ON STRONG COLLISIONS IN HYDROGENIC LINE BROADENING

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Received December 27, 1967; revised July 15, 1968

ABSTRACT

The degeneracy of hydrogenic states is used to sum approximately the $S$-matrix to all orders in Stark-broadening calculations. It is found that the usual strong-collision cutoff for lower lines should represent a reasonable approximation. However, there could be a significant difference between our results and previous calculations for transitions among levels with large principal quantum numbers.

I. INTRODUCTION

The Stark-broadening theories of Kolb and Griem (1958) and of Baranger (1958) made possible realistic calculations of Stark-broadened profiles of spectral lines (Griem, Kolb, and Shen 1959; hereinafter referred to as GKS). These calculations were made utilizing the impact and classical-path approximations for the perturbing electrons and the static approximation for the ions. In averaging over the impact parameters of the electrons, divergences were encountered at both zero and infinite impact parameters. The divergence at large impact parameters can be removed by cutting off the integral at a distance of the order of the Debye length. The divergence at the zero impact parameter is attributed to the breakdown of perturbation theory for strong collisions. A cutoff at $p_{\text{min}}$ was introduced in the GKS calculations, which corresponds to the first non-vanishing term of the $S$-matrix becoming unity, i.e., breakdown of the perturbation expansion. An estimate was made for the strong-collision contributions in the calculation of the H$\beta$ profile (Griem, Kolb, and Shen 1962).

The purpose of this paper is not to review the approximations of the formal theory, i.e., impact, classical-path, and static approximations; these approximations are known to be valid near the line center for most temperature and density ranges. Rather, our purpose is to point out that within these approximations one can take advantage of the degeneracy of the atomic states. Then it is possible to make an approximation by which the $S$-matrix may be summed to all orders (and still retain its unitarity properties). The resultant classical-path $S$-matrix no longer diverges in the limit of the zero impact parameter. Thus we can "extend" the cutoff to the quantum-mechanical limit of $\sim \hbar/mv$, or to a distance where the multipole expansion breaks down.

In § II, the general theory is presented. Various averages are performed in § III (using only the dipole term of the multipole interaction series), and the necessary integrals are evaluated. These integrals can be reproduced almost exactly by a suitable cutoff similar in spirit to the older strong-collision corrections. The results for the Ly-$\alpha$ line are compared with the corresponding results of GKS and with the alternative cutoff procedure. In § IV the results are critically examined. For the lower hydrogenic lines we can conclude that the $p_{\text{min}}$ cutoff of GKS probably represents a very good approximation. For higher series members, there may be significant differences between our results and those of GKS.

II. THEORY

The shape of a Stark-broadened line in the classical-path approximation is given by the Fourier transform (Baranger 1958) of

$$\Phi(t) = Tr[dT^+(t,0)dT(t,0)\rho^{(a)}]_{2\nu},$$

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where the trace is taken over the atomic states, $\rho^{(a)}$ is the density matrix for the atom, $d$ is the dipole operator, $T(t,0)$ is the time-development operator, and $[ \ ]_{\text{av}}$ is an average over the parameters characterizing the perturber (i.e., over impact parameters and velocities in the classical-path approximation).

The equation for the operator $U(t,0) = \exp (i\hbar t/\hbar) T(t,0)$ is

$$i\hbar \frac{\partial U(t,0)}{\partial t} = [\tilde{V}(t) + eE\tilde{z}] U(t,0),$$

(2)

where $\tilde{V}(t) = \exp (i\hbar t/\hbar) V(t) \exp (-i\hbar t/\hbar)$, $V(t)$ is the interaction energy of the free electrons with the atomic electron, and $\tilde{z}$ is the $z$-component of the position vector of the atomic electron. The quantity $E$ is a fixed electric field equal to the electric field produced by the ions at the atom, but it does not contain the ion coordinates, i.e., the static approximation. The assumption that we need matrix elements of $U$ only between states having the same principal quantum number (no quenching assumption) implies in equation (2) that $\tilde{V}(t) = V(t)$ and $\tilde{z}(t) = z$, because all hydrogenic levels of the same principal quantum number have the same energy. Then an approximate solution of equation (2) is

$$U(t,0) = \exp \left\{ - (i/\hbar) \int_0^t V(t')dt' + eEz \right\}.$$

(3)

This solution was used by Callaway (1965) in studying inelastic collisions of slow atoms, and by Byron and Foley (1964) in investigating line broadening.

The series equivalent to equation (3) (without the $z$-term) was also used by Griem (1965). The solution is exact if $V(t)$ commutes with itself at different times. This at first sight appears to be the case; however, it is not true when we restrict the $V(t)$ matrix elements to those between states of the same principal quantum number. Expression (3) does, however, retain unitarity, and to second order (after the required angular averages are performed) it does agree with the exact solution (see Smith, Vidal, and Cooper 1968 for details).

The time-dependent part of equation (1) is $T_a^+(t,0) T_b(t,0)$, where the subscripts restrict $T(t,0)$ to operate in the subspace corresponding to energy $E_a$ or $E_b$. An "equation of motion" can be constructed for this term using equation (3) and the impact approximation.

Then from equation (3) we have

$$U(t,0) = e^{-(i/\hbar) Ezt} U_a(t,0),$$

(4)

where $U_a(t,0)$ is the time-ordered exponential,

$$\exp \left[ - (i/\hbar) \int_0^t e^{iEzt/\hbar} V(t') \left( e^{-iEzt/\hbar} d t' \right) \right].$$

Since the electric field $E$ is static, we need to consider only $U_a^+(t,0) U_a(t,0)$. This is done as in GKS, and the result is

$$[U_a^+(t,0) U_a(t,0)]_{ab} = \exp \left[ -i(z_a - z_b)eEz/\hbar \right] \exp \left[ i(z_a - z_b)eEz/\hbar + \phi_{ab} \right],$$

(5)

with $z_a$ and $z_b$ operators in the subspaces of energies $E_a$ and $E_b$, and

$$\phi_{ab} = \sum_j P_j [U^a_{e\gamma}(\infty, -\infty) U_{ab}(\infty, -\infty) - 1],$$

(6)

where $P_j$ is the probability per unit time for a collision of a free electron and an atom. The quantity $P_j$ is given by
and the position vector of the atomic electron, let 
where the de Broglie wavelength is chosen such

\[ \rho = \frac{m \dot{r}}{2} \]

\[ \mathbf{r} = \mathbf{R} \]

\[ \mathbf{p} = \mathbf{P} \]

\[ \frac{\partial}{\partial \mathbf{p}} \frac{\partial}{\partial \mathbf{p}} = \frac{\partial}{\partial \mathbf{p}} \frac{\partial}{\partial \mathbf{p}} \]

\[ \int d^3 \mathbf{p} \]
that $u$ is along the $z$-axis. Then $U(\infty, -\infty)$ is diagonal in the $E_a$ subspace if the basic states are chosen to be the Stark eigenstates $|n_1n_2m\rangle$. This allows us to sum the infinite series (see Griem 1965) implied by expression (11):

$$
\langle n_1n_2m | U_e | n_1'n_2'm' \rangle = \delta_{n_1n_1'} \delta_{n_2n_2'} f(n_1 - n_2),
$$

where $f(n_1 - n_2) = \exp\{-i[3n(n_1 - n_2)h]/m_e v\}$ and $n$ is the principal quantum number. The subscript $c$ indicates that $U$ is calculated in the collision axis. The angular average can now be carried out (Cooper 1967). In order to make use of the symmetry of wave functions, this average is best carried out in terms of wave functions in spherical coordinates. The transformation matrix elements between spherical and parabolic (or Stark) wave functions are given by Hughes (1967) in terms of Clebsch-Gordon coefficients. Using his results, expressed in $3-j$ symbols, we have

$$
\langle nlm | U_e | nlm \rangle = \sum_{n_1} \left( \begin{array}{ccc} \frac{1}{2}(n - 1) & \frac{1}{2}(n - 1) & l^2 \\ \frac{1}{2}(m + n_2 - n_1) & \frac{1}{2}(m - n_1 + n_2) & -m \end{array} \right)
\times (2l + 1)f(n_1 - n_2),
$$

where $n_1$ and $n_2$ are related by $n = n_1 + n_2 + |m| + 1$. In performing the angular average, the atomic axes (in an arbitrary fixed direction) are rotated through the Euler angles $\alpha$, $\beta$, and $\gamma$ into the collision axes defined by $u$ as being in the $z$-direction. The angular average is then performed by integrating over the Euler angles, since the collisions occur at random with respect to a fixed direction. Then

$$
U_{AV} = \frac{1}{8\pi^2} \int_0^{2\pi} da \int_0^\pi d\beta \sin \beta \int_0^{2\pi} d\gamma D^+(a, \beta, \gamma) U_e D(a, \beta, \gamma),
$$

where $D(a, \beta, \gamma)$ is the rotation operator (Edmonds 1960). The matrix elements of $U_{AV}$ can easily be obtained from equation (14):

$$
\langle nl'm' | U_{AV} | nlm \rangle = \delta_{l'l'} \delta_{nm'-m} (2l + 1)^{-1} \sum_{m=-l}^{l} \langle nlm | U_e | nlm \rangle.
$$

Substituting equation (13) in equation (15), we have

$$
\langle nlm | U_{AV} | nlm \rangle = \Gamma(l) = \sum_{n_1n_2} \left( \begin{array}{ccc} \frac{1}{2}(n - 1) & \frac{1}{2}(n - 1) & l^2 \\ \frac{1}{2}(m + n_2 - n_1) & \frac{1}{2}(m - n_1 + n_2) & -m \end{array} \right)
\times f(n_1 - n_2).
$$

Finally, we need the angular-averaged matrix elements in parabolic wave-function basis, since this is the representation which diagonalizes $z$ (see equation [10]). It is given by

$$
\langle n_1n_2m | U_{AV} | n_1'n_2'm' \rangle = \sum_{l}(2l + 1)(-1)^{n_1 + n_2 + |m| - m}
\times \Gamma(l) \left( \begin{array}{ccc} \frac{1}{2}(n - 1) & \frac{1}{2}(n - 1) & l \\ \frac{1}{2}(m + n_2 - n_1) & \frac{1}{2}(m - n_1 + n_2) & -m \end{array} \right)
\times \left( \begin{array}{ccc} \frac{1}{2}(n - 1) & \frac{1}{2}(n - 1) & l \\ \frac{1}{2}(m + n_2' - n_1') & \frac{1}{2}(m + n_1' - n_2') & -m \end{array} \right).
$$

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Because of the symmetry of the first $3-j$ symbol in expression (16) with respect to interchanging the first two columns, only terms with $f(n_1 - n_2) + f(n_2 - n_1)$ contribute. Hence we have only real matrix elements. In general, expression (17) will be different from the corresponding results of GKS in that different components are now weighted differently by the vector-coupling coefficients.

For the Ly-$\alpha$ case ($n = 2$) we have calculated this matrix numerically. With the rows and columns specified in the order $|001\rangle$, $|00-1\rangle$, $|100\rangle$, and $|010\rangle$, $U_{AV}$ can be expressed using parabolic wave function as basis:

$$U_{AV}^{(P)} - 1 = 2[\cos \left(\frac{6\hbar}{mpv}\right) - 1]$$

We note here that the first term of the expansion of $\cos(6\hbar/mpv)$ gives numerical results identical with those of equation (15) of GKS. In general, the required matrix elements can be expressed as a sum of integrals of the following type (multiplied by the appropriate vector-coupling coefficients):

$$I = 2\pi N \int_{r_D}^{\infty} \int_{r_D}^{\infty} \rho_D \rho 2 \{ \cos \left[ \frac{3n(n_1 - n_2)\hbar}{mpv} \right] - 1 \}$$

where $\rho_D$ is the Debye length and $n_1 > n_2$. The lower cutoff for $r \sim 1$ corresponds to the validity range of the classical-path approximation (Baranger 1962). The parameter $r$ is included to show that the final result is not sensitive to the values of $r$. The integral is evaluated in the Appendix for the case

$$I = \frac{3n(n_1 - n_2)\hbar}{mpD} \left(\frac{m}{2kT}\right)^{1/2} = \frac{3n(n_1 - n_2)\hbar}{mpD} \left(\frac{m}{2kT}\right)^{1/2}$$

(20)

(In most plasma problems for the lower series members, relation (20) is well satisfied.)

The result is

$$I = 3n(n_1 - n_2)N \left(\frac{8\pi m}{\hbar kT}\right)^{1/2} \left[ K(r) - \frac{3}{2}(1 - \gamma) + \ln A + O(A^2) \right],$$

where

$$K(r) = \sin \left(\frac{g}{r}\right) - \cos \left(\frac{g}{r}\right) - \frac{1}{(g/r)^2},$$

and where $g = 3n(n_1 - n_2)$, and $\text{Ci}$ is the cosine integral.

The values of $K(r)$ are slowly varying with $r$, and $K(1) = 0.025$. For $n = 2$, i.e., Ly-$\alpha$,

$$I(n = 2) = 36N \left(\frac{8\pi m}{\hbar kT}\right)^{1/2} \left[ 0.025 - \frac{3}{2}(1 - \gamma) + \ln A \right],$$

where $r$ has been set equal to unity, and terms of $O(A^2)$ have been neglected.

b) Comparison with Results of GKS

We shall now reproduce the results of GKS for comparison with ours. The usual perturbation-theory approach amounts to replacing the cosine term in equation (19) with the first two terms of its expansion ($\cos \theta \simeq 1 - \theta^2/2$). This obviously breaks down at small impact parameters, when the term corresponding to $\theta$ exceeds unity. However,
for large values of $\theta$, the cosine oscillates rapidly (see Fig. 1), and a strong-collision correction is made by replacing the cosine in the integral by its average (zero) for all $\rho$ less than $\rho_{\text{min}}$ (for which $\theta \approx 1$). We then obtain

$$I' = 2\pi N \int_{\rho_{\text{min}}}^{\infty} \rho f(v)dv \left\{ \int_{\rho_{\text{min}}}^{\rho} \rho dp \left[ \frac{-9n^2(n_1 - n_2)^2h^2}{2m^2p^2v^2} \right] - \rho^2 \right\}.$$  \hspace{1cm} (23)

Since the cosine lies between +1 and −1, the limits on the correction term are between 0 and $2\rho^2_{\text{min}}$ (which gives an estimate of the maximum possible error). In GKS, $\rho_{\text{min}}$ is estimated to be $(2/3)^{1/2} \hbar n^2/mv$ with no $\rho^2_{\text{min}}$ term added, whereas in equation (23) it is $3(n_1 - n_2)n\hbar/mv$ (with $\rho_{\text{min}}$ defined by $\theta = 1$). In later papers (Griem, Kolb, and Shen 1962), $\rho^2_{\text{min}}$ has been included. For Ly-α, the ratio of the two $\rho_{\text{min}}$'s is 1.8. However, for higher members of the Lyman series, detailed calculations are needed to compare the two cutoffs, since the cutoff proposed here depends on $n_1$ and $n_2$ but the GKS cutoff does not. When used to estimate the integral of equation (19), the cutoff proposed here is equally good, irrespective of the $n_1$ and $n_2$. This has significant advantages, since it means that the integral is well represented for all $n_1$ and $n_2$, whereas this is definitely not the case with a single cutoff. For Ly-α, the results of integration of equation (23) for GKS are

$$I = 18N \left( \frac{8\pi m}{kT} \right)^{1/2} \left( \frac{\hbar}{m} \right)^2 \left( \gamma + \ln Y_{\text{min}} \right),$$  \hspace{1cm} (24)

using $\rho_{\text{min}} = (2/3)^{1/2} \hbar n^2/mv$ and $Y_{\text{min}} = (4\pi N/3m)(4e\hbar/kT)^2$ with no $\rho^2_{\text{min}}$ added, and

$$I'' = 18N \left( \frac{8\pi m}{kT} \right)^{1/2} \left( \frac{\hbar}{m} \right)^2 \left( \gamma + \ln Y_{\text{min}} - 0.683 \right),$$  \hspace{1cm} (25)

using $\rho_{\text{min}} = 3(n_1 - n_2)n(\hbar/mv)$. Equation (22), expressed in $Y_{\text{min}}$, is

$$I = 18N \left( \frac{8\pi m}{kT} \right)^{1/2} \left( \frac{\hbar}{m} \right)^2 \left( \gamma + \ln Y_{\text{min}} - 0.579 \right).$$  \hspace{1cm} (26)

For comparison, we usually have $\ln Y_{\text{min}} \sim -10$, so here the difference is at most $\sim 5$ per cent. The difference between the three expressions can be understood easily by inspec-
tion of Figure 1. In equation (24) the $S$-matrix in the integrand is overestimated by replacing it with the first two terms of the expansion of the cosine term. This overestimate is not enough to compensate for the neglect of the strong collisions. Unfortunately, comparison generally is not easy for the higher lines. One would expect, however, that $\rho_{\text{min}}$ of GKS would be too large to give good numerical results for the higher lines. We would also like to add that the summation of the perturbation series (Griem 1965) gave the result $-0.582$ as compared with $-0.579$ in equation (26). Since the cutoff proposed here is a good estimate of the integral for all $n_1$ and $n_2$, it indicates that if a strong-collision correction does have to be introduced, considerable advantage in accuracy can be obtained by imposing the unitarity condition on each of the $S$-matrix elements separately (rather than on some sum or average of them).

IV. DISCUSSION

We have shown that for Ly-$\alpha$ even the neglect of strong collisions with a $\rho_{\text{min}}$ cutoff appears to be a good approximation. However, for higher members of the series, equation (17) implies that different components of a line are weighted differently, and this may cause a significant difference from the results of GKS. Detailed calculations are needed to show the difference numerically. However, some advantage in accuracy will be obtained by cutting off each term separately, since each term (eq. [19]) obeys the unitarity condition on the $S$-matrix elements. Since the integral of equation (19) does not diverge as $\rho \to 0$, we could extend to this limit. The procedure of Vainshtein and Sobelman (1959) also does not diverge as $\rho \to 0$. However, they do this by replacing the second-order perturbation term by a function of the type $\exp i \theta^2/2$ rather than by a cosine function as in this case. Our angular-averaged $S$-matrix retains unitarity and also is correct to second order. Notice that the over-all error of the half-width in terms of percentage is usually much smaller than the error in the electron-impact contribution (Griem, Kolb, and Shen 1962).

The results we have obtained strictly apply only to a dipole perturbation. If we crudely estimate the breakdown of the multipole expansion of the interaction $V(\ell)$ at the impact parameter $\rho \simeq n^2 \alpha_0$ (or, roughly, $n^2(kT/\text{Ryd})^{1/2} \hbar/mv$), we find that for $n > 2$ this impact parameter is typically greater than $\hbar/mv$ (using $kT/\text{Ryd} \sim 1/10$).

In the same way as in § III it is possible to diagonalize the approximate classical-path $S$-matrix in which $V(\ell)$ is taken to higher orders. However, this is a cumbersome procedure, and for the most important lines ($n \leq 10$), it appears that this breakdown of the multipole expansion is unimportant. Inspection of equation (21) shows that the integral of equation (19) is not very sensitive to the values of $r$. When the expansion breaks down, the oscillations of the $S$-matrix change; hence we would reinstate in equation (19) a cutoff for each term at $r (\simeq n^2(kT/\text{Ryd})^{1/2})$ and retain the strong-collision contribution from $\hbar/mv < \rho < r\hbar/mv$. This leads to subtracting $(r^2 - 1)/g^2$ from $K(r)$, which again leaves only a slowly varying part if $g/r \geq 1$. For $n \leq 10$, $g/r \geq 1$ for all values of $n_1 - n_2$. (For $n \geq 10$, this is true only for some values of $n_1 - n_2$; for these the effect of the multipole interaction should be considered in more detail.) The difference between this and the dipole-only case will then usually be negligible. This is small, because, if $g/r > 1$, the cutoff for the breakdown of the multipole expansion comes in a region where the $S$-matrix element has already begun to oscillate. This indicates that the usual procedure (GKS) of considering the dipole term only should lead to only small corrections for the most important lines. Similar conclusions were reached by Griem (1965) for Ly-$\alpha$.

It is a pleasure to thank Drs. Earl Smith and R. Vidal for helpful discussions and Dr. David Hummer for pointing out the method of evaluating the integral involved in equation (19).
This work was supported in part by the Advanced Research Projects Agency (Project DEFENDER) monitored by the U.S. Army Research Office–Durham under contract DA-31-124-ARO-D-139.

APPENDIX

The average over impact parameter and velocity involves evaluating the following integral:

\[
G = \int_{-\infty}^{\infty} e^{-mv^2/2kT} v^3 dv \int_{0}^{\infty} \rho d\rho \cos \frac{\hbar}{m\rho v}.
\]

(A1)

The integral over \( \rho \) can be performed, and \( G \) reduces to

\[
G = \frac{1}{2} \left( \frac{\hbar}{m} \right)^2 \left[ \frac{\sin (g/r)}{(g/r)} - \frac{\cos (g/r)}{(g/r)^2} - \text{Ci} (g/r) \right] G_1 + \frac{1}{2} \rho_D^2 G_2
\]

\[
- \frac{1}{2} \left( \frac{\hbar}{m} \right)^2 \rho_D G_3 + \frac{1}{2} \left( \frac{\hbar}{m} \right)^2 G_4,
\]

(A2)

\[
G_1 = \int_{\rho_D/m}^{\infty} v^2 e^{-mv^2/2kT} dv; \quad G_2 = \int_{\rho_D/m}^{\infty} v^2 e^{-mv^2/2kT} \cos \left( \frac{\hbar}{m\rho_Dv} \right) dv;
\]

\[
G_3 = \int_{\rho_D/m}^{\infty} v^2 e^{-mv^2/2kT} \sin \left( \frac{\hbar}{m\rho_Dv} \right) dv; \quad G_4 = \int_{\rho_D/m}^{\infty} v^2 e^{-mv^2/2kT} \text{Ci} \left( \frac{\hbar}{m\rho_Dv} \right) dv.
\]

For \( (\hbar/m\rho_D)(m/2kT)^{1/2} \ll 1 \), the lower limit of \( G_1, G_2, \) and \( G_3 \) can be replaced by zero. The integrals \( G_2 \) and \( G_3 \) are given by Harrison, Hummer, and Fite (1964). The results are

\[
G_1 = \frac{kT}{m}; \quad G_2 = 2 \left( \frac{kT}{m} \right)^2 - \frac{A^2}{2} \left( \frac{kT}{m} \right)^2 + O(A^4);
\]

(A3)

\[
G_3 = \frac{A}{2} \left( \frac{2kT}{m} \right)^{3/2} + O(A^3), \quad \text{where} \quad A = \frac{\hbar}{m\rho_D} \left( \frac{m}{2kT} \right)^{1/2}.
\]

(A4)

In \( G_4 \) the following substitution is made (Abramowitz and Stegun 1964):

\[
\text{Ci} \left( \frac{\hbar}{m\rho_Dv} \right) \simeq \gamma + \ln \left( \frac{\hbar}{m\rho_Dv} \right).
\]

(A5)

The lower limit is again replaced by zero after using relation (A5). The result is

\[
G_4 = \frac{kT}{m} \left( \frac{3}{2} \gamma + \ln A \right),
\]

(A6)

where \( \gamma \) is Euler's constant. Using equations (A3), (A4), and (A6), we obtain equation (21).

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