Line shape measurement and isolated line width calculations: Quantal versus semiclassical methods

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In a recent paper Griem, Ralchencko, Bray [Phys. Rev. E **56**, 7186 (1998)] perform quantum-mechanical calculations of the line width of the B III $2s$-$2p$ transition and find agreement with previous quantum-mechanical results. The quantum-mechanical widths are a factor ~ 2 smaller than those measured in a recent experiment where the full width at half maximum for the B III $2s$-$2p$ transition was measured in a plasma with a *measured* electron temperature and density of 10 eV and 2×10^{18} cm^{-3}. The quantum-mechanical results also disagree with a nonperturbative semiclassical calculation. We will illustrate that Griem, Ralchencko, and Bray are incorrect in stating that the experimental results are in error and that the semiclassical calculations are inapplicable. [S1063-651X(99)07311-0]

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INTRODUCTION

In the study of the Stark broadening of spectral lines emitted from charged emitters, the role of isolated lines is of great importance. The isolated lines are, by definition, a purer study of the effects of the plasma collisional broadening as the complicating effects of the overlapping line transitions are removed. This provides a great simplification. Moreover, when the spectral line arises from a transition wherein the principle quantum number does not change, the so-called $\Delta n=0$ transitions, the width of the transition is due largely to the electron collisional broadening and the quasistatic contributions are reduced greatly. These two considerations make the study of these isolated transitions a critical test bed of the theoretical and calculational aspects of the collisional broadening. Thus, one has the possibility of studying a case that will potentially expose the problems in the calculations. Indeed, the same problems may exist in cases other than the isolated line case, but the effects may be masked by the ion broadening, overlapping lines, and/or the complexities of the level structure.

For the reasons, the fact that the quantum-mechanical calculations for isolated ion lines have not agreed with experimental data has been of concern [1]. Thus, when in a recent paper by Griem, Ralchencko, and Bray (GRB) [2] it was confirmed by two new independent calculations that the quantal approaches do not agree with a measurement of the width of the B III $2s$-$2p$ transition [3], there is definitely cause for concern. In this comment we will show that GRB are incorrect in claiming both that the semiclassical calculations are inapplicable and that the experimental data are comprised by turbulence.

CALCULATION

Since this is a comment, we will restrict our discussion first to the points made in GRB concerning the semiclassical calculations and second to those concerning the experiments.

To address the criticism of the semiclassical (SC) theory of Stark broadening, we present the most recent development [1], a nonperturbative SC calculation (NPSC), since this removes many of the former deficiencies associated with previous SC calculations, providing a clear picture of the method and its limitations. The NPSC does not include quantal effects, as the name implies, but does include the interactions of the ions and electrons with the charged radiator. The dipolar and quadrupolar terms are calculated rigorously while an absolute bound on the monopole contributions as well as the entire nonsemiclassical (i.e., quantal) contribution is determined. Here the nonsemiclassical contribution includes collisions that penetrate the ion and those with large de Broglie wavelength. Thus, we have a half width calculated by the NPSC, $\Delta_{\rm NPSC}$, that can be parametrized as

$$\Delta_{\rm NPSC}=\Delta_{\rm SC}+\delta_b,$$

where $\Delta_{\rm SC}$ is the contribution to the width due to all interactions that are nonquantal and δ_b is the bound on the contribution to the half width from all other interactions. The NPSC method satisfies unitarity so that there is no need for an additional unitarity-based cutoff, requiring only a cutoff at the point where the interactions become quantal.

Within the context of line broadening in the NPSC, where other processes such as quantal resonances are not included, the only source of error in the width calculation would arise from the choice of the boundary where quantal effects come into play. This boundary is manifested in a velocity-dependent minimum impact parameter cutoff, $\rho_{\rm min}(v)$, given by

$$\rho_{\rm min}=\max\left[\mathcal{A}\frac{n^2a_0}{Z},\mathcal{B}\frac{\hbar}{mv}\right], \tag{1}$$

where n is the principal quantum number, a_0 is the Bohr radius, Z is the spectroscopic charge number, $\hbar$ is Planck's constant, and m is the electron mass. The choice made in the

NPSC calculations are that $\mathcal{A}=\mathcal{B}=1$, which is the value used in all published literature (see, for example, Griem [4]). However, the assertion has been made by GRB that all SC calculations are inapplicable. First, in the NPSC calculations of the B III $2s$-$2p$ [1] the contribution δ_b was estimated to be half the upper bound; this half represents 17% of the total width. Thus, the maximum would be an additional 17%, which would increase the discrepancy between the quantum-mechanical and NPSC full-width-at-half-maximum calculations. On the other hand, this increase in the NPSC maintains the magnitude of the NPSC/experimental deviation at 8%.

Thus, contrary to the comments in GRB, this brief discussion indicates that the problems are *not* due to neglect of the monopole term—included in δ_b, neglect of the ion broadening—included in NPSC, or incorrect treatment of the strong collisions—bounded by δ_b.

The NPSC cannot bound those contributions that are quantum-mechanical in nature; nevertheless, the two possibilities that could cause error in the NPSC would not improve agreement with GRB. The first possibility is that there are substantial quantal effects arising from impact parameters smaller than those defined by Eq. (1). However, the quantal calculations show small contributions from this region and δ_b is consistent with the *relative* size of the contribution found in the quantal calculation. The second possibility is that we have incorrectly chosen the limit $\mathcal{A}$ and/or $\mathcal{B}$ in Eq. (1) and this can be examined by increasing $\rho_{\min}$. For example, if $\mathcal{B}$ is increased to 2π, NPSC results in a width that is still *greater* than the GRB calculation. Moreover, since contributions from $\rho<\rho_{\min}$ can only increase the width, it is clear that the discrepancy would remain large.

Finally, we point out that there is a large body of literature where the SC calculations have been proven to agree with experimental data, but no such literature exists for the quantum-mechanical calculations of line widths. To assume that calculations performed using the quantum-mechanical methods are *a priori* correct—without validation—while the NPSC calculations, which are in agreement with *all* available experimental results [1] are incorrect is not a supportable position.

EXPERIMENT

To justify the correctness of their calculations of the B III $2s$-$2p$ line width, GRB invoke the argument that turbulence from ‘‘high-Reynolds-number flows’’ decays on long time scales. The characteristic times are then estimated from a scale length, which also is the estimate of the eddy size and the velocity difference. The important aspect here is not the details of this analysis, which is dubious when applied to plasma (as opposed to neutral gas flow), but the fact that on several counts this analysis presented in GRB of the experiments does not stand up to scrutiny.

First, in GRB the characteristic length chosen is 1 cm. This eddy size, according to GRB, must be smaller than the Thomson scattering volume for the eddies to contribute to the signal. In fact, this is incorrect, since the scattering volume in the experiment is bounded by 500 μm. Thus, by the arguments in GRB the Thomson signal is indicative of the local temperature and density.

Second, one can show that even if the scattering signal somehow samples the turbulent velocities as assumed in GRB, in addition to the thermal ones, a required 5 eV of Gaussian distribution of turbulence when sampled will *not* reproduce the observed signal, as opposed to the erroneous suppositions of GRB. This is shown in Fig. 1, where we plot an example of an experimental Thomson scattering spectrum along with a fitted theoretical spectrum and a turbulence spectrum following the suppositions of GRB. The theoretical spectrum is calculated using the form factor after Evans [5] for multiple-ion-species plasmas. This form factor was derived from first principles in Ref. [6] and was experimentally verified in Ref. [7]. As can be seen, the theoretical spectrum provides an excellent fit for $T_e=T_i=10$ eV. On the other hand, the turbulence spectrum calculated after GRB and which represents the convolution of a theoretical Thomson scattering spectrum for $T_e=T_i=5$ eV with a Gaussian turbulence spectrum is clearly in disagreement with the observed spectrum. We note that the symmetry of the observed scattering signal militates against non-Gaussian components in the signal, whether turbulent or not. Further, the Thomson scattering spectrum is used in its entirety to infer the ion and electron temperatures, since a fit to the whole scattered spectral profile is employed. Thus, it is the total shape of the ion features that provides the information, not only its width.

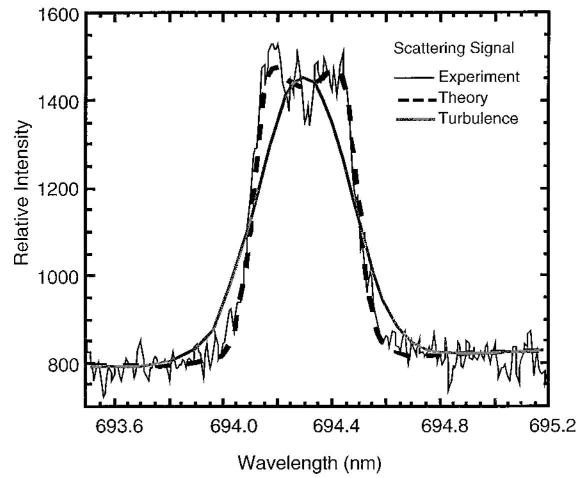

FIG. 1. Comparison of the Thomson scattering signal to theoretical models. Observed Thomson scattering signal (——); theoretical fit due to a 10-eV plasma (- - - -); and, a 5-eV plasma with 5 eV of turbulent eddying (——).

Third, we re-emphasize that the Thomson scattering signal is absolutely calibrated with an intensity error of $\pm 5\%$. The measured Thomson scattering signal, see Fig. 1, is within the expected value of the thermal plasma results. Any turbulence would provide a signal level enhanced by orders of magnitude and this would be easily detectable. For this reason small enhancements of the Thomson scattering signal by turbulence would further increase the discrepancy between the experimentally determined width and the quantal calculations. Thus, turbulence does not play a role in the measured line widths.

Fourth, the fact that it is necessary for GRB to require strong turbulence in order to compromise the B III $2s$-$2p$ results makes it clear that turbulence does not play a role in the width. The fact is that this strong turbulence, where the turbulent energy is on the order of the kinetic energy, would have signatures in the spectral features of the line profiles of other transitions. Since the plasma is collisional and weakly coupled, with coupling parameters of ~ 0.05 for ions and electrons, the ion-ion thermalization time, as well as the inverse ion plasma frequency, are on the order of 10 ps, which indicates that the possibility of long-lived hydrodynamic instabilities, requiring an ion-ion relative drift would be damped on these time scales. It is dubious that hydrodynamic instabilities can be supported in conditions of the gas-liner *Z*-pinch, which is magnetic-field free, collisional, and weakly coupled.

SUMMARY

The assertion in GRB that the semiclassical method of calculation is invalid for the width of the B III $2s$-$2p$ transition is not correct. The NPSC, in particular, provides a robust method by which to calculate arbitrary isolated line widths, since it provides both exact results and a bound on all nonquantal contributions that are otherwise excluded. We emphasize that strong collisions of a fundamentally quantal nature, e.g., recombination, are not bounded by the SC unitarity, since the *S* matrix used does not include these possible channels. However, what we exclude (and bound) are electrons that can have various effects—such as quenching the line by recombining—but no matter what their effect, these either do not contribute to broadening (for example, by quenching) or else contribute additively to the width. That is, the inclusion of the additional effects *cannot* reduce the width.

Next, the assertions in GRB suggesting that turbulence is the reason the experiments are wrong does not stand up to scrutiny. The supporting information from other experiments, the absolute calibration of the Thomson scattering signal, the agreement of the shape of the scattering signal with the theoretical spectrum and the unrealistic possibility of a plasma that would have macroscopic turbulence, which starts at wavelengths of 1 cm as ascertained, would decay to the scale of fluctuations contributing to the Thomson scattering signal, all indicate that the data is sound.

That there is an important discrepancy we have no doubt. That the difficulty is with the experimental data we believe is doubtful. We firmly believe that the first step toward resolving this discrepancy should come from a detailed comparison between the semiclassical and quantum-mechanical methods. One can be certain that there is error in the calculations.

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