AN ADIABATIC TREATMENT OF ION DYNAMICS FOR
FORBIDDEN LINE PROFILES

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A correction to the static ion approximation near the center of forbidden lines is proposed. In essence this correction consists of folding the usual static profile into a function $A(\omega)$ which is essentially just the Fourier transform of the normalized ion field autocorrelation: $\langle E_i(t) \cdot E_i(0) \rangle / \langle E_i^2(0) \rangle$. This result should permit a very simple calculation of the turbulent broadening of forbidden lines produced by nonthermal excitation of ion oscillations.

It is well known that the static ion approximation is invalid near the center of forbidden lines [1]. In this paper we propose a particularly simple correction to the static result using an adiabatic approximation to the ion dynamics.

Using the classical path method, the line shape is given by [2]

$$I(\omega) = \pi^{-1} \operatorname{Re} \int_0^\infty \exp(i\omega t) C(t) \, \mathrm{d}t \tag{1}$$

$$C(t) = \sum_{ab} \left\{ \langle \psi_b | d | \psi_a \rangle \cdot \langle \psi_a | T(t) \rho d T^\dagger(t) | \psi_b \rangle \right\}_{\mathrm{Av.}} \tag{2}$$

where $\{ \ldots \}_{\mathrm{Av.}}$ denotes an average over perturber positions and velocities. The time development operator T satisfies the equation

$$i\hbar \frac{t}{\partial t} T(t) = [H_a + V_e(t) + V_i(t)] T(t) \tag{3}$$

where H_a, V_e and V_i are the unperturbed radiator Hamiltonian, the electron-radiator interaction, and the ion-radiator interaction respectively. This operator may be written in the product form

$$T(t) = T_i(t) U_e(t) \tag{4}$$

where

$$i\hbar \frac{t}{\partial t} T_i(t) = [H_a + V_i(t)] T_i(t) \tag{5}$$

$$i\hbar \frac{\partial}{\partial t} U_e(t) = [T_i^\dagger(t) V_e(t) T_i(t)] U_e(t) . \tag{6}$$

The U_e equation can be simplified by using an interaction representation $T_i = \exp(-itH_a/\hbar) U_i$ and ignoring the effect of the ions on the electron dynamics (the ion fields produce only small level shifts [3]); we thus obtain

$$i\hbar \frac{\partial}{\partial t} U_e(t) \approx [\exp(itH_a/\hbar) V_e(t) \exp(-itH_a/\hbar)] U_e(t) . \tag{7}$$

The correlation function in eq. (2) can now be given by

$$C(t) = \sum_{ab} \{\langle \psi_b(t)| \, d \,|\psi_a(t)\rangle \cdot \langle \psi_a(0)| \, U_e(t)\rho d U_e(t) \,|\psi_b(0)\rangle\}_{\text{Av.}} \tag{8}$$

where $\psi_a(t) = T_i(t)\psi_a(0)$, or

$$i\hbar \frac{\partial}{\partial t}\psi_a(t) = [H_a + V_i(t)]\psi_a(t) . \tag{9}$$

This equation may be solved, using the adiabatic approximation [3,4], to yield

$$\psi_a(t) = \exp(-i\eta_a(t))\left[|a\rangle + \sum_{c \neq a} |c\rangle \langle c |V_i(t)| a\rangle / E_{ac} + \ldots\right] \tag{10}$$

$$\hbar\eta_a(t) = \int_0^t ds \left[E_a + \sum_{c \neq a} |\langle c |V_i(s)| a\rangle|^2 / E_{ac}^2 + \ldots\right] \tag{11}$$

where $|a\rangle$, $|b\rangle$, $|c\rangle$, etc. and E_a, E_b, E_c, etc. denote eigenstates and eigenvalues of the unperturbed radiator Hamiltonian H_a and we have used the fact that the diagonal elements $\langle c |V_i| c\rangle$ all vanish.

The adiabatic approximation is valid [4] when $\hbar(dV_i/dt) \ll E_{ac}^2$ which is normally easily satisfied when the forbidden component is well resolved. The problem of m-degeneracy in the adiabatic approach is treated by averaging over m states [3], We thus consider a three-state radiator having an allowed transition $|1\rangle \rightarrow |0\rangle$ and a forbidden transition $|2\rangle \rightarrow |0\rangle$. We assume that the forbidden line is well resolved, $E_{12} \gtrsim \langle 1 |V_i| 2\rangle$, and that quenching transitions are negligible, $E_{10} \gg \langle 1 |V_i| 0\rangle$. $C(t)$ can now be written as the sum of an allowed term $C_a(t)$ and a forbidden term $C_f(t)$,

$$C_f(t) = \langle 0| \, d \,| 1\rangle \cdot \{\exp(-i\eta_{20})\langle 1 |V_i(t)| 2\rangle\langle 2 |V_i(0)| 1\rangle\}_{\text{ion}} \langle 1 |\{U_e(t)\rho d U_e^\dagger(t)\}_{\text{el.}} |0\rangle / E_{21}^2 \tag{12}$$

where the electron and ion averages are denoted by $\{\ldots\}_{\text{el.}}$ and $\{\ldots\}_{\text{ion}}$. In evaluating $C = C_a + C_f$, we have noted that coupling terms of the form $\{V_i e^{-i\eta}\}$ vanish because $V_i = -d \cdot E_i$ is an odd function of the ion field whereas η is even.

The phase difference η_{20} can be written in the form [3] $\omega_{20}t + P_{20}(t)$ where $P_{20}(t) = \int_0^t \Delta\omega_{20}(s)ds$ and $\Delta\omega_{20}(s)$ denotes the difference between the static ion shifts of the levels $|1\rangle$ and $|0\rangle$. Using $\{V_i V_i\} = d \cdot d\{E_i \cdot E_i\}$, eq. (12) becomes

$$C_f(t) = A(t)C_f^{(0)}(t) \tag{13}$$

$$A(t) = \{E_i(t) \cdot E_i(0) \exp[-iP_{20}(t)]\}_{\text{ion}} / \{E_i^2(0) \exp[-it\Delta\omega_{20}(0)]\}_{\text{ion}} \tag{14}$$

$$C_f^{(0)}(t) = \exp(-i\omega_{20}t)\{E_i^2(0) \exp[-it\Delta\omega_{20}(0)]\}_{\text{ion}} \langle 0| \, d \,| 1\rangle \cdot \langle 1 |\{U_e(t)\rho d U_e^\dagger(t)\}_{\text{el.}} |0\rangle / E_{21}^2 . \tag{15}$$

The function $C_f^{(0)}$ is just the result obtained using the static ion approximation. Since the correlation function C_f is given in product form, its Fourier transform will be given by the convolution

$$I_f(\omega) = \int_{-\infty}^{\infty} d\omega' \, A(\omega - \omega')I_f^{(0)}(\omega') \tag{16}$$

where $I_f^{(0)}(\omega)$ is the real part of the transform of $C_f^0(t)$ and $A(\omega)$ is the real part of the transform of $A(t)$. [See eq. (1) noting that $A(t) = A^*(-t)$ and $C_f^{(0)}(t) = C_f^{(0)*}(-t)$.] Notice too that the total forbidden line intensity, obtained by integrating over ω, is just $C_f(0) = C_f^{(0)}(0)$ since $P(0) = 0$; this means that our correction does not change the total intensity.

The correlation function $\{E_i(t) \cdot E_i(0)\}$ falls to zero in a correlation time τ which is the average duration of an ion-radiator collision or something like the reciprocal of the ion plasma frequency. The phases $P(t)$ and $t\Delta\omega(0)$ are usually small during τ; for very large static fields where this is not the case, these phases may be replaced by impact parameter cutoffs (here at small impact parameters) similar in spirit to the ion field cutoff used in electron broadening [5]. In this manner we obtain

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$$A(t) = \langle E_i(t) \cdot E_i(0) \rangle / \langle E_i^2(0) \rangle \qquad (17)$$

where the averages $\langle \ldots \rangle$ contain the appropriate cutoffs. This result should adequately represent the effect of ion dynamics on most resolved forbidden profiles; if eq. (17) is not sufficient for some particular problem, a calculation of the more accurate result in eq. (14) is not difficult.

References

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