High Energy Density Physics 6 (2010) 9–14

Contents lists available at ScienceDirect

High Energy Density Physics

journal homepage: www.elsevier.com/locate/hedp

Review

Plasma line broadening and computer simulations: A mini-review

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ARTICLE INFO

Article history:
Received 2 July 2009
Accepted 2 July 2009
Available online 9 July 2009

Keywords:
Spectral line broadening
Stark effect
Computer simulations
Molecular dynamics

PACS:
32.70.-n
31.15.xv
52.70.-m
01.65.+g

ABSTRACT

Over the fifty years that have passed since its foundation, the modern theory of spectral line broadening in plasmas has made great strides in explaining countless phenomena. The theory has been in constant development and, increasingly, the computer simulation methods have played an important and unique role in this process. In this short Review we outline this development, describe the current status, and discuss the future of computer simulations for plasma line broadening.

It is nice to know that the computer understands the problem. But I would like to understand it, too.
E. Wigner.

1. Introduction

1.1. Outlook

The foundation of the modern theory of spectral line broadening in plasmas, based on contributions of several scientists, had been laid out by the 1960s [1]. For over a decade, there appeared a large number of successful applications of the theory to various experiments [2]. With a large number of applications in many areas of plasma physics, applied to plasmas with particle density ranging from several atoms per cubic centimeter to that of solid state and temperature from close to absolute zero to billions kelvin, the theory of line broadening has been in perpetual development and remains at the heart of plasma spectroscopy [3].

The 1960s were also the years of a rapid progress in development of computers. It was then that Moore's law – the prediction of exponential growth of the computational power with time – was foreseen [4] for the next decade and, somewhat surprisingly, still holds true [5]. It is only natural, then, that one clear trend in the development and applications of line-broadening calculations is a significant increase in the computational results, in particular, using computer simulations [6]. Evidently, this is not specific to the subject of line broadening, as other fields of science in general show clear signs of intrusion of computers in what used to be a sovereign patrimony of theoreticians (e.g., see [7]).

1.2. The "standard theory"

We recall, see the more detailed overview [8] in this issue, that the line shape is given by

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

where $C(t)$ is the autocorrelation function of the light amplitude, which in the dipole approximation and neglecting stimulated emission can be expressed (up to a numerical factor) as

$$C(t) = \mathrm{Tr}\langle \vec{d}\,(0)\,\vec{d}\,(t)\rho(0)\rangle. \tag{2}$$

Here, $\vec{d}$ is the dipole momentum of the radiator, ρ is the statistical or density operator, and the trace (Tr) is taken over both the initial and final states of the transition. The problem, thus, is reduced to (*i*) finding time evolution of $\vec{d}$ and (*ii*) averaging its autocorrelation

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doi:10.1016/j.hedp.2009.07.001

function over a statistically-representative ensemble of the plasma particles. In Eq. (2), this average is denoted by the angle brackets $\langle\rangle$.

Evidently, the problem in its general form cannot be treated analytically. In order to make it solvable, several fundamental assumptions and approximations are used. First, the density operator of the perturbers ρ_p and that of the radiator ρ_r are assumed to be independent. Second, it is usually assumed that the kinetic motion of the radiator as a whole, which is responsible for the Doppler broadening, and the evolution of its bound electron(s), which gives rise to the Stark broadening, are not correlated, i.e., the internal (electronic) and external (translational) degrees of freedom of the radiator are not coupled. Thus, the total density operator can be factorized:

$$\rho = \rho_p \otimes \rho_r^{(\mathrm{ext})} \otimes \rho_r^{(\mathrm{int})}, \tag{3}$$

where $\otimes$ denotes a tensor product. Third, the effects of the plasma environment on the radiator are split into two parts characterized by two radically different frequency regions: the slow ions and fast electrons. Indeed, the typical frequency of the electric field due to a perturber species p with a thermal velocity v_p and a particle density n_p is

$$\nu_p \sim v_p n_p^{1/3}, \tag{4}$$

thus, the perturbation due to electrons is (assuming equal temperatures and plasma quasi-neutrality)

$$\frac{\nu_e}{\nu_i} \sim \left(\frac{m_i}{m_e}\right)^{1/2} Z_i^{1/3} \tag{5}$$

times faster than that of ions with mass m_i and charge Z_i. This large factor, two orders of magnitude or more, allows the averaging in Eq. (2) to be performed in two stages, first over the electrons and then over the ions:

$$\langle\ldots\rangle = \big\langle\langle\ldots\rangle_{\mathrm{electrons}}\big\rangle_{\mathrm{ions}}. \tag{6}$$

While evaluating the inner average in Eq. (6), over electrons, the ions are assumed to be essentially stationary, collectively producing a slowly varying electric field F_i that results in a static shift $w(F_i)$. The electrons are assumed to perturb the radiator by means of "collisions", treated in the impact approximation. These collisions cause a change of the radiator state, thus interrupting the spontaneous radiation, or alter the energy levels of the radiator, which results in a phase shift. The net effect of these processes is a shifted Lorentzian shape conveniently expressed using the impact operator ϕ:

$$\langle\ldots\rangle_{\mathrm{electrons}} \to \frac{1}{\omega - w(F_i) - i\phi(F_i)}. \tag{7}$$

The real and imaginary parts of ϕ have, respectively, the meaning of the half-width and shift of the Lorentzian.[1] On the other hand, the outer average in Eq. (6), over ions, is performed as a mere averaging over all possible fields corresponding to the different ion configurations near the perturbed atom or ion, which is called the quasi-static approximation:

$$\langle\ldots\rangle_{\mathrm{ions}} \to \int_0^\infty \mathrm{d}F_i W(F_i)(\ldots), \tag{8}$$

where $W(F_i)$ is the ion microfield distribution function.[2] Finally, we obtain

$$L(\omega) = -\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\int_0^\infty \mathrm{d}F_i \frac{W(F_i)|\vec{d}|^2\rho_r^{(\mathrm{int})}}{\omega - w(F_i) - i\phi(F_i)}. \tag{9}$$

The above expression, and the set of assumptions in Eqs. (3), (6)–(8) that led to its derivation, often collectively referred to in the contemporary line-broadening literature as the "standard theory" (ST). It should also be noted that in all calculations of the microfield distribution $W(F)$ and almost all calculations of the impact operator ϕ, classical motion of, respectively, the ions and the electrons is assumed. Because of the mixture of classical treatment of the perturbers and the quantum approach to evolution of the radiator, such calculations are called "semiclassical".

1.3. Computer simulations

Computers have been used in science since their invention. The main use of a computer, however, was at first like that of an arithmometer – a very powerful one, but still an instrument for solving more or less straightforward numerical problems, like those that in principle could be solved, albeit in a very laborious way, by a human. The line-broadening theory is not an exception. For example, soon after the formulation of the ST, a computer code was developed [9] employing the ideas of the ST; other implementations (e.g., [10,11]) followed. The focus of the present review, however, is not computer calculations in general, but a very specific subset called "computer simulation" (CS) methods.

Computer simulation is the discipline of designing an abstract model of an actual physical system, executing the model on a computer, and analyzing the execution output. The scale of models being simulated by computer simulations today far exceeds anything possible (or perhaps even imaginable) using traditional paper-and-pencil mathematical modeling. Often it is practically impossible to trace an entire execution of CS; for this reason, the results obtained using a CS are, in a sense, considered as results of an experiment. In fact, there is a certain controversy as to whether a CS approach to a given problem should be considered a theoretical or experimental one [12]. Indeed, the simulation results are *used* like experiments in some studies, e.g., to test theories, and, like experimental results, are prone to problems of reproducibility and statistical errors. On the other hand, no measurements are done on real systems using a CS, because what is investigated in computer simulations are *models*. Thus, in order to write reasonable simulation code one needs to have sound ideas about the underlying nature of the physical processes and, like in theoretical studies, to make hard choices about including only the most relevant physical phenomena and neglecting the rest. However, by leveraging the computational power, it can be afforded to employ models at a more fundamental level, i.e., one may need fewer approximations. For example, as discussed in the next Section, the use of the CS methods (CSMs) in line-shape calculations began with simulating the motion of ions, thus removing the quasi-static approximation (8), that was then followed by progressively removing most of the other ST approximations assumed in arriving at Eq. (9).

Therefore, with properly chosen models, computer simulations play a very important role as "ideal" experiments, ones that allow us to "switch off" certain effects and examine others, thus providing a unique insight into how different, but similar – at least

[1] Note that w and ϕ are operators in the Hilbert space of the radiator.

[2] In realistic calculations of $W(F_i)$ the ions are replaced by Debye quasiparticles, thus, the ion-electron interactions are phenomenologically accounted for.

– in appearance, effects interfere. For example, one can study the correlation between the Stark and Doppler broadenings, which can be difficult to distinguish experimentally by line-shape measurements. Also, some quantities that are not directly observable in experiments yet have a profound theoretical meaning (e.g., various microscopic correlation functions) can only be extracted using CS.

2. Milestones

First attempts to incorporate ion motion into theoretical models (i.e., eliminating the quasi-static approximation expressed by Eq. (8)) were made in late 1960s to early 1970s [13–16]. Concomitant with the development of these models experimental techniques improved and there began accumulating experimental data of Stark broadening of hydrogen and hydrogen-like transitions that showed significant disagreements with the "mainstream" theoretical calculations. Kelleher and Wiese [17] studied the shape of the Balmer β line of hydrogen and deuterium and showed that the dip in the center of the spectral line is significantly "shallower" than predicted. By varying the plasma composition, it was unambiguously shown that the effect depends on the reduced mass of the radiator and the perturbing ion species $\mu = \mu_r\mu_p/(\mu_r + \mu_p)$; furthermore, an extrapolation of the experimental results to $\mu = \infty$ matched the theoretical results fairly well. These and similar results [18] clearly indicated that it was an effect of ion motion that was missing in the standard theory; measurements of first members of the Lyman series by Grutzmacher and Wende [19,20] showed further significant disagreements.

Dubbed as "ion dynamics",[3] the phenomenon inspired the use of the *N*-body molecular-dynamic (MD) simulations in line-shape calculations. Since the pioneering work of Stamm and Voslamber [21], such calculations are made based on the scheme given in Fig. 1. The calculations are split into two largely independent computational pieces. The first one is the MD simulation that models the motion of plasma particles. Clearly, the volume of the plasma simulated should be large enough to encompass a few Debye radii in each dimension, thus, a typical number of the particles included is of the order of $10^2 - 10^3$. The fields produced at the radiators, as a result of the essentially chaotic motion of the plasma particles modeled, are stored as a function of time for a subsequent use in the second computational piece. The latter piece treats these "field histories" as a time-dependent perturbating potential, $V(t)$, while solving the Schrödinger equation for a radiating atom or ion:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}U(t) = [H_0, U(t)] + V(t)U(t), \tag{10}$$

where H_0 is the unperturbed Hamiltonian and $U(t)$ is the time-development operator, or, in the interaction representation,

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\overline{U}(t) = \overline{V}(t)\overline{U}(t). \tag{11}$$

As a result, the time evolution of the dipole operator $\vec{d}(t)$ is obtained:

$$\vec{d}(t) = U(t)^\dagger \vec{d}(0)U(t), \tag{12}$$

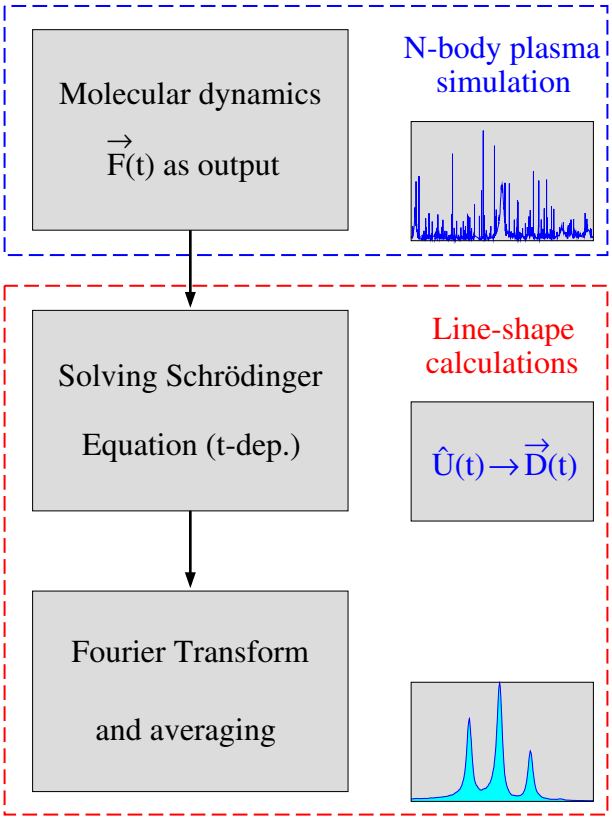

Fig. 1. Schematic diagram of CS line-shape calculations.

that, in turn, is further used to calculate the line-shape in the dipole approximation (Eqs. (2) and (1)).[4] The entire procedure is repeated many times in order to average over a statistically-representative ensemble. This directly corresponds to the averaging $\langle\ \rangle$ in Eq. (2). Finally, any broadening effects not accounted for in a specific model, e.g., Doppler broadening, are calculated at a post-processing stage, which is not shown in Fig. 1.

From the basic properties of the Fourier transform it is evident that the simulation time of a single run, t_r, should be sufficiently long to provide the required accuracy $\delta\omega$ for the line shapes, i.e., $t_r \gtrsim 2\pi/\delta\omega$.[5] The total simulation time t should be long enough to collect representative statistics of the field histories, i.e., it should be a few orders of magnitude larger than it takes the slowest particles (usually ions) to cross the inter-particle distance: $t \gg \nu_i^{-1}$, see Eq. (4). The number of runs contained in the average should be $N_r \equiv t/t_r \gg \delta\omega/(2\pi\nu_i)$, commonly reaching values of the order of 10^3 for calculations aimed at a few-percent accuracy. In practice, it is often more efficient to let the MD simulations run for the entire time t and then split the resulting field history into N_r parts than to make many short runs of duration t_r.[6] Thus, the statistical ensemble

[3] The term is somewhat ambiguous; indeed, for sufficiently fast ions, their effect can adequately be described within the framework of the ST, namely, using the impact approximation. What is meant by "ion dynamical" effects are, in fact, intermediate cases when neither the quasi-static nor the impact approximation is applicable to the Stark broadening effect of ions. Similar intermediate regimes of *electron* broadening can be realized in dense and/or cold plasmas, or when considering Rydberg transitions.

[4] Extension to the magnetic dipole and higher orders of the multipole expansion should be straightforward, although no such studies, to the best of our knowledge, have been published.

[5] This is a rather challenging requirement, since the relative accuracy $\delta\omega/w$ depends on the final line width w that is not known in advance.

[6] The reason is that, especially for moderately- or strongly-coupled plasmas, some time is required for the simulated plasma to equilibrate, i.e., to relax – both in configuration and momentum space – from the arbitrarily assigned initial conditions. Clearly, the field histories during the equilibration time are unusable for the line-shape calculations; therefore, the time needed for equilibration can represent a significant overhead if the MD simulations are repeated many (N_r) times.

averaging is replaced with the time averaging, justified by the ergodic hypothesis. We note that the resulting line shape is "noisy", with the "noise" diminishing as the number of runs grows. Consequently, the parameters that define a line shape, such as the full width at half maximum (FWHM), will gradually converge to a certain value in the course of the calculations. The convergence process has an inherently random character, thus substantiating the similarity between CSMs and experiments as mentioned in the previous section. This also makes the estimation of the accuracy of the obtained values a non-trivial task.

In spite of the common general structure shown in Fig. 1 for all line-shape computer simulations, the details of different approaches vary widely. First, only the motion of ions was simulated [21], while the effect of electrons was still considered in the impact approximation; thus, the electron broadening was accounted for by convolving the CS-modeled line shapes with a respective Lorentzian at the post-processing stage. Furthermore, the ions were assumed non-interacting, moving along straight-path trajectories (the screening effects were accounted for by using, instead of the Coulomb potential, the Debye potential when calculating the field histories). Evidently, using straight-path trajectories is applicable to cases of neutral radiators or, in general, when the neglect of any correlations between the motion of perturbers and radiators is justified. The next important development, by Stamm et al. [22], was taking into account interactions between the ions and between the ions and the (charged) radiators. In addition to extending the applicability range to strongly-coupled plasmas, where evidently the straight-path-trajectory approximation breaks down, the inclusion of the radiators in the MD calculations allowed for investigating "in situ" correlations between the Stark and the Doppler effects. We note that this corresponds to dropping the approximation of independent ρ_p and $\rho_r^{(ext)}$ in Eq. (3).

Strictly speaking, only this type of MD modeling can be called a true N-body simulation. Here we refer to it as the full MD (FMD) approach, and the CS using non-interacting quasiparticles as the trivial MD (TMD) one. Since in an FMD implementation, at each time step, forces between all pairs of the particles need to be evaluated, the required computational resources scale as $\sim N^2$, where N is the number of particles simulated.[7] This is in a striking contrast to a TMD scheme, for which the processing time scales as N.

In the studies we have reviewed so far, the electrons were treated in the impact approximation, i.e., outside of the MD modeling, because of the difficulty in including the electrons in the same framework of simulation as the ions. The reason arises from the radically different time scales of the field variations (see Eq. (5)). As a result, carrying out simulations of both electrons and ions is about two orders of magnitude more expensive computationally. This large factor is especially prohibitive in the case of FMD simulations. Hence, quite expectedly, the first CS-based line-shape calculations with both electrons and ions, performed by Gigosos and Cardeñoso [25] and Hegerfeldt and Kesting [26], utilized a variant of TMD.

In addition to being the first joint simulations, i.e., having both electrons and ions, these studies included other noteworthy developments. In Ref. [25] the evolution operator was obtained based on a special technique [27] which is very simple and advantageous for numerical calculations. It is based on the $SO(4)$ symmetry of the hydrogen states (and, therefore, may only be applied to the hydrogen-like radiators when the fine structure, as well as the coupling between states with different quantum numbers can be neglected). Also worth noting is that the method allows for a straightforward generalization [28] to account for the magnetic field.[8] The authors of Ref. [26] used a collision-time simulation technique, avoiding re-injection of the plasma particles. During the course of a plasma CS, at each time step part of the particles cross the boundary of the simulation volume and have to be re-injected back in order to preserve the particle density. The simplest approach, using the mirror walls, is inapplicable for simulating non-interactive (quasi)particles of TMD, since it results in periodic trajectories and, therefore, artifacts in the calculated line shapes. Instead of using more complex re-injection techniques, in the collision-time method [26] the simulation volume and, hence, the number of particles, are chosen large enough so that the loss of the particles during a time typical for the dipole autocorrelation function has a negligible effect. However, in order to reduce the computational time, in the calculation of the perturbation field only particles sufficiently close to the center of the volume are accounted for.

It took another decade and a half until the joint FMD simulations became feasible. Used first for investigating correlation effects in many-component plasmas [30–32], these types of simulation were soon applied to realistic line-shape calculations in the studies of Ferri et al. [33] and Stambulchik et al. [34]. At the same time, calculational approaches assuming a generic, non hydrogen-like form of radiator Hamiltonian were implemented by Gigosos et al. [35] and Stambulchik and Maron [29].

3. Current status and prospects for future studies

After three decades of development, computer simulation methods in line-shape calculations have matured to become an important asset in the spectroscopist's toolbox. Evidently, there has also been significant progress [3] in the theoretical understanding of many complex phenomena that fall outside the basic ST assumptions. Nevertheless, in several cases accurate and detailed calculations are yet impossible without CSMs. As examples we note that CSM results are widely used as plasma diagnostic tables [36], sought as a definite arbitrator in comparing competing theories [37,38], applied in situations when the Stark line shapes are significantly altered by either the fine-structure effects [29] or magnetic field [39,40], employed for studying effects of correlations in plasma-particle motion on line shapes [33,34,41], and used for the analysis of line-shape asymmetries [42,43]; this list is far from being exhaustive.

An observant reader may have noticed that, in the vast majority of the CSM studies, hydrogen or hydrogen-like radiators were considered. One reason for this is historical: the very birth of the line-shape CS methods was urged by observing the ion dynamical effects on line shapes of hydrogen[-like] species. There is also a technical reason favoring radiative transitions in hydrogen-like radiators: these atomic systems are characterized by a near degeneracy of the dipole-connected atomic states and, as a result, the Stark effect is linear and the line broadening is strong. On the other hand, radiative transitions between non-degenerate states are characterized by quadratic Stark effect and, hence, the broadening is relatively small. However, in order to obtain an accurate line-shape one needs to run the calculations for a time well exceeding the inverse line width: $t_r \gg w^{-1}$. On the other hand, the time step of the calculations should be much smaller than the inverse typical frequency of the field variation (4) due to the

[7] There are numerical algorithms allowing for reducing the computational complexity of the N-body calculations from the "brute-force" $\mathcal{O}(N^2)$ to lower powers of N, down to $\mathcal{O}(N)$ [23]. However, these advanced algorithms become efficient for particle numbers exceeding $\sim 10^4 - 10^5$ [24], whereas the needs of the line-shape modeling are usually satisfied with significantly lower $N(\sim 10^2 - 10^3)$.

[8] Contrary to an erroneous remark in [29].

lightest perturbers, i.e., electrons: $\Delta t \ll \nu_e^{-1}$. Therefore, for a given plasma density and temperature, the number of time steps the calculations should be carried over is much larger for a narrow isolated line, and may reach hundreds of thousands or even more per single run of which there need to be many to provide a time average that is equivalent to the statistical average in Eq. (2). Beyond the corresponding growth of the computational resources required [35], this also poses problems of keeping the accumulated numerical error, which also scales up with the number of steps, within reasonable bounds.

There are, however, more fundamental problems. Presently, the CSM line-shape calculations are semiclassical, that is: (*i*) the perturbers are assumed to move along classical trajectories and (*ii*) there is no connection between the evolution of the internal degrees of freedom of the radiator and that of the "bath" of perturbers (cf. Eq. (3)). While justified for ions, applying these assumptions to electrons is, in general, questionable. Indeed, let us consider a hypothetical three-level radiator with the ground state $|0\rangle$ and two excited states $|1\rangle$ and $|2\rangle$ that give rise to $|1\rangle \to |0\rangle$ and $|2\rangle \to |0\rangle$ radiative transitions, respectively. We further assume, for simplicity, that only the interaction between $|1\rangle$ and $|2\rangle$ is essential for the Stark broadening of both spectral lines. When immersed in a thermal bath with the temperature T, the populations of the excited states, i.e., the diagonal elements of the density matrix of the radiator should satisfy the statistical ratio $\langle\rho_{22}^{(\mathrm{int})}\rangle/\langle\rho_{11}^{(\mathrm{int})}\rangle = \exp(-\Delta E_{12}/kT)$, where ΔE_{12} is the energy separation between the two excited states, k is the Boltzmann constant, and averaging $\langle\,\rangle$ is done over a sufficiently long time to smooth out fluctuations. However, if calculated within a CSM approach, the ratio would be exactly unity. This result can easily be understood if one considers a physical problem corresponding to the employed model in which the motion of the perturbers is unaffected by the internal state of the radiator. This would be the case for very massive (literally, infinitely heavy) perturbers, moving with the velocities of the real plasma particles – so that the time evolution of the *field* they form is kept the same.[9] Clearly, this corresponds to $T = \infty$ of the particles in the bath and, thus, the Boltzmann factor of unity.

The consequences of the failure to reproduce the correct Boltzmann populations are more serious than the mere fact of wrong relative line intensities, which are trivial to correct unless there is a significant overlap of their shapes. Indeed, from the detailed balance principle it follows that the excitation $|1\rangle \to |2\rangle$ and de-excitation $|2\rangle \to |1\rangle$ rates should be different, as determined by the same $\exp(-\Delta E_{12}/kT)$ factor. On the other hand, these rates correspond to the inelastic part of the Stark broadening [44], which typically constitutes a major part of the total Stark width of isolated lines (e.g., [45]). Thus, the Stark broadening calculated within the CSM approach as it exists today is prone to uncertainties of the order of $|1 - \exp(-\Delta E_{12}/kT)|$.[10] Evidently, also certain non-equilibrium effects [46] cannot be reproduced. For the errors to be small one requires $\Delta E_{12}/kT \ll 1$. This is easily satisfied for degenerate systems (as far as electrons are considered, the static Stark splitting due to a typical ion field can be substituted for ΔE_{12}), however, in the case of isolated lines kT can be comparable to ΔE_{12} or even be smaller.

Low-temperature cases are also problematic since the exchange term in the excitation amplitude due to a near-threshold electron can be significant. This problem arises as pure quantum exchange phenomenon cannot be reproduced when electrons are simulated by a classical MD. Further difficulties arise for low-temperature cases particularly for transitions between levels with low principal quantum number when the contribution of electron collisions with very low impact parameters, which are comparable to the dipole matrix element of the transition, contribute significantly. Therefore, in these cases penetrating collisions need to be accounted for [47].

To summarize: the treatment of the electron perturbers beyond the classical picture *and* allowing for "back-reaction" from the radiator to the perturber are needed in order to extend the applicability domain of line-shape CSM calculations beyond spectral lines of hydrogen-like radiators while preserving high accuracy. Including the "back-reaction" effects implies that the principal scheme of the CSM calculations (Fig. 1) should undergo an essential upgrade: the MD simulations and the Schrödinger solver will no longer be independent computational pieces but, instead, run in parallel allowing for a bidirectional interaction between them. We note that going beyond the fundamental approximation of independent ρ_p and $\rho_r^{(\mathrm{int})}$ would have benefit beyond the calculations of Stark broadening of isolated lines. For example, correlation effects between the internal state of the radiator and the distribution function of perturbers are believed to contribute to the shift of hydrogen-like lines [48,49]. Finally, resonance broadening [3, Chap.4.8], which is often important for neutral species in dense but weakly ionized plasmas, is another candidate for modeling within this approach.

4. Conclusions

The theory of spectral line broadening has a large number of applications in many areas of plasma physics. The theory has been in perpetual development, resulting in deepening our understanding of plasma physics, extending the applicability limits, discovering new challenges, and sparking enlightening discussions. The computer simulation methods have played an increasingly important role in this development. Presently, line shapes of hydrogen-like species are treated very well by the computer simulation methods, however, the suitability to the modeling of isolated lines is less satisfactory. Including in the calculations quantum-level interactions between the radiator and perturbers is considered a future direction in the development of the simulation methods.

Acknowledgments

We are indebted to S. Alexiou, A. Calisti, J.W. Dufty, D. Fisher, M.A. Gigosos, M.Á. González, H.R. Griem, P.C. Kepple, Yu. Ralchenko, R. Stamm, and J. Wrighton for reading the manuscript and providing critical comments.

This work was supported in part by the Minerva Foundation (Germany) and Sandia National Laboratories (USA). Y.M. is the incumbent of the Stephen and Mary Meadow Professorial Chair.

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