Problems with the Standard Semiclassical Impact Line-Broadening Theory

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In this work we study in detail the Ne VII $2s3p$-$2s3s$ singlet line, which was also the object of a recent experiment. The standard perturbative impact theory predictions are tested against a fully nonperturbative semiclassical impact calculation, taking into account dipole and quadrupole interactions. Potentially very significant problems with the standard perturbative theory are encountered and discussed, and a simple remedy is proposed.

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The calculation of plasma-broadened line spectra provides a very useful diagnostic tool and additionally is a necessary ingredient for large-scale computations in astrophysics and plasma physics. A major cornerstone, reducing the many-body problem of line broadening to the computation of one-body quantities, is the impact approximation [1,2]. For practical calculations, the impact theory is usually employed in its perturbative version, and even then simplified formulas are often used.

Isolated lines [2], by being relatively simple and usually unaffected by ion microfield effects, whether static or dynamic [3] are an excellent testing ground for the theories of electron collisional broadening. Such tests require reliable experimental profiles, and much progress has been made in this direction in recent years mainly by the Bochum group [4–10]. These studies have revealed significant discrepancies with simplified expressions that are often used for the electron collisional broadening [2,11–14]. Furthermore, serious discrepancies with close-coupling (CC) calculations [15] were found in [5]. Even more impressive is a recently obtained factor of 2 discrepancy between CC calculations [15] and experiment [10], for a line and parameter range where CC should be at its best. In both cases, much better agreement (roughly by a factor of 2) is obtained by semiclassical (SC) calculations. This means that SC calculations are in fact *the best* available today, in the sense of giving agreement with experiment.

At the foundation of any sophisticated [3,16–20] SC perturbative calculation is the requirement that unitarity is not violated. This is important, of course, since unitarity violation can lead to a serious overestimation of the width [17,21]. Unitarity is preserved for over 30 years by using a criterion, thought to be both necessary and sufficient. This "fact" has gone unchallenged over this period of time. Hence, a minimum impact parameter $\rho_{\min}(v)$ is determined, such that unitarity is satisfied for larger impact parameters, by numerically solving the equation

$$\left| \left\{ \frac{\sum_{a'} \int_{-\infty}^{\infty} V'_{aa'}(t_1)\, dt_1 \int_{-\infty}^{t_1} dt_2\, V'_{a'a}(t_2) + \sum_{b'} \int_{-\infty}^{\infty} V'_{bb'}(t_1)\, dt_1 \int_{-\infty}^{t_1} dt_2\, V'_{b'b}(t_2)}{\hbar^2} \right\} \right| \leq d\,, \tag{1}$$

where $\{\cdots\}$ denotes an angular average, V' denotes the SC [1] emitter-perturber interaction in the interaction picture, a and b denote upper and lower level states, respectively, a' and b' denote a complete set of states that perturb a and b, respectively, and d is a number less than or equal to 1. The condition $d = 1$ is sufficient to preserve unitarity, but to keep the expansion parameter small, frequently $d = 0.5$ is also used [19]. Often, the real part of the left-hand side of Eq. (1) is substituted for the absolute value sign, because the imaginary part is usually much smaller. The test in Eq. (1) is then carried out using the A function [2,3,18] for which analytic expressions have been recently given [22]. Thus, one hopes that perturbation theory is reliable for $\rho \geq \rho_{\min}(v)$ and that this region gives the dominant contribution, so that one may either neglect or estimate very roughly the unknown (within a SC perturbative framework) $\rho \leq \rho_{\min}(v)$ contribution. In this work, we demonstrate by means of a *specific case* that checking unitarity in this manner is not sufficient and the error associated with the breakdown of this test can be substantial.

The main problem of the impact approximation has always been the so-called strong collisions, i.e., the collisions at small impact parameters $\rho \leq \rho_{\min}(v)$. It has been known for a long time that the contribution of such collisions can be bounded, but usually some fraction of this bound is then used as an additive contribution to the width. Whereas for, say, large-scale computations, returning a single value for the width is desirable, for detailed comparisons with experimental results it is best to return an error bar for the contribution of these strong collisions, which cannot be computed reliably. This is the approach adopted here [3]. In other words the theoretical width lies between the weak collision width $[\rho \geq \rho_{\min}(v)]$, which is *presumed* to have been reliably computed by the usual perturbative (PR) treatment, and the sum of the weak

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and strong [$\rho \leq \rho_{\min}(v)$] collision widths. Sometimes these bounds were satisfactory [3], while other times [7] they were rather too large and reducing them would be desirable.

Although one loosely speaks of small impact parameters and/or small velocities as giving rise to strong collisions, it is important to distinguish between collisions that fall into this group because unitarity is violated as the perturbation expansion fails and collisions that fall into this group because the SC approximation is no longer valid. Whereas there is no way within the SC approximation to avoid the latter, the collisions that violate unitarity are still treatable within the SC impact approximation, by means of a nonperturbative (NP) approach. There are essentially two such known NP approaches. The first one is an analytic solution under the approximation of neglecting time-ordering effects, while the second [23] is a fully numerical solution of the Schrödinger equation. To avoid ambiguities, we have chosen the second approach here. Thus, if the $\rho_{\min}(v)$ required to satisfy unitarity is significantly larger than then $\rho_{\min}(v)$ required to preserve the SC approach, as is very often the case [6–10] a NP calculation achieves a *very significant* reduction of the error bars given by the PR calculation.

As a reminder, the half width at half maximum (HWHM) is written as [18]

$$\text{HWHM} = 2\pi n \int \rho\, d\rho \int dv\, v f(v) Q(\rho, v), \quad (2)$$

where n is the electron density, $f(v)$ is the Maxwellian velocity distribution, and Q is given by

$$Q(\rho, v) = \{I - S_a(\rho, v) S_b^{-1}(\rho, v)\}, \quad (3)$$

where the subscripts a and b denote the upper and lower levels, respectively, I is the unit matrix, S is the S matrix, and $\{\cdots\}$ denotes angular average. When one formulates the problem on the collision axes, one finds for isolated lines [18]

$$Q(\rho, v) = (2J_a + 1)^{-1} \sum_{M, m_a, m_a', m_b, m_b'} \langle J_b m_b' 1M \mid J_a m_a' \rangle \langle J_b m_b 1M \mid J_a m_a \rangle \times [\delta_{m_b, m_b'} \delta_{m_a, m_a'} - \langle J_a m_a' \mid S_c(\rho, v) \mid J_a m_a \rangle \langle J_b m_b' \mid S_c(\rho, v) \mid J_b m_b \rangle^*], \quad (4)$$

where the subscript c denotes that the S matrix has been computed for a given direction of the perturber trajectory (collision axes).

For ion lines, the trajectory is parametrized in terms of the "time" variable u, defined by [3,18]

$$t = s(\epsilon \sinh[u] - u)/v, \quad (5)$$

with $s = Z_{em} e^2 / 4\pi\epsilon_0 m v^2$ and with the eccentricity $\epsilon = \sqrt{1 + (\rho/s)^2}$.

All calculations described in this work refer to the singlet $2s3p$-$2s3s$ Ne VII 3643.6 Å line, which has been the subject of a recent experimental study [9]. The combination of available experimental data and the fact that broadening is determined by a small set of three levels makes this line suitable for illustrating the important points. We first give an example of a *pure dipole* calculation. When we calculate $Q(\rho, v)$ for a velocity of 2×10^6 m/sec and an impact parameter of 5 Å ($\epsilon = 1.653$), the PR result is $Q(\rho, v) = 0.051\,08$, and is in good agreement with the NP result of 0.049 97. This is understandable, since $Q(\rho, v)$ is small (= 0.051 08), so the perturbation expansion should be accurate. But when we attempt the same calculation for an impact parameter of 0.68 Å ($\epsilon = 1.0158$), which also has a relatively small expansion parameter of $Q(\rho, v) = 0.16$, the NP result is 0.0868. Figure 1, which shows the real part of $\{I - U_a(u) U_b^{-1}(u)\}$ versus the "time" variable u, illustrates what has happened: If the U matrices remain close to the unit matrix, then the perturbation expansion is certainly valid. This is the case of the solid line, which represents the larger eccentricity. However, we may get a small $Q(\rho, v)$ without this being the case, as is demonstrated by the dashed line, which represents the smaller eccentricity. In other words, it is only for small times (or u) that the U matrices evolve according to perturbation theory in the smaller ϵ case. Consequently, the unitarity criterion is insufficient and the NP result is substantially different from the PR one. We note the flat initial and final regions for both cases in Fig. 1, which show that the U matrix has indeed converged to the S matrix.

Nevertheless, the PR and NP HWHM for a dipole-only interaction turn out to be close: 0.535 vs 0.5094 Å,

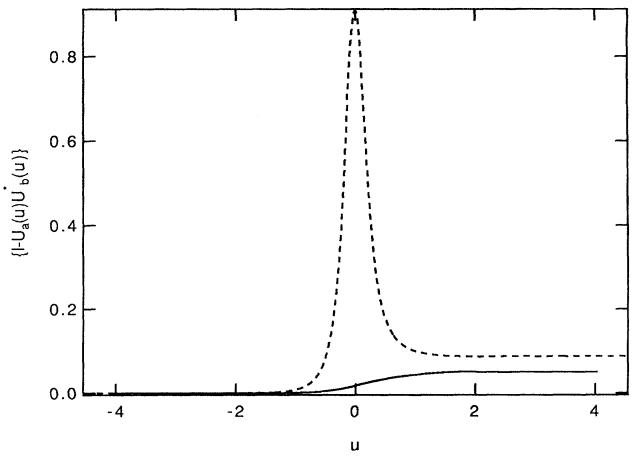

FIG. 1. Real part of $\{I - U_a U_b^{-1}\}$ vs u. The solid and dashed lines correspond to a NP calculation for $v = 2 \times 10^6$ m/sec and $\rho = 5$ and $\rho = 0.68$ Å, respectively.

respectively. The reason for this agreement can be seen in Fig. 2, where the PR (solid line) and NP (dashed line) $Q(\rho, v)$ are shown as a function of ρ for different velocities. Keeping in mind that the average velocity is 2.9×10^6 m/sec, it is clear why the differences between the PR and NP calculations are small: The main contribution comes from weak collisions for which the PR and NP calculations are in good agreement.

Things are different in the quadrupole case where the dominant contribution comes from smaller impact parameters and velocities. In PR calculations, unitarity requires a cutoff at larger impact parameters compared to a pure dipole calculation, with an associated, often very significant, increase in the strong collision error bars. In such calculations including quadrupole impact broadening often [18] only the diagonal channels are included. In [20] this assumption was discussed and a rough criterion was adopted for including the "near hydrogenic" nondiagonal channels. Although tables of the relevant nondiagonal functions exist [24], analytic expressions have not been developed for these functions, unlike the dipole case, and it would be desirable to do so, in order to be able to determine which quadrupole channels should be included in the calculation. We here present concrete examples where the near hydrogenic nondiagonal channels must be included: For the line in question, the only diagonal quadrupole channel is $3p$-$3p$, since $3s$-$3s$ is not allowed. However, the $3s$-$3d$ channel is allowed, and this is often neglected [18]. Figure 3 shows a comparison of pure quadrupole calculations. There are basically two regimes, the perturbative regime and the strong collision regime, at small impact parameters. The first thing to note is that *even* in the PR regime, *it makes* a significant difference whether the $3s$-$3d$ channel is included or not. On the other hand, because perturbation theory is valid, the $3d$-$3d$ channel makes no difference in the results. This changes in the strong collision regime, and the addition of the $3d$-$3d$ channel makes an important difference, resulting in a peak rather than a trough. This result confirms that as we move to smaller ρ, progressively more and more perturbing levels and channels come into play.

Figure 4 is a similar graph, but with the dipole terms included. It should be noted that the strong collision regime shrinks to smaller ρ for a pure dipole interaction or if the velocity is increased. The remarks made about the importance of the "nearly hydrogenic" $3s$-$3d$ channels still hold true.

With regard to the effect on the final line profile, the electron temperature (average velocity) and density (average impact parameter) are very important in determining the relative significance of the strong collision regime. For the neon line considered here [9], the strong collision regime is very important for a dipole plus quadrupole calculation: the PR result is 0.563 Å with an error bar of 0.477 Å, as opposed to error bars of about 0.13 Å for the NP results, for which the calculations involving the (a) $3p$-$3p$, (b) $3p$-$3p$ and $3s$-$3d$, and (c) all $3p$-$3p$, $3s$-$3d$, and $3d$-$3d$ quadrupole channels yield HWHMs of 0.85, 0.977, and 0.975 Å, respectively. (The experimental result is [9] 0.865 Å). It is noteworthy that the $3s$-$3d$ channel accounts for about 15% of the *total* (i.e., including the dipole interaction) electronic width, whereas the $3d$-$3d$ channel results in a

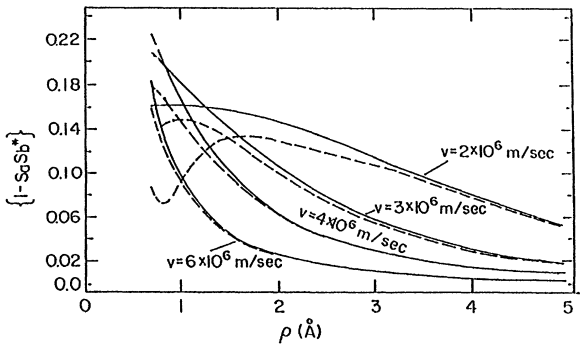

FIG. 2. $Q(\rho, v)$ vs ρ for different velocities v. The solid and dashed lines represent, respectively, PR and NP dipole calculations.

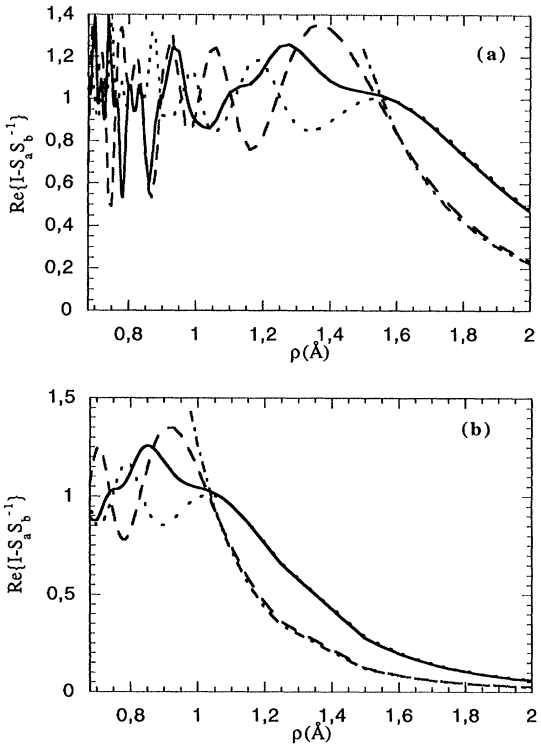

FIG. 3. $Q(\rho, v)$ vs ρ for a pure quadrupole interaction. (a) $v = 2 \times 10^6$ m/sec, (b) $v = 3 \times 10^6$ m/sec. The solid, dotted, and dashed lines correspond, respectively, to NP calculations including all, all except the $3d$-$3d$, and only the $3p$-$3p$ channels, respectively. The dash-dotted line corresponds to a PR calculation including only the $3p$-$3p$ channel.

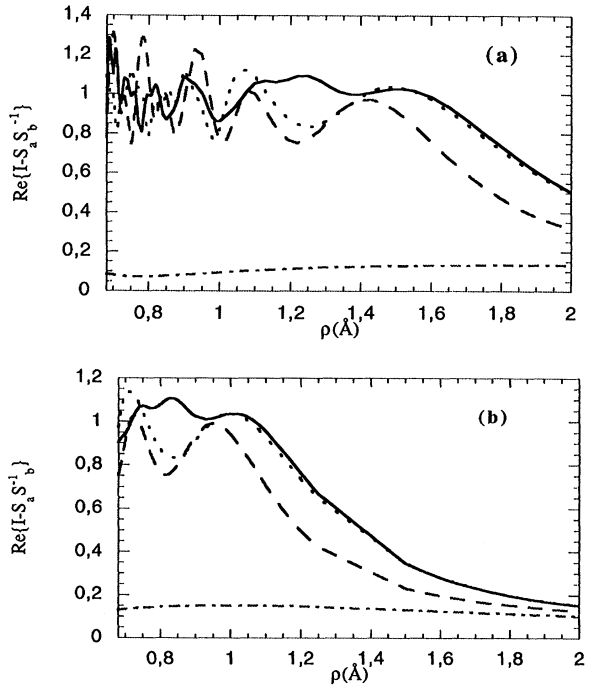

FIG. 4. $Q(\rho, v)$ vs ρ for dipole and quadrupole interactions. (a) $v = 2 \times 10^6$ m/sec, (b) $v = 3 \times 10^6$ m/sec. The solid, dotted, and dashed lines correspond, respectively, to NP calculations including all dipole channels and, respectively, all, the $3p$-$3p$ and $3s$-$3d$, and the $3p$-$3p$ only quadrupole channels. The dash-dotted line is a pure dipole NP calculation.

decrease of the *total* electronic width by less than 0.5%. These results thus demonstrate the need for analytical approximations of the relevant nonhydrogenic quadrupole broadening functions [24], which should then be included in existing codes. These results (with their error bars) are absolutely rigorous (within the number of states used), if one trusts the "demarcation line" between what may and what may not be treated semiclassically, and for which the convention in [3] was adopted. It is then interesting that even for this case, where relatively low partial waves are involved, i.e., under conditions not most favorable for SC, good agreement is obtained. Furthermore, the effects described here were *responsible for* the seemingly excess broadening observed in Ne VIII [5] for which NP calculations give an electron FWHM contribution between 0.9 and 0.13 Å, with the latter number corresponding to the (unlikely) maximum possible contribution from nonsemiclassical collisions, compared with an experimental result of 1.2 ± 0.1 Å at the highest density considered.

In summary, we have demonstrated that the standard practice of even the most sophisticated current perturbative impact theory calculations cannot enforce unitarity reliably and that a more reliable verification of the unitarity is essential. Such a procedure would involve additional information and could be implemented by evaluating, at intermediate times, the function $\{I - U_a U_b^{-1}\}$ to ensure that it is monotonic. One possible implementation of this could involve using an upper limit of the t_1 integrations of 0 rather than ∞ in Eq. (1); this check would allow the diagnosis of the situation shown by the dashed line in Fig. 1. Even without any additional checks, it is still much better to check than not to, since for large impact parameters, the unitarity check *is* reliable.

Further, it has also been demonstrated that to the extent that quadrupole interactions are important, it is not always sufficient to include only the diagonal quadrupole channels. An analytic solution to the problem of strong collisions is the subject of current research.

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