Interaction of an excited hydrogenlike atom with a charged particle in the dipole approximation

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The quantum scattering of a charged particle from an excited hydrogenlike atom or ion is treated, using the dipole approximation for the interaction and neglecting transitions involving change of the principal quantum number n. The scattering wave functions thus found are used to calculate the collisional broadening of the spectrum lines of atoms or ions in the binary approximation. The use of a specific additional symmetry in the dipole approximation made it possible to obtain compact expressions for the scattering amplitude with mixing of the degenerate states of the atom and for the line contour for the case of arbitrary n, and also to trace the transition to various limiting cases (especially to the cases of quasiclassical and classical motion of the incident particle and to the adiabatic limit).

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1. INTRODUCTION

The scattering of a charged particle from an excited hydrogenlike atom or ion leads to inelastic transitions and also to broadening of the spectrum lines emitted by the atom. These two processes are related to one another, are of considerable practical interest, and have been investigated many times.

An interesting feature of the problem from the theoretical point of view is the presence of additional degeneracy of the energy levels of the hydrogenlike system in the nonrelativistic approximation. As a result of this, on the one hand, transitions between the n^2 degenerate states of the atom (n is the principal quantum number) change not only the direction of the orbital angular momentum of the atomic electron, but also its magnitude. On the other hand, the possibility of the atom's having a constant dipole moment (i.e., of the linear Stark effect) is associated, as is well known, with the degeneracy of states of opposite parity. The potential for the interaction of the atom with a distant charged particle therefore falls off in inverse proportion to the square of the distance and depends on the state of the atom. Because the potential falls off so slowly, the contributions from large distances, i.e., from distant collisions or large angular momenta, become especially important in the scattering and line-broadening problems. In this case one uses the dipole approximation for the interaction potential[1], writing

$$\frac{Z_B}{|\mathbf{R}-\mathbf{r}|}-\frac{Z_B}{R}\approx Z_B\frac{\mathbf{rN}}{R^2},\quad \mathbf{N}=\mathbf{R}/R. \tag{1.1}$$

Here $\mathbf{R}$ and $\mathbf{r}$ are the radius vectors of the incident particle B (with charge Z_B) and the atomic electron, respectively (atomic units are used throughout).

The classical approximation for the motion of the incident particle and the dipole approximation for the interaction have previously been used to treat the scattering problem[2–4] and the line broadening problem.[5,6] Atomic transitions involving change in the principal quantum number n were neglected in these studies. A quantum treatment of the motion of the incident particle becomes necessary if the particle is light, or if its energy is low. Such a treatment has been given for the scattering problem by Seaton,[1] Gailitis and Damburg,[7] and Burke and Macek,[8] and very recently, for the line broadening problem, by Tran Minh, Feaurtier, and Van Regemorter[9,10] (also see Ref. 11). We note that because of the above mentioned strong dependence of the interaction potential on the state of the atom and the necessity of taking interference effects into account, the calculation of the differential cross sections requires the use of the quasiclassical approximation,[12] even in the case of the collision of a heavy particle with a hydrogen atom.

Using the classical description of the motion of the colliding particles, a general solution for the case of arbitrary n has been obtained[4,5] on the basis of the hidden symmetry properties of the Coulomb problem and, in particular, the manifestation of these properties when a hydrogenlike system is placed in crossed electric and magnetic fields.[13]

No use has been made up to now of the symmetry properties in the quantum description, so the latter has been limited to the simplest particular case, $n=2$.[7–10]

Some approximate symmetry properties of the electron-electron interaction operator in the dipole approximation have recently been investigated by Herrick,[14] but his results are not applicable to the case of large values of the total angular momentum L, which is just the case that is important in the scattering and line-broadening problems. S. I. Nikitin and the present author[15,16] have investigated both exact and approximate symmetry properties that manifest themselves in addition to other symmetry properties in the limit of large L.

The purpose of the present work is to apply these results to the scattering (Secs. 2 and 3) and line-broadening (Sec. 4) problems for arbitrary n. In both cases one must know the continuum wave functions (Sec. 2). However, the scattering is entirely determined by the asymptotic behavior of the wave functions in coordinate space (or by the scattering angle in the case of classical mechanics), whereas for the line-broadening problem one

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requires the wave function, generally speaking, throughout all of space (or the entire trajectory in the classical case). We shall first derive exact formulas (within the limitation of the dipole approximation) for the quantities of interest (i.e., for the scattering amplitude, Eq. (2.11), and for the line contour, Eq. (4.2)) and discuss their properties. Then we consider the case of distant collisions, i.e., of large L, in which the formulas can be written in explicit form (Eqs. (3.6) and (4.5)) because of the possibility of using a quasiclassical description of the angular correlations between the incident particle and the atomic electron.[15,16] Here a quantum-mechanical treatment of the radial motion of the scattered particle may still be used, or one may use the quasiclassical approximation (Eqs. (3.9) and (4.10)). The difference between hydrogenlike atoms and ions becomes important when the deviations of the trajectories from straight lines is to be taken into account. In the case of an ion it is sufficient to assume a Coulomb trajectory as the simplest approximation (see Eq. (3.14)), whereas in the case of an atom there is no unique trajectory since the interaction depends on the state of the atomic electron (see Eqs. (3.9)–(3.11) and the discussion in Sec. 4).

Still another important parameter is the ratio of the splitting of the adiabatic terms of the quasimolecule consisting of the atom and the stationary charge ($\Delta E \sim 3Z_B n/2Z_A R^2$) to the frequency characterizing the rate of change of the interaction ($\nu \sim v/\rho$, where ρ is the impact parameter and v is the collision velocity). If $\nu/\Delta E \sim 2Z_A L/3Z_B \mathcal{M}_n \ll 1$ ($\mathcal{M}$ is the reduced mass), the system will develop adiabatically during the collision and there will be no transitions between the terms. In the opposite limit the passage is rapid and perturbation theory can be used to treat the scattering (Sec. 3).

2. SCATTERING IN THE DIPOLE APPROXIMATION

In the dipole approximation, the Hamiltonian for the system takes the form

$$\mathcal{H} = -\frac{1}{2\mu}\nabla_r^2 - \frac{1}{2\mathcal{M}}\nabla_R^2 - \frac{Z_A}{r} + \frac{(Z_A-1)Z_B}{R} - gZ_B\frac{\mathbf{rN}}{R^2}, \qquad (2.1)$$

where the radius vector $\mathbf{R}$ of the incident particle is measured from the center of mass of the atom, the radius vector $\mathbf{r}$ of the electron is measured from the atomic nucleus, whose charge and mass are Z_A and M_A, respectively, M_B is the mass of the incident particle,

$$\mu = M_A/(M_A+1), \quad \mathcal{M} = (M_A+1)M_B/(M_A+M_B+1).$$

The factor $g = (M_A+Z_B)/(M_A+1)$ arises in the separation of the motion of the common center of mass and is usually close to unity.

We introduce the projection operator Q_n onto the subset of states of the atomic electron with the fixed principal quantum number n. The assumption that the atom remains always in a state with a given n is equivalent to the substitution of the operator $\mathcal{H}_n = Q_n \mathcal{H} Q_n$ for the Hamiltonian operator $\mathcal{H}$. Using the fact that the operator $\mathbf{r}$ is equivalent on the n shell to the Runge-Lenz vector $\mathbf{A}$,[13] we obtain (also see Refs. 12 and 14)

$$\mathcal{H}_n = Q_n\left\{-\frac{1}{2\mathcal{M}}\frac{1}{R^2}\frac{d}{dR}R^2\frac{d}{dR} + \frac{\Lambda}{2\mathcal{M}R^2} + \frac{(Z_A-1)Z_B}{R} - \frac{\mu Z_A^2}{2n^2}\right\}Q_n. \qquad (2.2)$$

The operator Λ that occurs here, which is given by

$$\Lambda = \mathbf{I}_1^2 - \frac{3gZ_B\mathcal{M}n}{\mu Z_A}(\mathbf{AN}) \qquad (2.3)$$

($\mathbf{I}_1$ is the angular momentum of the relative motion of the particle and the atom), acts only on the angular coordinates of the incident particle and those of the atomic electron. As was emphasized in Ref. 12, Λ is an additional integral of motion, and by diagonalizing it one can separate the scattering channels and classify them (also see Ref. 14).

Since the total angular momentum $\mathbf{L} = \mathbf{I}_1 + \mathbf{I}_2$ of the system ($\mathbf{I}_2$ is the angular momentum of the atomic electron) is also an integral of motion and commutes with Λ, it is convenient in dealing with Λ to use basis functions having definite values of L and its projection M:

$$|nl_1l_2LM\rangle = \sum_{m_1m_2} C^{LM}_{l_1m_1l_2m_2}|nl_2m_2\rangle Y_{l_1m_1}(\mathbf{N}_1), \qquad (2.4)$$

where $|nl_2m_2\rangle$ are hydrogenlike atomic wave functions, l_i and m_i are the orbital angular momentum and its projection for the particle B ($i=1$) and the electron ($i=2$), and the $C^{LM}_{l_1m_1l_2m_2}$ are Clebsch-Gordan coefficients. Since the orbital angular momenta l_1 and l_2 are not fixed ($0 \leq l_2 \leq n-1$), there is still a number of the functions (2.4) for fixed L and M (there are n^2 of them when $L \geq n-1$).

Let us suppose that we have diagonalized Λ on the subspace spanned by the functions $|nl_1l_2LM\rangle$:

$$\Lambda|n\gamma LM\rangle = \lambda_\gamma(L)|n\gamma LM\rangle, \qquad (2.5)$$

$$|n\gamma LM\rangle = \sum_{l_1l_2} U_L(\gamma|l_1l_2)|nl_1l_2LM\rangle. \qquad (2.6)$$

Here the new quantum number γ labels the eigenvalues $\lambda_\gamma(L)$ and eigenvectors $|n\gamma LM\rangle$ of Λ, and the matrix U_L transforms the initial representation using the quantum numbers l_1 and l_2 to the Λ representation using the quantum number γ. The eigenfunction of $\mathcal{H}_n$ can be expressed in the form (E is the collision energy)

$$|kn\gamma LM\rangle = f_{k\gamma}(R)|n\gamma LM\rangle, \quad E = k^2/2\mathcal{M}, \qquad (2.7)$$

where $f_{k\gamma}(R)$ is a solution of the radial wave equation

$$-\frac{1}{2\mathcal{M}R^2}\frac{d}{dR}\left(R^2\frac{d}{dR}f_{k\gamma}\right) + \left(\frac{\tilde{l}(\tilde{l}+1)}{2\mathcal{M}R^2} + \frac{(Z_A-1)Z_B}{R} - E\right)f_{k\gamma} = 0. \qquad (2.8)$$

Here we have introduced the effective orbital angular momentum $\tilde{l}$: $\tilde{l}(\tilde{l}+1) = \lambda_\gamma$.

Thus, the radial motion of the colliding particles has been separated: it is described by Eq. (2.8), whose well-known solutions we shall not write down here. We note only that the positive-energy ($E>0$) wave functions have the following asymptotic behavior for large R:

$$f_{k\gamma}(R) \approx \sin\left(kR - \eta\ln 2kR - \frac{\pi\tilde{l}}{2} + \arg\Gamma(\tilde{l}+1+i\eta)\right)\Big/ kR,$$
$$\eta = \mathcal{M}(Z_A-1)Z_B/k. \qquad (2.9)$$

There may exist negative-energy solutions corresponding to bound states that become quasistationary when n-subshell mixing is taken into account. They can be used to describe doubly excited autoionization states of the atom and the corresponding scattering resonances.[16-18] We also note that when L is large enough we have $\lambda_\gamma > -1/4$, i.e., we may ignore the possibility of a $\sim 1/R^2$ fall off the potential at the origin[19] (actually such a fall does not occur because of the difference at small R between the actual interaction and its dipole approximation).

It should be emphasized that the representation of the eigenfunctions of Λ introduced above is not the same as the proper representation of the scattering matrix S that is frequently used in various problems in collision theory (see, e.g., Ref. 20). Actually, the amplitude of the outgoing wave is obtained by the action of the operator $\hat{S}\hat{P}_R$ on the amplitude of the incoming wave, where $\hat{P}_R$ is the operator that inverts the collision coordinate $\mathbf{R}$.[19] The incoming and outgoing waves in solution (2.9) have the same amplitude, which is therefore an eigenfunction of $\hat{S}\hat{P}_R$, but not of $\hat{P}_R$ or $\hat{S}$ separately. Thus, the S matrix and Λ are determined by the same functions, but they do not commute. The reason why they do not commute is that Λ, while it commutes with the projected Hamiltonian $\mathscr{H}_n$, does not commute with $\mathscr{H}_n^{(0)}$, which represents the projected Hamiltonian with the interaction responsible for the scattering turned off and is obtained by setting $Z_B = 0$ in the expression for $\mathscr{H}_n$. At the same time, the scattering matrix can be expressed in terms of the product of wave operators defined by the limiting processes[21]

$$\lim_{t\to\pm\infty} \exp(i\mathscr{H}_n t)\exp(-i\mathscr{H}_n^{(0)} t).$$

The situation here is quite analogous to that which obtained in a potential scattering problem that admits separation of variables in spheroidal coordinates (Abramov and Komarov[22]).

In view of Eq. (2.9) we define the proper phases in the Λ representation as follows:

$$\delta_\gamma(L,E) = -\frac{\pi}{2}(l-L) + \arg\Gamma(l+1+i\eta). \tag{2.10}$$

Then after some calculation we obtain the following expression for the amplitude for inelastic scattering with transition of the atom from the state $|nl_0m_0\rangle$ to the state $|nlm\rangle$:

$$F_{nl_0m_0\to nlm}(\mathbf{N}_0,\mathbf{N}) = \frac{2\pi}{ik}\sum_{\gamma LM}\{\exp(2i\delta_\gamma(L,E) - i\pi L) \times A_{\gamma LMnl_0m_0}(-\mathbf{N}_0)^* - A_{\gamma LMnl_0m_0}(\mathbf{N})^*\} A_{\gamma LMnlm}(\mathbf{N}), \tag{2.11}$$

$$A_{\gamma LMnlm}(\mathbf{N}) = \sum_{l_1m_1} U_L(\gamma|l_1l_2) C^{LM}_{l_1m_1lm} Y_{l_1m_1}(\mathbf{N}). \tag{2.12}$$

Here $\mathbf{N}_0$ and $\mathbf{N}$ are unit vectors in the direction of the incident and scattered particle, respectively, and for definiteness the quantization axis for the angular momenta has been taken parallel to $\mathbf{N}_0$. In view of the above discussion, formula (2.12) may be compared as regards structure with the general expressions for scattering amplitudes for noncentral potentials.[20,22]

3. LARGE ANGULAR MOMENTA

As was noted in Sec. 1, the case of large L is especially important because of the long range of the interaction. In the limit of large L, the operator Λ has an additional approximate symmetry[15,16] that makes it convenient to replace the quantum number γ by two quantum numbers n' and n'' which range independently from $-j$ to $+j$ in integral steps ($j = (n-1)/2$). The following approximate expressions for the eigenvalues λ_γ and the matrices U_L are valid[15,16]:

$$\lambda_{n'n''} = L(L+1) - 2\Omega(n'+n'') + (n'+n'')^2 + O(\mathscr{M}^2/L^2), \tag{3.1}$$

and

$$U_L(n'n''|l_1l_2) = \sum_{j_1j_2} C^{l_2L-l_1}_{j_1j_2} D^{(j_1)}_{n'j_1}(0,\beta,0) D^{(j_2)}_{n''j_2}(0,-\beta,0), \tag{3.2}$$

where

$$\Omega = \left[\left(L+\frac{1}{2}\right)^2 + \left(\frac{3gZ_B\mathscr{M}n}{2\mu Z_A}\right)^2\right]^{1/2}, \quad \operatorname{tg}\beta = -\frac{3gZ_B\mathscr{M}n}{2\mu Z_A(L+1/2)}$$

$$-\frac{\pi}{2} < \beta < 0,$$

and the $D^{(j)}_{mm'}(\alpha,\beta,\gamma)$ are Wigner functions. To calculate the scattering phase shifts we can use the following approximate expression for $\tilde{l}$:

$$\tilde{l} = L - \frac{\Omega(n'+n'')}{L+1/2} - \frac{\Omega^3(n'+n'')^3}{2(L+1/2)^5} + O(L^{-3}). \tag{3.3}$$

In the weak-interaction limit ($Z_B\mathscr{M} \to 0$ with $Z_A = 1$) we have

$$\exp(2i\delta_{n'n''}(L,E) - i\pi L) = e^{i\pi(n'+n''-L)}(1 + O(Z_B^2\mathscr{M}^2)). \tag{3.4}$$

For large L, the first two terms in the expansion of $U_L(n'n''|l_1l_2)$ in powers of the small quantity $Z_B\mathscr{M}$ can be calculated with the aid of the differentiation formulas for Wigner functions and can then be transformed with the aid of the recursion relations for the Clebsch-Gordan coefficients[23] so as to give the expansion in the form

$$U_L(n'n''|l_1l_2) = C^{l_2L-l_1}_{j-n'\,j-n''} + \frac{3gZ_B\mathscr{M}n}{2\mu Z_A(L+1/2)}(-1)^{1-(L+l_1+l_2)} \times \sum_{\mu,\nu=\pm1} C^{l_2+\mu\,L-l_1+\nu}_{j-n'\,j-n''} \langle nl_1l_2LM|\mathbf{N}r|n\,l_1+\nu\,l_2+\mu\,L\,M\rangle + O(Z_B^2\mathscr{M}^2). \tag{3.5}$$

It is not difficult to see, with the aid of Eqs. (3.4) and (3.5), that the first linear term in the expansion of the scattering amplitude (2.11) arises solely from the corresponding term in the expansion of the matrix U_L. In this approximation the amplitude calculated with the aid of Eq. (3.5) is identical with the amplitude as calculated in the first Born approximation for large angular momentum (we omit the details of the calculations).

Now let us consider the quasiclassical case. To make the transition to the quasiclassical case in expression (2.11) for the scattering amplitude we assume that $L \gg n-1 \gtrsim l, l_0$, drop the term representing the unscattered wave, and make use of the asymptotic behavior of the spherical functions[23] at $L\theta \gg 1$ (the angles θ and Φ define the direction of the vector $\mathbf{N}$ in a spherical coordinate system with its axis along $\mathbf{N}_0$); this yields

$$F_{nlom_0\to nlm}(\theta)=\frac{1}{ik(2\pi\sin\theta)^{1/2}}e^{i(m_0-m)\Phi}\sum_L\left(L+\frac{1}{2}\right)$$
$$\times\sum_{n'n''}\exp(2i\delta_{n'n''}(L,E))\,b^{n'n''}_{lom_0}(L,\pi)\cdot\left[\exp\left(i\left(L+\frac{1}{2}\right)\theta\right.\right.$$
$$+i\left(m_0-m-\frac{1}{2}\right)\frac{\pi}{2}\Big)\,b^{n'n''}_{lm}(L,\theta)+\exp\Big(-i\Big(L+\frac{1}{2}\Big)\theta$$
$$\left.\left.-i\left(m_0-m-\frac{1}{2}\right)\frac{\pi}{2}\right)b^{n'n''}_{lm}(L,-\theta)\right],\qquad(3.6)$$

$$b^{n'n''}_{lm}(L,\theta)=\sum_{l_1}U_L(n'n''|l_1l_2)C^{Lm'+m}_{l_1m'lm}e^{i((l_1-L)\theta}.\qquad(3.7)$$

When L and l_1 are both much larger than m' and m, the expression for $b^{n'n''}_{lm}$ is actually independent of m' and can be transformed, with the aid of the asymptotic behavior of the Clebsch-Gordan coefficients[23] and the approximate formula (3.2), to the form

$$b^{n'n''}_{lm}(L,\theta)=\sum_{i_1i_2}C^{l\,i_1+i_2}_{ji_1i_2}D^{(l)}_{m\,i_1+i_2}\left(0,\frac{\pi}{2},0\right)D^{(j)}_{n''i_1}(0,\beta,0)$$
$$\times D^{(j)}_{n'''i_2}(0,-\beta,0)e^{-i((i_1+i_2)\theta}.\qquad(3.8)$$

Finally, if we replace the summation over L in (3.6) by an integration, perform the integration by the method of stationary phase, and proceed in the usual manner,[19] we obtain

$$F_{nlom_0\to nlm}(\theta)=\frac{1}{k(\sin\theta)^{1/2}}e^{i(m_0-m)\Phi}\Big\{\sum_{n'n''}\left[L_{n'n''}\frac{dL_{n'n''}}{d\theta}\right]^{1/2}$$
$$\times\exp\left[2i\delta_{n'n''}(L_{n'n''},E)+i\left(L_{n'n''}+\frac{1}{2}\right)\theta+i\left(m_0-m-\frac{1}{2}\right)\frac{\pi}{2}\right]$$
$$\times b^{n'n''}_{lom_0}(L_{n'n''},\pi)\cdot b^{n'n''}_{lm}(L_{n'n''},\theta)+\sum_{n'n''}\left[L_{n'n''}\frac{dL_{n'n''}}{d\theta}\right]^{1/2}$$
$$\times\exp\left[2i\delta_{n'n''}(L_{n'n''},E)-i\left(L_{n'n''}+\frac{1}{2}\right)\theta-i\left(m_0-m-\frac{1}{2}\right)\frac{\pi}{2}\right]$$
$$\times b^{n'n''}_{lom_0}(L_{n'n''},\pi)\cdot b^{n'n''}_{lm}(L_{n'n''},-\theta)\Big\}.\qquad(3.9)$$

The first summation here is taken over those values for which there exists a solution to the equation

$$2\frac{d}{dL}\delta_{n'n''}(L,E)+\theta=0,\qquad(3.10)$$

which also serves to determine the functional relationship $L_{n'n''}(\theta)$ in this sum. The second sum is related in just the same way to the equation

$$2\frac{d}{dL}\delta_{n'n''}(L,E)-\theta=0.\qquad(3.11)$$

For example, for scattering from a neutral atom ($Z_A=1$) in the absence of orbiting in the potential $\sim-(n'+n'')\Omega/R^2$, the first sum encompasses the terms with $(n'+n'')<0$, and the second sum, those with $(n'+n'')>0$. With the aid of Eq. (3.8), one can show that in this case Eq. (3.9) agrees, except for an unimportant common phase factor, with a result obtained elsewhere[12] in a different manner.[1)]

In a collision with an ion one may assume that the motion of the colliding particles is determined mainly by the Coulomb interaction $V_C(R)=(Z_A-1)Z_B/R$ and neglect the interaction of the charge Z_B with the dipole induced in the atom in connection with the linear Stark effect. Then one may neglect the dependence on the quantum numbers n' and n'' in Eqs. (3.10) and (3.11) and give these equations the unified form

$$2\frac{d}{dL}\delta_c(L,E)-\varepsilon\theta=0,\quad\delta_c(L,E)=\arg\Gamma(L+1+i\eta),\qquad(3.12)$$

where δ_C is the scattering phase shift for the purely Coulomb potential $V_C(R)$ and $\varepsilon=\mathrm{sign}((Z_A-1)Z_B)$. The resulting dependence $L_C(\theta)=|\eta|\cot(\theta/2)$ should be used in Eq. (3.9), where the dependence on n' and n'' remains in the phase $\delta_{n'n''}$. Expanding the latter in the small difference $\tilde{l}-L$ and making use of Eq. (3.3), we obtain

$$\delta_{n'n''}(L,E)\approx\delta_c(L,E)+\frac{\Omega(n'+n'')}{L+1/2}\frac{\pi-\varepsilon\theta}{2},\qquad(3.13)$$

$$F_{nlom_0\to nlm}(\theta)=\exp\Big\{i(m_0-m)\Phi+2i\delta_c+i\varepsilon\Big(L_c+\frac{1}{2}\Big)$$
$$\times\theta-i\varepsilon\Big(m_0-m-\frac{1}{2}\Big)\frac{\pi}{2}\Big\}\frac{1}{ik}\left[\frac{L_c}{\sin\theta}\frac{dL_c}{d\theta}\right]^{1/2}\sum_{n'n''}\exp\Big\{i\Omega(n'+n'')(\pi-\varepsilon\theta)\Big/$$
$$\Big(L_c+\frac{1}{2}\Big)\Big\}\,b^{n'n''}_{lom_0}(L_c,\pi)\cdot b^{n'n''}_{lm}(L_c,-\varepsilon\theta).\qquad(3.14)$$

With allowance for the explicit dependence of L_C on θ, this result is equivalent to that obtained in Ref. 4.

Finally, if we neglect the curvature of the trajectories we should use an amplitude that depends on the impact parameter $\rho=L/k$ and set $\theta=0$ under the summation sign:

$$F_{nlom_0\to nlm}(\rho)=e^{i\xi}\sum_{n'n''}\exp\{i\Omega(n'+n'')\pi/k\rho\}$$
$$\times b^{n'n''}_{lom_0}(k\rho,\pi)\cdot b^{n'n''}_{lm}(k\rho,0),\qquad(3.15)$$

where ξ is an unimportant phase shift. For $n=2$, this result corresponds to that obtained by Chibisov[2] and by Gurevich *et al.*[3]

In the adiabatic case (see Sec. 1) it is not difficult to show, using the limiting expressions[16] for U_L, that the scattering amplitude corresponds to the development of the system in accordance with the adiabatic terms of the quasimolecule that are specified by the parabolic quantum numbers n_1 and n_2 in a coordinate system with its axis along **R**. Then on different terms the system acquires different phases

$$-\int\Delta E\,dt,\quad\Delta E=-3Z_Bn(n_1-n_2)/2Z_AR^2,$$

and this leads to a change in the orbital angular momentum of the atomic electron. An analogous description is possible in the general nonadiabatic case within the framework of dynamic terms; this has been thoroughly discussed elsewhere.[4,12] The condition for the applicability of the adiabatic approximation (Sec. 1) is violated at sufficiently large impact parameters, i.e., for small-angle scattering. With further decrease in the scattering angle the quasiclassical approximation becomes applicable and one should use the eikonal approximation or perturbation theory.

The conditions for the applicability of the approximations used in the present work have been thoroughly discussed before (see, e.g., Refs. 1, 4, and 12). Here we merely emphasize that the calculation of the total cross sections requires, generally speaking, that the relativis-

tic splitting of the energy level with a given principal quantum number be taken into account.[1,2] Since the scattering amplitude contains several interference terms, in the quasiclassical region the differential cross sections oscillate as functions of the scattering angle. Even though the quadrupole interaction is negligibly small as compared with the dipole interaction, it can still make an appreciable contribution to the phase of these oscillations (this was brought to the author's attention by E. E. Nikitin). This effect is small if the condition

$$2Z_B\mathcal{M}D/k\rho^3\ll 1 \tag{3.16}$$

is satisfied (D is the quadrupole moment of the atom), and this leads to a significant limitation on the collision energy E. If condition (3.16) is not satisfied, the oscillations remain but turn out to be shifted.

4. LINE BROADENING

In the binary approximation, the quantum mechanical part of the line broadening problem reduces to the calculation of the quantity (cf. Refs. 9, 10, and 25, for example)

$$\Phi(\Delta\omega)=\sum_{\varkappa}\sum_{\substack{\gamma_a L_a M_a\\ \gamma_b L_b M_b}}|\langle k_a\gamma_a L_a M_a|r_\varkappa|k_b\gamma_b L_b M_b\rangle|^2. \tag{4.1}$$

Here the states $|k_a\gamma_a L_a M_a\rangle$ describe the scattering of the perturbing particle B with the kinetic energy $k_a^2/2\mathcal{M}$ of relative motion from the atom in the upper level a of energy E_a, while the state $|k_b\gamma_b L_b M_b\rangle$ describes the scattering of particle B of energy $k_b^2/2\mathcal{M}$ from the atom in the lower level b of energy E_b. For brevity we omit the principal quantum numbers n_a and n_b of the atomic levels. The quantity $\Delta\omega=\omega_{ab}-\omega$ is the difference between the frequency $\omega_{ab}=E_a-E_b$ of the unperturbed spectrum line and the observed frequency ω. Because of energy conservation, we have $\Delta\omega=(k_a^2-k_b^2)/2\mathcal{M}$. The summation on $\varkappa$ is taken over the components of the radius vector $\mathbf{r}$ of the atomic electron. The shape of the spectrum line is determined by averaging (4.1) over the energy distribution of the particles. Neglecting transitions in which n changes in scattering, as we are doing, is frequently referred to in line-broadening theory as neglecting the damping.

In the dipole approximation for the scattering of a charged perturbing (line-broadening) particle one can use Eqs. (2.6) and (2.7) to put formula (4.1) into the form

$$\Phi(\Delta\omega)=\sum_{\gamma_a\gamma_b}\sum_{l_1 L_a L_b}(2L_a+1)(2L_b+1)|\langle k_a l_a|k_b l_b\rangle|^2$$
$$\times\left|\sum_{l_{2a}l_{2b}}U_{L_a}(\gamma_a|l_1 l_{2a})U_{L_b}(\gamma_b|l_1 l_{2b})^*\begin{Bmatrix} l_{2a} & l_{2b} & 1\\ L_b & L_a & l_1\end{Bmatrix}\langle l_{2a}\|r_2\|l_{2b}\rangle\right|^2, \tag{4.2}$$

where $\langle l_{2a}\|r_2\|l_{2b}\rangle$ is the reduced matrix element for the atomic electron, while

$$\langle k_a l_a|k_b l_b\rangle=\int_0^\infty f_{k_a l_a}(R)f_{k_b l_b}(R)R^2dR,$$
$$(l_a(l_a+1)=\lambda_{\gamma_a l_a},\quad l_b(l_b+1)=\lambda_{\gamma_b l_b}) \tag{4.3}$$

is the radial overlap matrix element between the initial- and final-state wave functions of the perturbing particle.

Assuming that the main contribution to the line broadening comes from distant collisions, we use the asymptotic formula[23]

$$\begin{Bmatrix} l_{2a} & l_{2b} & 1\\ L_a & L_b & l_1\end{Bmatrix}\approx\frac{(-1)^{l_{2a}+l_{2b}+1}}{(2l_1+1)^{1/2}}\begin{pmatrix} l_{2a} & l_{2b} & 1\\ L_a-l_1 & l_1-L_b & L_b-L_a\end{pmatrix}, \tag{4.4}$$

which is valid when $L_a, L_b, l_1\gg l_{2a}, l_{2b}$, to reduce Eq. (4.2) to the form

$$\Phi(\Delta\omega)=\sum_{l_1}\sum_{\substack{n_a' n_a''\\ n_b' n_b''}}\sum_{\varkappa}(2l_1+1)|\langle k_a l_a|k_b l_b\rangle|^2$$
$$\times|\langle n_a n_a' n_a''|r_\varkappa|n_b n_b' n_b''\rangle|^2. \tag{4.5}$$

Here the $|nn'n''\rangle$ are dynamic states of the hydrogen-like atom between which no transitions take place during the passage of a classical charged particle with orbital angular momentum l_1. These states can be expressed in terms of the ordinary spherical-basis atomic wave functions $|nlm\rangle$ with the aid of the matrix introduced above:

$$|nn'n''\rangle=\sum_{l_2 m_2}U_{l_1}(n'n''|l_1+m_2\,l_2)|nl_2m_2\rangle. \tag{4.6}$$

The states $|nn'n''\rangle$ were introduced earlier in solving the scattering problem[4] and the line-broadening problem[5] for the case in which the motion of the incident particle is assumed to be classical. Formula (4.5) shows that these states have a somewhat more general significance, since the radial motion of the charged particle, which determines the matrix elements $\langle k_a\tilde{l}_a|k_b\tilde{l}_b\rangle$, can be treated quantum mechanically. When using exact dipole-approximation wave functions, these matrix elements can be calculated analytically in terms of the hypergeometric function of one or two variables (for the case of the broadening of the spectrum lines of an atom,[9] or of an ion, respectively).

Passing from Eq. (4.5) to the limit in which the motion of the perturbing particle is treated classically involves replacing the summation over l_1 by an integration over the impact parameter and passing to the limit for the matrix elements $\langle k_a\tilde{l}_a|k_b\tilde{l}_b\rangle$. The classical limit corresponding to rectilinear trajectories for the perturbing particle that is broadening the lines of an atom has been treated by Tran Minh *et al.*[9] on the basis of an analytic expression for the matrix element. Having in mind the more general case of curved trajectories (e.g., for broadening of the lines of an ion) we shall briefly describe how such a transformation is to be carried through in the integral (4.3) itself, which assumes the following form when the simplest quasiclassical wave functions are used in the region of classically allowed motion:

$$\langle k_a l_a|k_b l_b\rangle\approx 4\int_{R_0}^\infty dR(p_a(R)p_b(R))^{-1/2}\cdot$$
$$\times\sin\left(\int_{R_0}^R p_a(R')dR'-\frac{\pi}{4}\right)\sin\left(\int_{R_0}^R p_b(R')dR'-\frac{\pi}{4}\right), \tag{4.7}$$

$$p_{a,b}=[k_{a,b}^2-(l_{a,b}+1/2)^2/R^2+2\mathcal{M}(Z_A-1)Z_B/R]^{1/2}, \tag{4.8}$$

where R_0 is the classical turning point. Replacing the product of trigonometric functions by the appropriate sum and dropping the rapidly oscillating term, we obtain

$$\langle k_a l_a | k_b l_b \rangle \approx 2\int_{R_0}^{\infty} dR (p_a(R) p_b(R))^{-1/2} \times \cos\left(\int_{R_0}^{R} p_a(R')dR' - \int_{R_0}^{R} p_b(R')dR'\right). \quad (4.9)$$

Further simplification is possible if we can assume that the emission of a photon by the atom has little effect on the momentum of the particle, i.e., that $p_a(R) \approx p_b(R) \equiv p(R)$. Then the difference $p_a(R) - p_b(R)$ is negligibly small, although this cannot be said of the integral of this difference over the trajectory. Under the integral sign we keep the next term in the expansion of $p_a - p_b$ for $p_a \approx p_b$ and then transform to an integration over the time t: $p \approx \mathcal{M} dr/dt$ (cf. Ref. 25); this gives

$$\langle k_a l_a | k_b l_b \rangle \approx 2\int_0^{\infty} dt \cos[\Delta\omega t + (l_a - l_b)\varphi(t)]. \quad (4.10)$$

Thus, both before and after the emission of the photon, the particle moves in a single classical trajectory with the angular coordinate $\varphi(t)$ measured in the collision plane from the position of closest approach. In the case of a rectilinear trajectory, the expression for the line contour with (4.10) and (3.3) taken into account agrees with the result of an earlier calculation in the theory of line broadening by a classical particle[5] in which the integral (4.10) was calculated in terms of a Bateman function. However, the assumption that $p_a(R) \approx p_b(R)$, which may be called the generalized Franck-Condon principle,[26] makes it possible to treat curved trajectories too. In calculating the broadening of the lines of an ion it is natural to use the Coulomb trajectory

$$v = [k^2 - (l_i + 1/2)^2/R^2 + 2\mathcal{M}V_C(R)]^{1/2}, \quad V_C(R) = (Z_A - 1)Z_B/R. \quad (4.11)$$

For an atom one may adopt some average of the effective centrifugal potentials $\sim (\bar{l}_a + 1/2)^2/R^2$ and $\sim (\bar{l}_b + 1/2)^2/R^2$ of the initial and final states (cf., Ref. 26). Thus, each pair $|n_a n'_a n''_a\rangle$ and $|n_b n'_b n''_b\rangle$ of initial and final dynamic states (4.6) in (4.5) will have its own potential.

The states $|nn'n''\rangle$ reduce in the adiabatic limit to states of the hydrogen atom with definite parabolic quantum numbers. In the more general case there is a peculiar separation of the effects of the adiabatic mixing of the states from the character of the radial motion, where they manifest themselves only through the single parameter $\bar{l}$. Thus, many results of the adiabatic theory[26] can be carried over to the general case.

[1)]It must be borne in mind that the Wigner functions were used in Ref. 12 as defined in Ref. 24, whereas they were used in the present work as defined in Ref. 23, and that the two groups of Wigner functions differ by phase factors; the relation between the two definitions is given in Ref. 23.

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