial distribution of the state amplitudes over the projections of the angular momentum is obviously conserved, but in the *u*-system it varies, i.e., M exchange takes place. Our next task is to calculate the angles ψ, θ, φ . The angular-velocity components of the rotation of the moving M system along the axes of the *u* system can be obtained from the equation [obtained by substituting (2.4) in (2.1)]

$$\sum_{m} (-1)^{m} \omega_{-m} \hat{T}_{im}^{JJ} = \left(\frac{4\pi}{3}\right)^{\frac{1}{2}} C \sum_{m} Y_{im} \cdot (\alpha, 0) \, \hat{T}_{im}^{JJ} \, . \tag{2.5}$$

The circular components of the angular velocity are of the form

$$\omega_0 = \dot{\phi} \cos \theta + \dot{\psi}, \quad \omega_{\pm 1} = (-i\theta \mp \dot{\phi} \sin \theta) e^{\pm i\phi} / \sqrt{2}. \tag{2.6}$$

From the completeness of the algebra of the operators \hat{T}_{1m}^{IJ} and from Eq. (2.5) follow the classical Euler equations of motion of a solid with equal moments of inertia

$$\overline{V}_{2\omega_1} = -C \sin \alpha, \quad \omega_0 = C \cos \alpha. \tag{2.7}$$

This equation can be written in vector form

$$\mathbf{n} = [\mathbf{C} \times \mathbf{n}],$$

$$\mathbf{n} = (\sin \theta \cos \psi, \sin \theta \sin \psi, \cos \theta), \quad \mathbf{C} = C(\sin \alpha, 0, \cos \alpha). \quad (2.8)$$

For the initial conditions n(0) = (0, 0, 1) we easily obtain from (2, 8)

$$n_{\mathbf{x}}(\alpha) = \sin \alpha - \cos \alpha \sin (\alpha \nu) / \nu - \sin \alpha (1 - \cos \alpha \nu) / \nu^2,$$

$$n_{\mathbf{y}}(\alpha) = -C (1 - \cos \alpha \nu) / \nu^2,$$

$$n_{\mathbf{z}}(\alpha) = \cos \alpha + \sin \alpha \sin (\alpha \nu) / \nu - \cos \alpha (1 - \cos \alpha \nu) / \nu^2, \quad \nu = (1 + C^2)^{\frac{\nu}{2}}.$$

(2.9)

Knowing the components of the unit vector, it is easy to determine the Euler angles θ and ψ after the flight of the charge ($\alpha = \pi$):

$$\theta = \arccos \left[(-C^2 - \cos \pi v) / v^2 \right], \quad \psi = - \arctan \left[(C \operatorname{tg} (\pi v / 2)) / v \right].$$
 (2.10)

We can next obtain the angle φ from Eqs. (2.7). In practice the situation reduces to a complicated integral which could not be evaluated here directly. However, all the Euler angles can be easily determined in a different coordinate frame, with z axis perpendicular to the collision plane (the z-system):

$$\begin{aligned} &\cos \bar{\theta} = (1 + C^2 \cos \pi \nu) / \nu^2, \\ &\bar{\psi} = \pi / 2 + \arctan \left(\nu \cot g \left(\pi \nu / 2 \right) \right), \\ &\bar{\phi} = -\arctan \left(tg \left(\pi \nu / 2 \right) \right) / \nu. \end{aligned}$$

We now transform the S matrix from the z-system to the *u*-system of coordinates, making both systems congruent by clockwise rotation through an angle $\pi/2$ about the x axis:

 $\hat{s}(\psi, \theta, \varphi) = \hat{D}(\pi/2, -\pi/2, -\pi/2) \hat{s}(\tilde{\psi}, \tilde{\theta}, \tilde{\varphi}) \hat{D}(\pi/2, \pi/2, -\pi/2).$

. As a result of straightforward but cumbersome spherical-geometry transformations¹² we obtain

$$p = \arctan \left[(C/\nu) tg (\pi \nu/2) \right] = -\psi.$$
 (2.12)

Thus, the DS of the interaction, if it reduces to the SU(2) group, can describe the dynamics of an angular momentum that is directed on the average along n, using the solution of the Bloch equation or of the corresponding Euler equations. We can stop here if we are not interested in the angular-momentum motion due to an interaction having a different DS. In such cases an approach in a basis of quasiclassical states may turn out to be effective.

The anisotropic part of the interaction potential is usually characterized by an ITO or by a set of ITO. The construction of the classical equations of motion that generalize the Bloch Eq. (2.8) is carried out in two stages. During the first stage the ITO are realized in a basis of quasiclassical states $|Jn\rangle$ (Ref. 4), which are the eigenstates of the operator

$$\mathbf{n} \cdot \mathbf{J} | J \mathbf{n} \rangle = J | J \mathbf{n} \rangle. \tag{2.13}$$

From analytic considerations, it is more convenient to use the complex variable

$$\mu = \operatorname{tg} (\theta/2) e^{i \psi}, \qquad (2.14)$$

which is obtained as a result of a stereographic projection from the sphere $n^2 = 1$ on the plane μ . We define these coherent states in the following manner:

$$|J\mu\rangle = \sum_{M=-J}^{J} {\binom{2J}{J-M}}^{\frac{J}{2}} \mu^{J-M} |JM\rangle, \qquad (2.15)$$

which differs from the definition of Refs. 3 and 4 in that the norm of the states is included in the measure $\delta_{J} \mu$ of the "expansion of unity":

$$\hat{I} = \int \delta_J \mu |J\mu\rangle \langle \mu J|, \quad \delta_J \mu = \frac{2J+1}{\pi} \frac{d \operatorname{Re} \mu d \operatorname{Im} \mu}{(1+|\mu|^2)^{2+2J}}.$$

The realization of the ITO, e.g., from the left for \hat{T}_{1q}^{IJ} , has in the basis (2.15) the form

$$\hat{T}_{10}^{\prime\prime} = J - \mu^{*} \frac{\partial}{\partial \mu^{*}}, \quad \hat{T}_{11}^{\prime\prime} = -\frac{1}{\sqrt{2}} \frac{\partial}{\partial \mu^{*}}, \quad \hat{T}_{1-1}^{\prime\prime} = \frac{1}{\sqrt{2}} \left(2J \mu^{*} - \mu^{*} \frac{\partial}{\partial \mu^{*}} \right). \quad (2.16)$$

In the general case a realization of an ITO of general form $\hat{T}_{x_q}^{JJ'}$ is specified by the operator function $\hat{F}_{x_q}^{JJ'}$ $(\mu^*, \partial/\partial\mu^*)$. For first-rank tensors these functions are given in Appendix 1.

During the second stage, we write down the quantum evolution equation $\psi(\mu^*) = \langle J\mu | \psi \rangle$ in the CS representation with a Hamiltonian realized in the same basis:

$$i\frac{\partial \Psi}{\partial t} = \hat{H}\left(J, \mu^{*}, \frac{\partial}{\partial \mu^{*}}\right)\Psi.$$
 (2.17)

The classical equations of motion of the angular momentum are obtained by the standard procedure of quasiclassical approximation of quantum mechanics. At large J, the function ψ is sought in the form

$$\psi = e^{j\Phi} \left\{ \psi_0 + \frac{1}{j} \psi_1 + \ldots \right\}. \tag{2.18}$$

From this we obtain in the zeroth approximation the classical Hamilton-Jacobi equation

$$i\frac{\partial\Phi}{\partial t} = \frac{1}{J}H\left(J,\mu,\frac{\partial\Phi}{\partial\mu}\right)$$
(2.19)

and if necessary the classical equation of motion.

We use the described procedure again to analyze the disorientation in scattering with CDI. In place of the S matrix we have here the scattering-operator symbol

$$S(\mu^{\bullet}, \alpha) = \langle J\mu | \hat{S}(\alpha) | JM' \rangle, \qquad (2.20)$$

which satisfies the equation

$$\frac{\partial S}{\partial \alpha} = -j(\mu^*, \alpha) \frac{\partial S}{\partial \mu^*} + J \frac{\partial j(\mu^*, \alpha)}{\partial \mu^*} S,$$

$$j(\mu^*, \alpha) = iC [2^{-1}(1-\mu^{*2}) \sin \alpha - \mu^* \cos \alpha].$$
(2.21)

The initial values for the S symbol, corresponding to a unit S matrix (prior to the collision, i.e., at $\alpha = 0$), are

$$S(\mu^{*},0) = \langle J\mu | JM' \rangle = \begin{pmatrix} 2J \\ J-M' \end{pmatrix}^{\prime \prime_{\mu}} \mu^{*J-M'}.$$
 (2.22)

The solution of Eq. (2.21) is determined by the equation of the characteristics, which is the classical equation of motion

$$d\mu^*/d\alpha = j(\mu^*, \alpha). \tag{2.23}$$

Thus, the quantity j has the meaning of the disorientation current, and the characteristics are the streamlines of j.

If we make the substitution

$$\mu^{*} = [\overline{\mu} + tg(\alpha/2)] / [1 - \overline{\mu} tg(\alpha/2)], \qquad (2.24)$$

which means a change to a rotating system with axis directed on the incident particle, then $\overline{\mu}$ satisfies the Riccati equation with constant coefficients

$$d\bar{\mu}/d\alpha = -iC\bar{\mu} - (1 + \bar{\mu}^2)/2. \qquad (2.25)$$

To illustrate the solutions of Eq. (2.25), Fig. 2 shows the phase portrait of the disorientation current. The form of the integral lines proves that the $\bar{\mu}$ -plane points move periodically around the singular points $\bar{\mu}_{\pm}$ = $-i(C \pm \nu)$.

On the characteristics (2.23) we have the solution of Eq. (2.21) (see Appendix 2)

$$S(\mu^*, \alpha) = (\partial \eta^* / \partial \mu^*)^{-J} S_0(\eta^*). \qquad (2.26)$$

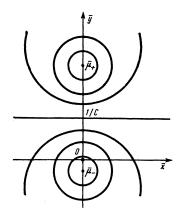


FIG. 2. Phase portrait of the disorientation current on the $\bar{\mu} = \bar{x} - i\bar{y}$ plane.

Here η^* is the Lagrange variable

$$\eta^{*}(\mu^{*}, \pi) = (\mu^{*} - A^{*})/(1 + \mu^{*}A),$$

$$S(\mu^{*}, \pi) = \left(\frac{2J}{J - M'}\right)^{\frac{1}{2}} (1 + |A|^{2})^{-J} (\mu^{*} - A^{*})^{J - M'} (1 + \mu^{*}A)^{J + M'}, \quad (2.27)$$

$$A = -iC + v \operatorname{ctg} (\pi v/2) = ae^{i\Psi}.$$

The matrix element $\langle JM | \hat{s} | JM' \rangle$ is obtained from (2.27) by a quadrature that leads us to the Wigner matrix:

c

$$\langle JM|S|JM'\rangle = \int \delta_{J}\mu \langle JM|J\mu \rangle S(\mu^{*},\pi)$$

= $e^{-i(M-M')\psi} \sum_{i} (-1)^{i} \frac{[(J+M)!(J-M)!(J+M')!(J-M')!]^{\gamma_{i}}}{(J+M-t)!(J-M'-t)!(M'-M+t)!t!}$
 $\times (1+a^{2})^{-j}a^{2i+M'-M} = D_{MM'}^{*}(\psi,\theta,-\psi).$ (2.28)

From the character of the phase trajectories we can determine the degree of disorientation after the collision. We note that the running angles $\theta(\alpha)$ and $\psi(\alpha)$ in the D matrix correspond to a trajectory that starts out from the origin $(\eta^* = 0)$. Therefore, if $|\mu| = \tan(\theta/2)$ changes weakly (or strongly) on this trajectory, the disorientation is weak (or strong). The corresponding angle $\theta(\pi)$ is close to zero or π . From Fig. 3 we can see that at $C \ll 1$ (remote flyby, large relative velocity) the disorientation is very weak, and in the other limiting case $C \gg 1$ it is strong. The latter can be easily explained by recalling that according to Eq. (2.8) the quantity C is also the rate of precession of the average angular momentum. Precessing rapidly around the interaction axis C/C, the angular momentum follows it adiabatically.

In the physics of atomic and molecular collisions one frequently uses a power-law model of interaction

$$\hat{V} = \frac{a_s}{r^{s+2}} (Y_{iq}^*(\alpha, 0) \hat{T}_{iq}^{IJ}).$$
(2.29)

The value s = 0 corresponds to the CDI, and s = 5 corresponds to the anisotropic part of the Buckingham potentials¹³ between the atoms of the inert gases and the polar molecules, etc.; the S matrix in the power-law model is also a rotation matrix. In the cases $s \neq 0$ all that changes is the character of the rotation, now described by the equation

$$d\bar{\mu}/d\alpha = -iC_{*}\sin^{*}\alpha\bar{\mu} - (1 + \bar{\mu}^{2})/2, \qquad (2.30)$$

where C_s is the Massey parameter [cf. (2.25)]. For an approximate solution of this equation we introduce the effective interaction region ε localized in the vicinity of the perturbed quantity, i.e., near the point $\alpha = \pi/2$,

$$\varepsilon = \int_{0}^{\pi} \sin^{*} \alpha \, d\alpha = 2 \cdot B\left(\frac{s+1}{2}, \frac{s+1}{2}\right), \qquad (2.31)$$

where B(x, y) is the Euler β function.

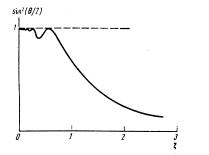


FIG. 3. Dependence of the disorientation on $\xi = 1/C$ (ξ is proportional to the impact parameter).

Replacing the smooth interaction $C_s \sin^s \alpha$ by a step function (Fig. 4), we easily obtain the disorientation parameters. To this end, using the known solution of Eq. (2.25) in the region of interaction with the Massey parameter C_s , we join it to the solution of the equation

$$d\bar{\mu}/d\alpha = -(1+\bar{\mu}^2)/2$$

outside the interaction region ε . As a result we obtain

$$\frac{\cos\theta_* = \nu^{-1} \sin e\nu \sin e + \nu^{-2} \cos e\nu \cos e}{-(1-\nu^{-2}) [\sin^2 (e/2) - \cos e\nu \cos^2 (e/2)],}$$

$$tg \psi_* = C_* [\cos (e/2) - \nu \operatorname{ctg} (e\nu/2)]^{-1}, \quad \nu = (1+C_*^2)^{\frac{\nu}{4}}.$$
(2.32)

In the case of remote flyby, under the condition $C_s \ll 1$ that the collision be nonadiabatic, the disorientation is, naturally, always weak:

$$\sin^2(\theta_*/2) \approx C_*^2 \sin^2(\epsilon/2). \tag{2.33}$$

In the other limiting case of adiabatic collisions, the disorientation in the power-law model differs somewhat from the disorientation in the CDI in that it is not necessarily strong. In fact, it follows from (2.32) that

$$\sin^{2}(\theta_{s}/2) = 1 - \cos^{2}(\varepsilon/2) \cos^{2}(\varepsilon C_{s}/2), \qquad (2.34)$$

i.e., the function $\sin^2(\theta_s/2)$ oscillates as $C_s^{-1} \neq 0$ about a value $1-2^{-1}\cos^2(\varepsilon/2)$. In the case of s=0, on the other hand, we have $\varepsilon = \pi$ and $\sin^2(\theta_0/2) = 1$.

3. RELAXATION MATRIX

In this section we study the consequences of the dynamic symmetry of the CDI, which manifests itself both in the structure of the relaxation matrix and in the values of the matrix elements.

We recall that if the velocity does not change the relaxation constants (RC) calculated in a coordinate frame whose z axis is directed along the velocity \mathbf{v} of the perturbed particle (the \mathbf{v} -system) is determined by the differential cross sections⁶

$$\sigma(JJ' \times p | JJ' \times_{i} p, \rho, u) = \sum_{MM, M'M_{i}} \{ \delta_{MM_{i}} \delta_{M'M_{i}} - D_{MM_{i}}^{J}(\Theta) D_{M'M_{i}}^{SJ'}(\Theta') \}$$

$$\times (-1)^{2J'-M'-M_{i}'} \langle JMJ'-M' | \times_{i} p \rangle \langle JM_{i}J'-M_{i}' | \times_{i} p \rangle, \qquad (3.1)$$

$$\sigma(\times_{i} L, \rho, u) = \sum_{p} (-1)^{\times_{i} - p} \langle \times_{p} \times_{i} - p | LO \rangle$$

$$\times [(2 \times +1) (2 \times_{i} +1)]^{V_{i}} \sigma(JJ' \times_{p} | JJ' \times_{i} p, \rho, u). \qquad (3.2)$$

The Euler angles $\vartheta = (\psi, \theta, \varphi)$ depend on ρ and u via the parameter C, and for the subsequent averaging over ρ and u it is useful to introduce the notation

$$\xi = 1/C = u\rho/\bar{v}_b\rho_0 = z\rho/\rho_0, \quad z = u/\bar{v}_b, \quad \zeta = v/\bar{v}_b$$

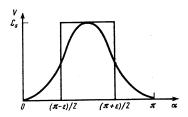


FIG. 4. Illustrating the replacement of the real interaction by a step.

where the Massey radius is

$$\rho_0 = e (nJ \|d\| nJ) / \hbar \bar{v}_b [J (J+1) (2J+1)]^{\prime h}, \qquad (3.3)$$

and \bar{v}_b is the average velocity of the perturbing charged particles.

The weighting density with which the averaging over the velocities is carried out, is given by⁶

$$\rho_b(L, \zeta, z) = (\sqrt{2}/\overline{v}_b)^3 \exp\left(-\zeta^2 - z^2\right) (2z\zeta)^{-\frac{1}{2}} I_{L+\frac{1}{2}}(2z\zeta). \tag{3.4}$$

Further integration of the cross sections (3.1) and (3.2) with respect to the impact parameter ρ must be cut off at the Debye radius ρ_D of the screening of the charges in the plasma. In the upshot we obtain the quantities

$$\Gamma(\varkappa \varkappa_{1}L, v) = N_{b}\overline{v}_{b}\rho_{0}^{2}\int_{0}^{\infty}\overline{v}_{b}^{3}\rho_{b}(L, \zeta, z) z dz 2\pi \int_{0}^{z\rho_{D}/\rho_{0}}\sigma(\varkappa \varkappa_{1}L, \xi) \xi d\xi, \quad (3.5)$$

which are needed for the calculation of the relaxation matrix elements in the v-system:

$$\sum_{L} (-1)^{\kappa_{1}-q} \langle \kappa q \kappa_{1}-q | L0 \rangle [(2\kappa+1)(2\kappa_{1}+1)]^{\nu_{1}} \Gamma(\kappa \kappa_{1}L, v).$$
 (3.6)

At $\overline{v} \gg \overline{v}_b$, the dependence of $\Gamma_{xx_1}^q$ on \varkappa , q, and v is specified directly by the cross sections (3.1) [see Eq. (2.4) of Ref. 6].

It is easy to show (we omit the proof) that the cross sections $\sigma(\varkappa_1 L)$, and consequently also the RC $\Gamma_{xx_1}^{q}$, are real. We emphasize that the latter is valid even in the case of different perturbation of the states nJ and n'J', although in the general case of arbitrary perturbation the quantities $\Gamma_{xx_1}^{q}$ are complex.

A second general property of the CDI is the logarithmic divergence of the integral with respect to ξ in (3.5). Assuming $\rho_D \gg \rho_0$, we consider the principal term of the integral with respect to ξ , which is proportional to $\ln (\rho_D z / \rho_0)$, and retain in it only $\ln (\rho_D / \rho_0) \gg 1$, assuming that $z \sim 1$ [see (3.4)]. In this case the integrals in (3.5) separate:

$$\Gamma(\varkappa \varkappa_{1}L, v) = N_{b}\overline{v}_{b}\rho_{0}^{2}K(2, L, \zeta) \cdot 2\pi \int_{0}^{\rho_{D}/\rho_{0}} \sigma(\varkappa \varkappa_{1}L, \xi)\xi d\xi, \qquad (3.7)$$

where $K(2,L,\zeta)$ are standard functions of $\zeta = v/\overline{v}_b$ (see Ref. 6), which in the case of CDI are expressed in terms of the probability integral and of elementary functions.

We analyze now the RC of the levels, and also the RC of the transitions for an identical perturbation of the combining states nJ and n'J'. In both cases the addition of the *D*-matrices in (3.1) leads to the expression

$$\sigma(\varkappa_p|\varkappa_i p, \xi) = \delta_{\varkappa_i} [1 - d_{pp}^{\ast}(\theta)]. \qquad (3.8)$$

Thus, under the indicated conditions the relaxation matrix is diagonal both in \varkappa and in p (in the v system), but depends on \varkappa and p. Consequently, the wind effect causes here only a dependence of the RC on p, and there are no off-diagonal terms in \varkappa , as in the general case.⁶

We investigate now the relation between the relaxation rates of the different multipole moments of the states and the polarizations. We call attention first to the fact that at $\kappa = 1$ the cross sections with p = 0 and p = 1 differ according to (3.8) by exactly a factor of 2. In the previously studied dipole-dipole and dispersion interactions⁷⁻¹¹ this difference reached only 30%. Next, for $\kappa \neq 1$ it is easy to separate the terms that yield the principal logarithmic members; since $\sin^2 \theta/2 + \xi^{-2}$ as $\xi \to 0$, we have

$$\sigma(\varkappa p | \varkappa_1 p, \xi) = \delta_{\varkappa \iota} \xi^{-2} (\varkappa^2 + \varkappa - p^2).$$
(3.9)

In particular, at the values of |p| that differ most the ratio of the cross sections increases with κ :

$$\sigma(\mathbf{x}0|\mathbf{x}0)/\sigma(\mathbf{x}\mathbf{x}|\mathbf{x}\mathbf{x}) = 1 + \mathbf{x}.$$

In the "logarithmic" limit (3.9) the cross section contains only the angular momenta L = 0 and 2. Indeed, from (3.2) and (3.9) it follows that

$$\sigma(\varkappa \varkappa_{1}L,\xi) = \frac{2}{3} \frac{\varkappa(\varkappa+1)}{\xi^{2}} \left(\delta_{L0} - \left[\frac{(2\varkappa-1)(2\varkappa+3)}{20\varkappa(\varkappa+1)} \right]^{\gamma_{2}} \delta_{L2} \right) \delta_{\varkappa \varkappa_{1}}.$$
 (3.10)

As κ increases from 1 to ∞ , the ratio of the anisotropic and isotropic parts ranges from $1/\sqrt{8}$ to $1/\sqrt{5}$.

If the collisions are isotropic $(\bar{v} \ll \bar{v}_b)$, we obtain with the aid of (3.10) the dependence of the relaxation constants on \varkappa :

$$\Gamma_{xx_{1}}^{q} = \Gamma_{x} \delta_{xx_{1}}, \quad \Gamma_{x} = \Gamma_{x} (x+1). \tag{3.11}$$

Thus, the CDI leads to a strong dependence of the RC on \varkappa , whereas for dipole-dipole and van der Waals interactions the values of Γ_{\star} are changed by approximately 10% in the range $\varkappa = 1-3$ (Refs. 14-16).

The polarization relaxation matrix has a somewhat different structure if the disorientation is not the same on the combining levels. An investigation of this case is cumbersome and is relegated to Appendix 3.

We confine ourselves here to the model with perturbation of one level. In the *v*-system the relaxation matrix $\hat{\Gamma}$ is then diagonal in the *M* representation.⁶ The corresponding cross sections and relaxation rates are given by

$$\sigma(JJL,\xi) = (2J+1)^{-\nu_{h}} \sum_{M} (-1)^{J-M} \langle JMJ - M | L0 \rangle [1 - d_{MM}^{J}(\theta)],$$

$$\Gamma(JJL,v) = N_{b} \overline{\nu}_{b} \rho_{0}^{2} K(2,L,\xi) 2\pi \int_{0}^{p_{D}/\rho_{0}} \sigma(JJL,\xi) \xi d\xi, \qquad (3.12)$$

$$\Gamma_{M}(v) = (2J+1)^{\nu_{h}} \sum_{r} (-1)^{J-M} \langle JMJ - M | L0 \rangle \Gamma(JJL,v).$$

In the principal-logarithm approximation we can obtain [cf. (3.9)]

$$\sigma(JJL,\xi) = \frac{2}{3} \frac{J(J+1)}{\xi^2} \left(\delta_{L_0} - \left[\frac{(2J-1)(2J+3)}{20J(J+1)} \right]^{\gamma_L} \delta_{L_2} \right),$$

$$\Gamma_M(v) = (K(2,0,\xi) - (-1)^{J-M} \langle JMJ - M | 20 \rangle$$

$$\times \left[\frac{(2J+1)(2J-1)(2J+3)}{20J(J+1)} \right]^{\gamma_L} K(2,2,\xi)) \Gamma,$$

$$\Gamma = N_b \bar{\nu}_b \rho_b c^2 J(J+1)(4\pi/3) \ln(\rho_D/\rho_0).$$

(3.13)

The dependence of the RC on the velocity v is concentrated in the functions $K(2,L,\zeta)$ (Fig. 5), which take at L=0 and 2 the form

K

$$K(2, 0, \zeta) = (1/\zeta) \Phi(\zeta),$$

(2, 2, ζ) = $(1/\zeta - 3/2\zeta^3) \Phi(\zeta) + 3\pi^{-1/2} \zeta^{-2} \exp(-\zeta^2),$ (3.14)

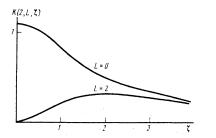


FIG. 5. Dependence of $K(2, L, \zeta)$ on the velocity $\zeta = v/\overline{v}_b$.

where $\Phi(\zeta)$ is the probability integral in accordance with the general formula (2.31) of Ref. 6.

4. SPECTRAL-LINE PROFILE

The relaxation matrix Γ investigated above makes it possible to calculate the impact broadening of spectral lines in CDI. In contrast to Ref. 1, where a model of isotropic collisions was used $(\overline{v} \ll \overline{v}_b)$, we present here results on the line profile in the opposite limiting case $\overline{v} \gg \overline{v}_b$, when the wind effect manifests itself to the utmost degree. The functions $K(2, L, \zeta)$ can be replaced by the asymptotic values $1/\zeta$, which are the same for all L, and all the elements of the relaxation matrix acquire the same dependence on the velocity:

$$\Gamma_{\rm xx_1}(v) = A_{\rm xx_1} \overline{v} / v. \tag{4.1}$$

The components of the spectral structure of the profile without Doppler broadening are given by special integrals:

$$I_{kq}(\Omega) = 4\pi^{-\eta_{t}} \overline{v}^{-3} \int_{0}^{\infty} \operatorname{Re}[\Gamma_{k}^{q}(v) - i\Omega]^{-1} v^{2} \exp(-v^{2}/\overline{v}^{2}) dv$$

$$= [z_{kq}^{-1} + z_{kq} \exp(z_{kq}^{-2}) \operatorname{Ei}(-z_{kq}^{-2})] \mathcal{J}_{kq}, \qquad (4.2)$$

$$\operatorname{Ei}(-x) = -\int_{x} t^{-1} \exp t dt, \quad \mathcal{J}_{kq} = 2\pi^{-\eta_{t}} A_{kq}^{-1}.$$

Here $z_{kq} = \Omega/A_{kq}$, \mathscr{I}_{kq} is the intensity of the component at the center ($\Omega = 0$), and A_{kq} are the roots of the matrix (4.1). Numerical calculations have shown that the functions $I_{kq}(\Omega)$ has, accurate to 3%, a Lorentz shape and a width 0.80 A_{kq} .

To illustrate the possible effects of the anisotropy of the collisions we discuss now the numerical calculations of the line profile in the model where one level is perturbed:

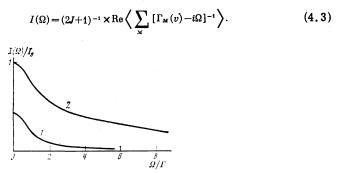


FIG. 6. Contour of spectral line in the limiting case of strongly anisotropic collisions (J = 10); 1) contour for transition with sublevel $M = \pm J$; 2) summary contour.

In the limiting case $\overline{v} \gg \overline{v}_{h}$ we have

$$\Gamma_{M}(v) = (1 - M^{2}/J(J+1)) \Gamma \bar{v}/v.$$
(4.4)

The maximum difference $\Gamma_{M}(v)$ as a function of M is characterized by the ratio $\overline{\Gamma}_0(v)/\Gamma_i(v) = J+1$. At large J, consequently, the set of Lorentzians (4.3) contains narrow $(J - M \sim 1)$ and broad $(M/J \ll 1)$ components. Therefore one can expect the total profile to contain an abrupt component against a broader background. The foregoing arguments are illustrated in Fig. 6, using a numerical calculation of an example with J = 10. The contribution of the terms with $M = \pm J$ to the intensity at $\Omega = 0$ is 41% (these terms are shown separately in Fig. 6). All the remain components |M| = 0-9 form a broad background with a width approximately six times larger. Such pronounced manifestations of the wind effects were unknown before. For comparison we recall that for other forms of the interaction the line shape, owing to the anisotropy of the collisions, changes by not more than 2% (Refs. 6,8,9).

5. CONCLUSION

The problem of disorientation in collisions with CDI occupies in M-exchange theory a special place, similar to the place of the harmonic oscillator in quantum mechanics. The quasiclassical description of rotations and of the elastic-scattering matrix in CDI ensures an exact quantum result (Appendix 2). The basis of the description is the classical Bloch equation which is obeyed by the motion of the angular momentum of the state perturbed upon collision. The DS group of the CDI and the matrix of the M exchange are connected with the rotation matrix, so that the relaxation matrix can be investigated analytically for all J. It has turned out that the CDI mechanism leads to maximum anisotropy for anisotropic collisions and to a strong dependence of the relaxation rate on the multipolarity of the angular momentum of the state in isotropic collisions. The level relaxation matrix has a diagonal structure, so that there are no transport and mixing of the multipole moment in the relaxation.

For other interactions, whose DS is determined by the set of ITO, we proposed above an approach with a quasiclassical realization of the ITO in a basis of coherent states. The complex variable μ of the phase transition, which characterizes this state, is connected with the direction of the average angular momentum.

To solve the dynamic Schrödinger equation in this phase space one makes use of the methods of the theory of analytic functions. At large J, it is also of interest to use the quasiclassical approximation and classical trajectories of motion in the μ plane. The trajectories are the characteristics of the dynamic equations. Consequently, formulation of the equations of the characteristics is a method of obtaining the generalized Bloch equation (of the classical equation of motion).

In conclusion, we consider it our pleasant duty to thank G.I. Surdutovich and A.M. Shalagin for helpful discussions.

REPRESENTATION OF ITO IN A BASIS OF COHERENT STATES

An ITO of rank \varkappa has in the quantum basis of the angular momentum the form

$$\hat{T}_{xq}^{JJ_i} = \sum_{\mathbf{M}M_i} |J_i M_i \rangle (-1)^{J_i - M_i} \langle J M J_i - M_i | \chi q \rangle \langle J M |.$$
(A1.1)

The analytic structure of this operator in a basis of coherent states is determined by the vector-addition coefficient. The ITO can be realized here both from the left and from the right. For example, in realization of the ITO from the left it is necessary to satisfy the equation

$$\langle J\mu | T_{nq}^{J_{1}} = T_{nq}^{J_{1}}(\mu^{*}) \langle J\mu |,$$
 (A1.2)

which in fact defines $T_{xq}^{IJ}(\mu^*)$. In particular, using (2.15) and (A1.1), we easily obtain for \hat{T}_{10}^{IJ}

$$\langle J\mu | \hat{T}_{10}^{JJ} = [J(J+1)(2J+1)/3]^{-\gamma_{h}} \sum_{\mathbf{M}} {J-M \choose 2J}^{\gamma_{h}} M\mu^{*J-\mathbf{M}} \langle JM |$$

= $a_{J} \left(J - \mu^{*} \frac{\partial}{\partial \mu^{*}} \right) \langle J\mu | = \hat{T}_{10}^{JJ} (\mu^{*}) \langle J\mu |.$ (A1.3)

This procedure can be used for any ITO. We confine ourselves below to realization of first-rank tensors:

$$\hat{T}_{11}^{JJ} = -\frac{a_J}{\overline{Y2}} \frac{\partial}{\partial \mu^*}, \quad \hat{T}_{1-1}^{JJ} = \frac{a_J}{\overline{Y2}} \left(2J\mu^* - \mu^{*2} \frac{\partial}{\partial \mu^*} \right),$$

$$\hat{T}_{10}^{JJ-1} = c_J\mu^*, \quad \hat{T}_{10}^{J-1J} = \frac{c_J}{2J(2J-1)} \frac{\partial}{\partial \mu^*} \left(\mu^* \frac{\partial}{\partial \mu^*} - 2J \right),$$

$$\hat{T}_{11}^{JJ-1} = c_J/\overline{Y2}, \quad \hat{T}_{11}^{J-1J} = \frac{c_J}{2^{2j}J(2J-1)} \frac{\partial^2}{\partial \mu^{*2}}, \quad (A1.4)$$

 $\hat{T}_{i-1}^{IJ-1} = c_{J} \mu^{*2} / \sqrt{2}, \quad \hat{T}_{i-1}^{J-1J} = \frac{c_{J}}{2^{\gamma_{j}} J(2J-1)} \left(2J - \mu^{*} \frac{\sigma}{\partial \mu^{*}} \right) \left(2J - 1 - \mu^{*} \frac{\sigma}{\partial \mu^{*}} \right), \\ a_{J} = [J(J+1)(2J+1)/3]^{-\gamma_{j}}, \quad c_{J} = [(2J+1)/6]^{-\gamma_{j}}.$

APPENDIX 2

HAMILTONIAN APPROACH

We seek the solution of (2.21) in the form

$$S(\mu^{\bullet}, \alpha) = \exp \{ J\Phi(\mu^{\bullet}, \alpha) \}.$$
(A2.1)

The eikonal obeys the Hamilton-Jacobi equation

$$\frac{\partial \Phi}{\partial \alpha} + H\left(\alpha, \mu^{*}, \frac{\partial \Phi}{\partial \mu^{*}}\right) = 0$$
(A2.2)

with the Hamiltonian

$$H=j(\mu^{\bullet}, \alpha)\Lambda - \partial j(\mu^{\bullet}, \alpha)/\partial \mu^{\bullet}.$$
 (A2.3)

The momentum here is $\Lambda = \partial \Phi / \partial \mu^*$. The equation of motion, of course, coincides with the equation of the characteristics (2.23):

$$d\mu^{*}/d\alpha = \partial H/\partial \Lambda = j(\mu^{*}, \alpha).$$
 (A2.4)

The eikonal is directly determined from (A2.2) by the quadrature

$$\Phi = \Phi_0 + \int_0^\infty d\alpha' \left(\frac{\partial j}{\partial \mu^*}\right) \mu^* = \mu^*(\eta^*, \alpha').$$
 (A2.5)

Here Φ_0 is the initial eikonal.

The second term, due to the divergence of the disorientation current, is expressed in accord with the theorem by the Jacobian of the transition $(\partial \mu^* / \partial \eta^*)$ over the collision time:

$$\Phi = \Phi_{\mathfrak{o}}(\eta^{*}) - \ln (\partial \eta^{*} / \partial \mu^{*}), \qquad (A2.6)$$

where $\eta^* = \eta^*(\mu^*, \alpha)$. Combining (A2.6) and (A2.1) we obtain (2.26).

APPENDIX 3

LINE BROADENING AT VARIOUS DISORIENTATIONS ON COMBINING LEVELS

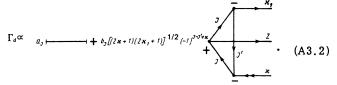
The general structure of the relaxation matrix (3.1) is determined in the principal logarithm approximation only by the diagonal (M, M) and off-diagonal $(M, M \pm 1)$ scattering channels. The diagonal-channel scattering matrix D_{MM}^{J} can be represented in the form

$$\left(1+\frac{a_{j}}{\xi^{2}}\right)$$
 + $\frac{b_{j}}{\xi^{2}}$ + $\frac{b_{j}}{\xi^{2}}$. (A3.1)

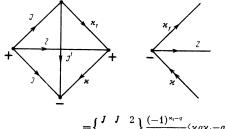
Here

$$a_J = -2J(J+1)/3, \quad b_J = -[J(J+1)(2J-1)(2J+1)(2J+3)]^{\frac{1}{2}}/3.$$

The corresponding part of the relaxation matrix of the irreducible polarization moments is then represented by the diagram



Using the standard transformation rules (cutting through three lines), we obtain the closed diagram of a 6J coefficient, whose values of well known, and the vector addition coefficient



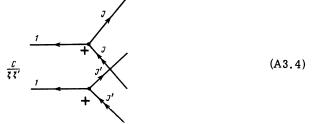
$$= \left\{ \begin{array}{c} J & J & 2 \\ \chi & \chi_1 & J' \end{array} \right\} \frac{(-1)^{\chi_1-q}}{\sqrt{5}} \langle \chi q \chi_1 - q | 20 \rangle = B_{\chi \chi_1 q}^{JJ},$$

 $\Gamma_{d} \propto (a_{J} + a_{J'}) \delta_{xx_{i}} + (-1)^{x_{i} - J - J'} [(2x + 1)(2x_{i} + 1)]^{\frac{1}{2}} [b_{J} B_{xx_{i}g}^{JJ'} + b_{J'} B_{xx_{i}g}^{J'J}] . (A3, 3)$

The contribution of the off-diagonal channels is made up in the logarithmic approximation by terms of the form

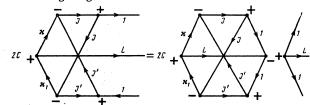
$$D_{MM-1}^{J}(\theta) D_{M'M'-1}^{J'}(\theta') = [(J+M)(J-M+1)(J'+M')(J'-M'+1)]^{\frac{1}{2}} \xi \xi'$$

which can be represented by the diagram



$C = 2 [JJ'(J+1)(J'+1)(2J+1)(2J'+1)]^{\frac{1}{2}}.$

The corresponding part of the RC is represented by the following diagram:



which leads to the 9J coefficient

 $\Gamma_{n}(\varkappa \varkappa_{1}L) \propto 6C[(2\varkappa+1)(2\varkappa_{1}+1)]^{\frac{1}{2}}(-1)^{\varkappa-\varkappa_{1}} \left\{ \begin{array}{cc} \varkappa \varkappa_{1}L\\ J & J \\ J' & J \end{array} \right\} \langle 111-1|L0\rangle.$ (A3.5)

Thus, in the principal-logarithm approximation, the relaxation rates contain isotropic contributions with L=0, and anisotropy only with L=2.

- ¹V. S. Lisitsa and G. V. Sholin, Zh. Eksp. Teor. Fiz. 61, 912 (1971) [Sov. Phys. JETP 34, 484 (1972)].
- ²M. L. Strekalov, Zh. Eksp. Teor. Fiz. 77, 843 (1979) [Sov. Phys. JETP 52, 426 (1979)].

³J. M. Radcliffe, J. Phys. A4, 313 (1971).

- ⁴A. M. Perelomov, Usp. Fiz. Nauk **123**, 23 (1977) [Sov. Phys. Usp. **20**, 703 (1977)].
- ⁵M. Ya. Vilenkin, Spetsial'nye funktsii i teoriya predstavleni⁴ grupp (Special Functions and Group Representation Theory), Nauka, 1965.
- ⁶S. G. Rautian, A. M. Shalagin, and A. G. Rudavets, Zh. Eksp. Teor. Fiz. **78**, 561 (1980) [Sov. Phys. JETP **51**, 274 (1980)].
- ⁷T. Manabe, T. Yabusaki, and T. Ogawa, Phys. Rev. 20A, 1946 (1977).
- ⁸A. P. Kazantsev, Zh. Eksp. Teor. Fiz. **51**, 1751 (1966) [Sov. Phys. JETP **24**, 1183 (1967)].
- ⁹Yu. A. Vdovin and V. M. Galitskil, Zh. Eksp. Teor. Fiz. **52**, 1345 (1967) [Sov. Phys. JETP **25**, 894 (1967)].
- ¹⁰V. K. Matskevich, I. E. Evseev, and V. M. Ermachenko, Opt. Spektrosk. 45, 17 (1978).
- ¹¹V. N. Rebane, Author's abstract of doctoral dissertation, Leningrad State Univ., 1960.
- ¹²D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskiĭ, Kvantovaya teoriya uglovogo momenta (Quantum Theory of the Angular Momentum), Nauka, 1975.
- ¹³A. D. Buckingham, J. Chem. Phys. 48, 3827 (1968).
- ¹⁴M. I. D'yakonov and V. I. Perel', Zh. Eksp. Teor. Fiz. 48, 345 (1965) [Sov. Phys. JETP 21, 227 (1965)].
- ¹⁵A. Omont, J. Phys. 35, 25 (1965).
- ¹⁶A. I. Okunevich and V. I. Perel', Zh. Eksp. Teor. Fiz. 58, 666 (1970) [Sov. Phys. JETP 31, 356 (1970)].

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