Pramāṇa – J. Phys., Vol. 29, No. 5, November 1987, pp. 455–460. © Printed in India.

Effects of Debye shielding in the electron broadening calculations

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MS received 25 November 1986

Abstract. The impact broadening by charged electron gas is calculated. A proper account of the Debye screening has been taken as also the curvilinearity of the perturber's trajectories. The results have been given in the form of graphs for a ready comparison with earlier results.

Keywords. Electron broadening; Debye shielding.

PACS Nos 31·30; 52·90

1. Introduction and formalism

Routine straight-line path approach in the semi-classical impact broadening calculations is equivalent to assuming that perturbers (electrons) move completely independently of each other particle. In the case of charged perturbers this assumption is not proper due to long-range interactions or the resulting correlation effects but mostly due to Debye shielding. At first approximation one may regard plasma as a swarm of statistically independent shielded electrons and ions, i.e. one can assume that these fictitious electrons and ions move along straight-line paths and produce Debye-shielded electric fields (Baranger 1962; Grabowski 1965; Grabowski and Beres 1968; Stamm and Smith 1984). In this approximation the phase shift in the case of the linear Stark effect ($n = 2$) is given by (Grabowski 1965 and Grabowski and Beres 1968):

$$\eta_{2,D}(x) = \pm \frac{\pi C_2}{2vD} f(x) = \eta_2^0 x f(x)/2, \tag{1}$$

where η_2^0 represents the zero-order approximation, ie the ordinary phase shift calculated in simple Coulomb straight-line model;

$$f(x) = \frac{4}{\pi}\int_0^{\pi/2}\left\{\frac{1}{x}\exp\left(-\frac{x}{\cos\varphi}\right) + \frac{1}{\cos\varphi}\exp\left(-\frac{x}{\cos\varphi}\right)\right\}\mathrm{d}\varphi$$

$$= \frac{2}{x} + \lim_{\beta\to\pi/2}\frac{4}{\pi}\sum_{k=0}^{\infty}(-1)^k a_k x^k, \tag{2}$$

$$a_k = \frac{k}{(k+1)!}\int_0^{\beta}\frac{\mathrm{d}\varphi}{\cos^{k+1}\varphi}; \tag{3}$$

$x = \rho/D$ is the impact parameter-to-Debye radius ratio, $f(x)\to 2/x$ when $x\to 0$. (Note: C_2 in (1) relates to C'_2 in (Grabowski 1965; Grabowski and Beres 1968), as $C_2 = 2\pi C'_2$). The impact of the screening effects on the phase shift as compared with the Coulomb calculations increases with x. In particular (Grabowski and Beres 1968)

$$\eta_{2,D}/\eta_2^0 \leqslant 0{\cdot}95 \quad \text{for} \quad x \geqslant 0{\cdot}075,$$
$$\leqslant 0{\cdot}90 \quad \text{for} \quad x \geqslant 0{\cdot}155,$$
$$\leqslant 0{\cdot}75 \quad \text{for} \quad x \geqslant 0{\cdot}420.$$

In the present paper we attempt to consider the screening effects together with the curvilinearity of the perturber trajectory (the so-called trajectory effect) (Dimitrijevic 1984; Grabowski and Dimitrijevic 1986) as a second approximation in the phase shift calculations. In this context the trajectory effect means a back reaction in the field of a net charge induced in the perturbed (macroscopically neutral) particle or in the field of its permanent dipole moment **p**.

However, the above approximation leads to integrals η which, in general, cannot be evaluated in elementary way. This concerns even the simplest case of a perturbed monopole particle. Therefore in further calculations we apply the approximate approach by Vallee *et al* (1976) in which mean perturbation $\bar{U}$ (mean trajectory effect) is evaluated and thereby η calculations are formally reduced to the rectilinear case.

The phase shift induced in a perturbed atom during history of collision is generally given by (cf. (2) in (Grabowski and Dimitrijevic 1986) and assumptions therein)

$$\eta_{n,l}^{\text{curve}}(\rho) = \frac{2}{v}\int_{R_{\max}}^{\infty} \frac{\Delta E_n(R) R\, \mathrm{d}R}{\{R^2[1-p_l(R)]-\rho^2\}^{1/2}}, \tag{4}$$

where $p_l(R) = U_l(R)/E$ is the potential-to-total energy ratio of the colliding pair as a function of the actual distance R; $\Delta E_n(R)$ is the atomic energy (or the line frequency) perturbation; n and l symbolically represent the laws of R-dependence of quantities ΔE and U, respectively.

For the linear Stark effect ($n = 2$) in the presence of Debye shielding the energy shift is expressed by

$$\Delta E_n(R) = \pm C_2\left(\frac{1}{R^2} + \frac{1}{RD}\right)\exp\left(-\frac{R}{D}\right) \tag{5}$$

and the solution of (4) in Vallee's (Vallee *et al* 1976) approximation becomes formally the same as (1),

$$\eta_{2,D}^{\text{curve}}(w) = \eta_2^0 w f(w)/2, \tag{6}$$

where

$$w = x/(1-\bar{p}_l)^{1/2}, \quad \bar{p}_l = \bar{U}_l/E. \tag{7}$$

Now we can numerically take into account the trajectory effect in a system of colliding particles in presence of Debye shielding. We apply the approach of Vallee *et al* (1976) and the function $f(x)$ tabulated in (Grabowski and Beres 1968). (To this end and for further purposes we have extended tabulation of $f(x)$ from $x = 1$ up to 700; cf. § 2.2

below.) The mean potential interaction energy U_l appearing in (7) depends on the type of perturber and should be evaluated for particular cases individually. In the straight-line model we can estimate:

$$\bar{U}_l = \frac{1}{\tau}\int_{-\tau/2}^{+\tau/2} U_l(R)\,\mathrm{d}t \approx \frac{1}{R_0}\int_{\rho}^{\infty} \frac{U_l(R)\,\mathrm{d}R}{[1-(\rho/R)^2]^{1/2}}, \tag{8}$$

where R_0 is maximum size of the interacting system. We assume here that R_0 is equal to the mean intermolecular distance in plasma, $R_0 \approx N_e^{-1/3}$.

In further calculations we consequently assume: (i) the impact parameter ρ is much larger than size of the target, (ii) $\rho \ll R_0$, and (iii) model of Debye shielding is justified.

2. Applications

2.1 *The mean potential interaction energy*

In the model calculations presented in this section we assume that the collisions are relatively strong, so the dipole moment of the radiator tends to align along the symmetry axis of the system.

(a) *The perturbed particle (radiator) has a permanent dipole moment* **p**. A perturber of charge $\pm Q$ moves in the field U_p of this particle, being the following function of the perturber-to-radiator distance R:

$$U_p(R) = -\frac{Qp}{R^2}\left(1+\frac{R}{D}\right)\exp\left(-\frac{R}{D}\right). \tag{9}$$

The mean value $\bar{U}_p$ becomes

$$\bar{U}_p = -\frac{\pi Qp}{4DR_0} f(x) = -\frac{\pi Qp}{2R_0\rho}\,[1+O(x)], \tag{10}$$

accordingly to (4) and (2).

(b) *The perturbed particle macroscopically neutral, with the polarizability* α. A perturber of charge $\pm Q$ induces in the particle the dipole moment $\mathbf{p}_\alpha(R)$ dependent on the distance R. So, the perturber moves in the field $U_\alpha(R)$of the induced dipole:

$$U_\alpha(R) = -\frac{\alpha Q^2}{2R^4}\left(1+\frac{R}{D}\right)^2 \exp\left(-\frac{2R}{D}\right), \tag{11}$$

and the mean value $\bar{U}_\alpha$ becomes

$$\begin{aligned}\bar{U}_\alpha &= -\frac{\alpha Q^2}{2R_0\rho^3}\int_0^{\pi/2} (x+\cos\varphi)^2 \exp\left(-\frac{2x}{\cos\varphi}\right)\mathrm{d}\varphi \\ &= -\frac{\pi\alpha Q^2}{8R_0\rho^3}\left[1-\frac{\xi^3}{4}\left\{\frac{2}{\xi}+\lim_{\beta\to\pi/2}\frac{4}{\pi}\sum_{k=0}^{\infty}(-1)^k b_k \xi^k\right\}\right], \quad \xi = 2x,\end{aligned} \tag{12}$$

$$b_k = \frac{k-1}{(k+1)!(k+3)}\int_0^{\beta}\frac{\mathrm{d}\varphi}{\cos^{k+1}\varphi}. \tag{13}$$

We now refer to the power series appearing in (2). This series, convergent to the sum being a small number as compared with $2/x$, is a majorant (eg at $x=1$) of the series occurring in (12), because always $a_k > b_k$. Therefore, in (12) we have $\{\ \} < f(\xi)$, and finally

$$\bar{U}_\alpha = -\frac{\pi\alpha Q^2}{8R_0\rho^3}\left[1-\frac{\xi^2}{2}+O(\xi^3)\right]. \tag{14}$$

Debye shielding appears mainly in the term $-\xi^2/2$; $O(\xi^3)$ represents small terms of the order ξ^3 and higher.

Result (*b*) is particularly useful in the electron–broadening calculations of lines related to weakly bounded electronic states, and therefore strongly susceptible to the polarizability, e.g. to excited states of hydrogen and hydrogenic atoms.

2.2 *Width and shift of the line.* The result of the numerical integration of the function $f(x)$ equation (2) can be nearly exactly (especially at $x \leqslant 0{\cdot}1$) fitted by the formula

$$f(x) = \frac{2}{x}\exp(-Bx^A). \tag{15}$$

Using the least square method we obtained the values:

$$A = 1{\cdot}0634 \pm 0{\cdot}0080, \quad B = 0{\cdot}7376 \pm 0{\cdot}0023 \tag{16}$$

for the whole interesting range of x $(0 < x \leqslant 100)$.

Now we can express the phase shifts (1) and (6) explicitly and can calculate the width (σ') and shift (σ'') cross sections (Traving 1960; Sobelman *et al* 1981) as follows:

$$\sigma'_{2,D} = 4\pi\int_0^\infty\left[\sin^2\frac{\eta_{2,D}(\rho)}{2}\right]\rho\,\mathrm{d}\rho = \pi\rho_w^2\int_0^\infty\left[\sin^2\frac{1}{t}\exp(-K_1t^A)\right]t\,\mathrm{d}t, \tag{17}$$

$$\sigma''_{2,D} = 2\pi\int_0^\infty[\sin\eta(\rho)]\rho\,\mathrm{d}\rho = 2\pi\rho_w^2\int_0^\infty\left[\sin\frac{1}{t}\exp(-K_2t^A)\right]t\,\mathrm{d}t, \tag{18}$$

where $K_1 = B(\rho_w/2D)^A$, $K_2 = B(\rho_w/D)^A$, ρ_w—the Weisskopf radius in the conventional meaning.

Figures 1 and 2 present the integrands of (17) and (18) in t variable. The numbers at the curves—the Weisskopf-to-Debye radius radio, ρ_w/D. When $D \to \infty$ our results reduce to the routine Coulomb results. As is well-known, in long range Coulomb forces σ' diverges as $\ln\rho_m$ and σ'' diverges as ρ_m, where ρ_m is the upper limit of integration (Traving 1960 and Sobelman *et al* 1981). As opposed to this, in the presence of Debye shielding the quantities $\sigma'_{2,D}$ and $\sigma''_{2,D}$ converge, and artificial cut-off of the integrals is unnecessary.

The integrals (17) and (18) are unwieldy. We calculated them approximately, expanding in the power series the exponential factor on the left of the point 1 on the abscissa axis, and the sine function on the right of that point, and integrating step by step. The results are as follows:

$$\sigma'_{2,D} \approx \pi\rho_w^2 \left\{ \frac{1}{A} E_1(2K_1) - \frac{1}{3A} E_3(4K_1) + 0{\cdot}3857 - 0{\cdot}1077K_1 + 0{\cdot}1754K_1^2 \right\}$$

$$\approx \pi\rho_w^2 \{ -0{\cdot}192 - \ln u + u - u^2/4 + \ldots \}, \tag{19}$$

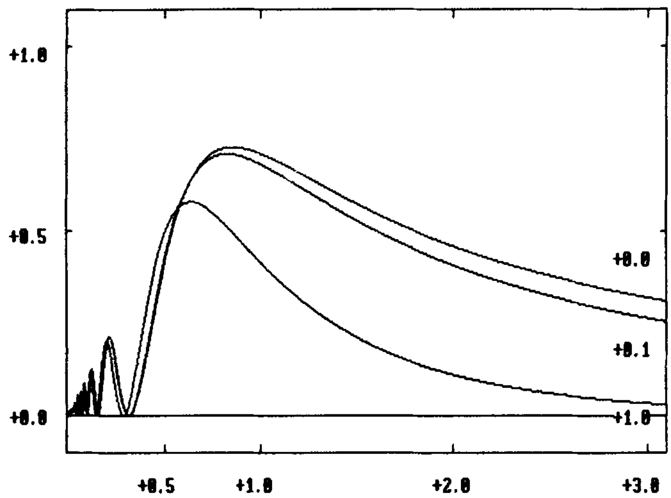

Figure 1. Contribution of impact phase shift to line width. The curves represent the integrand of (17) as a function of a reduced impact parameter t at some values of ρ_w/D ratio as marked from the right.

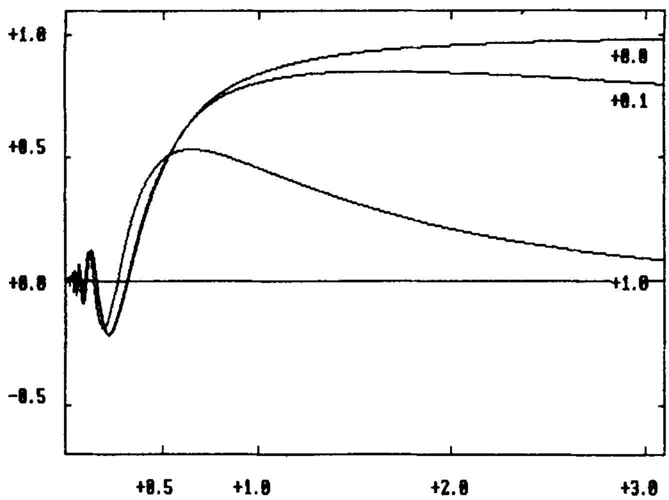

Figure 2. Contribution of impact phase shift to line shift. The curves represent the integrand of (18) at the same convention as in figure 1.

$$\sigma''_{2,D} \approx 2\pi\rho_w^2 \left\{ \frac{1}{A} K_2^{-1/A} \Gamma\left(\frac{1}{A}, K_2\right) - \frac{1}{6A} E_2(K_2) + 0{\cdot}3785 - 0{\cdot}0181 K_2 + 0{\cdot}0270 K_2^2 \right\}$$

$$\approx 2\pi\rho_w^2 \left\{ 0{\cdot}378 + \frac{B^{A-1}}{Au} \exp(-u) - \frac{1}{6A} E_2(3u) \right\}. \tag{20}$$

The formulae in the variable $u = B(\rho_w/D)$ concern the region $u \ll 1$ only.

All results (19) and (20) refer to the phase shift (1) in the rectilinear approximation. These results can easily be transformed to the curvilinear case (equation (6)) when the parameter B is consequently replaced by $B^l = B/(1-\bar{p}_l)^{A/2}$.

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