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Semiclassical calculations of line broadening in plasmas: Comparison with quantal results

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Abstract

We here report the resolution of (factor of 2) discrepancies in electron broadening of isolated ion lines between semiclassical nonperturbative and fully quantal close-coupling and convergent close-coupling calculations. The major reason for these discrepancies was the neglect of penetration by the semiclassical calculations. This, however, is not an inherent shortcoming of semiclassical calculations and has now been included. As a result the discrepancies between quantal and semiclassical calculations are much smaller. The most serious remaining discrepancy is due to the neglect of back-reaction by semiclassical calculations (which again may be included in principle, though doing so would be much harder). Further tests for hydrogen and H-like lines, for which back-reaction is not an issue, would be interesting.

Keywords: Semiclassical Stark broadening; Quantal Stark broadening

1. Introduction

Electron impact broadening of isolated ion bound–bound transitions has become a issue of great importance in recent years as large scale computational projects [1–4] and extremely elegant and accurate experiments [5] have been undertaken. However, difficulty has occurred as experimental results agree with previous nonperturbative semiclassical (NPSC) calculations, but

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disagree with fully quantum-mechanical (QM) close-coupling calculations [6–8]. The situation, which applies to virtually all lines studied so far [9], was discussed in [7,8,10,11]. Two points of view can be taken: (1) the experiments are incorrect or (2) one of the theories is incorrect. We note that the experiments have now been performed at different facilities and repeated at the same facilities confirming the data. Here, we report the resolution of the discrepancy between the QM and SC methods.

The weakest link of NPSC is the demarcation between what may, and what may not be treated semiclassically. The demarcation occurs at the point where the minimum impact parameter, $\rho_{\min}(v)$, exceeds the de Broglie wavelength, λ_{dB}, as quantal effects will not occur for $\rho \geqslant \rho_{\min}(v)$. Previous comments concerning SC methods were raised on two fronts [7,8]: first, it was suggested, in contrast to all previous references, e.g., [12,13], that the minimum impact parameter must be 2π times λ_{dB} for SC to be valid. This was tested in [14] using the fully quantum-mechanical Coulomb–Bethe method with no indication of a breakdown of SC for $\rho \geqslant \lambda_{\mathrm{dB}}$. At any rate contributions from the low-order partial waves are small for the conditions of the experimental studies. Second, it was suggested that penetrating impacts were incorrectly bound by the NPSC calculations. This turns out to be both true and, by far, the most important factor in resolving the QM–SC discrepancies and essentially renders discussions on the first point academic.

2. Importance of penetration

For NPSC it is essential to determine the "atomic wavefunction extent" (WFE) to estimate at what distance corrections associated with the long-range approximation to the full multipole expansion must be included. Previously, the WFE was estimated to be $n^2 a_0/Z$, [13] with n the principal quantum number, a_0 the Bohr radius and Z the spectroscopic charge number. In cases of interest for Stark broadening (SB) of isolated ion lines it turns out that this estimate can be inaccurate. For example, for the BIII 2s-2p line measured in [5]

$$F(R) = \int_0^R dr r P_{2s}(r) P_{2p}(r), \tag{1}$$

where P_{nl} is the reduced radial WF, one finds that for $R = 4a_0/3$ $F(R)$ is only 43% of its value at $R = \infty$, whereas it should have been ~100% for this cutoff to be applicable. This indicates that penetration *is* an issue, not only at the perihelion, but over a much larger part of the semiclassical hyperbolic trajectory.

Computationally this translates to a factor that corrects the dipole and quadrupole matrix elements between states with principal and orbital quantum numbers (n, l) and (n', l') in the multipole expansion of the interaction. The correction factor, C_λ, arises from the multipole expansion of $1/(|\mathbf{r} - \mathbf{R}(\mathbf{t})|) - 1/R(t)$ and is given by

$$C_\lambda(R; n, l, n', l') = \frac{\int_0^R P_{nl}(r) P_{n'l'}(r) r^\lambda \, \mathrm{d}r}{\int_0^\infty P_{nl}(r) P_{n'l'}(r) r^\lambda \, \mathrm{d}r} + R^{2\lambda+1} \frac{\int_R^\infty \mathrm{d}r P_{nl}(r) P_{n'l'}(r) r^{-(\lambda+1)}}{\int_0^\infty P_{nl}(r) P_{n'l'}(r) r^\lambda \, \mathrm{d}r} \tag{2}$$