Computer simulation technique for plasmas

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A computer simulation based on statistically independent, noninteracting, shielded ions is developed. This simulation procedure differs from the usual molecular-dynamics approach in several respects and, for some problems, provides less-time-consuming and more-accurate results. Simulation results are compared with analytically known plasma functions and the basic limitations of the method are discussed.

I. INTRODUCTION

In recent years, experiments[1-3] have shown that the dynamic properties of ions can have an important influence on the spectral line profile of atomic radiation emitted from plasmas. Previous theories for spectral line shapes had simply treated the ions as static, assuming that the more mobile electrons would dominate any observable dynamic plasma properties. Subsequent attempts to include a quantitative description of ion dynamics have been complicated by the necessity of retaining the observable many-body properties of the static ion distribution function and, at the same time, providing a realistic yet calculable treatment of ion motion. A wide variety of approximate methods have been proposed, many of which have improved the agreement with experimental data, but the different theoretical results do not agree with one another and there is as yet no theory which gives a satisfactory description of all the experimental data. A brief review of several different theoretical methods is given in Ref. 4.

At the present time, most theoretical calculations have been based on a model of the plasma in which the ions are treated as statistically independent quasiparticles which move on a straight line trajectory and interact with the radiating atom through Debye-shielded Coulomb fields. This model is probably adequate, but its validity is open to question until satisfactory agreement with experimental measurements is obtained.

The goal of this research is to develop a computer simulation technique which is valid for plasma line broadening, to use this model to analyze other theoretical methods, and to compare line profiles obtained by computer simulation with experimental data. For these goals, we will continue to employ the fundamental assumption that the ions may be treated as statistically independent quasiparticles. In this paper, we will discuss the development of our computer model and compare preliminary calculations with well-known plasma properties.

II. STATIC PROPERTIES

In our computer simulation for an ion density n, we use a random number generator to choose the r, ϑ, and ϕ spherical coordinates for N particles in a sphere of radius, R, where

$$\frac{4\pi}{3}R^3=N/n\ . \tag{2.1}$$

We then calculate the electric field at the center of the sphere due to these N ions using the expression

$$\vec{\epsilon}=\sum_j \vec{\epsilon}_j=\sum_j (e\vec{r}_j/r_j^3)(1+\xi r_j/\lambda_D)\exp(-\xi r_j/\lambda_D)\ , \tag{2.2}$$

where $\vec{r}$ is the position of the jth ion, $\lambda_D=\sqrt{kT/4\pi ne^2}$ is the Debye length, T is the plasma temperature, e is the electron charge, and ξ is a shielding parameter discussed below. This calculation is repeated N_c times to give N_c different values of the electric field $\vec{\epsilon}$, we then sort the values of $|\vec{\epsilon}|$ to determine a probability distribution for this ensemble of N_c configurations.

A typical result for $n=10^{17}$ cm^{-3}, $T=10^4$ K, $\xi=1$, $N_c=40000$, $N=125$ is shown in Fig. 1 plotted as a function of the dimensionless quantity $\beta=\epsilon/\epsilon_0$, where $\epsilon_0=e/r_0^2$ and $4\pi r_0^3/3=n$. Changing the number of configurations N_c only changes the statistical noise on $P(\beta)$ which goes as $1/\sqrt{N_c}$. Changing the number of ions N has a negligible effect on $P(\beta)$ provided that $N\gtrsim 125$; to see why this is so, note that, for a fixed density n, adding

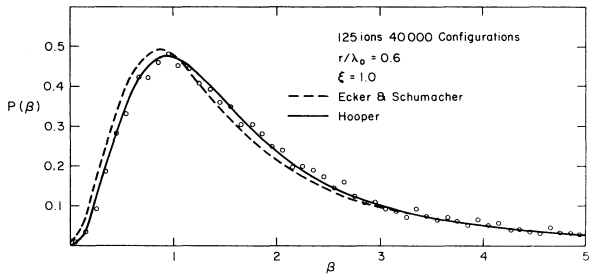

FIG. 1. Comparison of static electric microfield distribution $P(\beta)$ obtained from computer simulation (open circles) theoretical results of Hooper (Ref. 5) (solid curve) and Ecker and Schumacher (Ref. 6) (dashed curve).

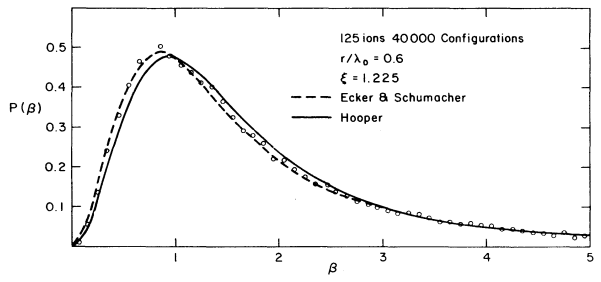

FIG. 2. Comparison of static electric microfield distribution $P(\beta)$ obtained from computer simulation (open cirlces) theoretical results of Hooper (Ref. 5) (solid curve) and Ecker and Schumacher (Ref. 6) (dashed curve).

more ions simply results in a larger volume R, as given by Eq. (2.1), which improves the calculation for large r or small β. That is, with $n=10^{17}$ cm^{-3} and $N\geq 125$, Eq. (2.1) gives $R\geq 5r_0$; the simulation neglects ions more distant than this value of R and this corresponds to $\beta\leq 0.04$ where $P(\beta)<0.01$ so the effect of these distant ions would be insignificant.

In Figs. 1 and 2, we have used $\xi=1$ and 1.225 and compared our results with the functions of $P(\beta)$ obtained by Hooper[5] and Ecker and Schumacher[6] for a microfield ratio $r_0/\lambda_D=0.6$. These values of ξ were chosen for illustration because $\xi=1$ represents the basic model with static shielding, and $\xi=1.225$ was the value obtained by Ecker and Schumacher from a model which approximates dynamic shielding effects with an effective statically shielded field. The value $\xi=1.11$ was used by Seidel[7] in his model microfield calculations and the domain $1\leq\xi\leq 1.225$ is the range of values normally found in the literature. Our $\xi=1.225$ results agree with those of Ecker and Schumacher as they should since, with this choice of ξ our models are identical, the only difference being the fact that Ecker and Schumacher employed numerical calculations of an analytic expression for $P(\beta)$, whereas we used a computer simulation. This agreement serves as a test of our numerical methods. For $\xi=1$, our results are essentially identical to those of Hooper, who used a more sophisticated static model containing collective effects; for this reason Hooper's shielding parameter α is not directly comparable to our ξ. Nonetheless, we obtain agreement to within 2% with all of Hooper's microfield distribution functions for $0\leq r_0/\lambda_D\leq 0.8$ using our simple statically shielded model. This close agreement with Hooper's results also shows that the interactions between shielded ions do not significantly affect $P(\beta)$ at small values of the plasma parameter.

III. DYNAMIC PROPERTIES

In representing ion motion, we use a random number generator to choose a set of velocities $\vec{v}_j$ for each of the ions such that the magnitudes v_j are distributed according to the Maxwellian law $v^2/v_0^3\exp(-v^2/v_0^2)$ where $v_0^2=2kT/m$. The ions then move on straight lines $\vec{r}_j(t)=\vec{r}_j(0)+\vec{v}_j t$; that is, there are no collisions in our model, so we may evaluate $\vec{r}_j(t)$ for any set of times t_i without concern that the increments $(t_{i+1}-t_i)$ may be large.

If a particle exits the sphere of radius R [defined by Eq. (2.1)] between the times t_i and t_{i+1}, it is replaced by a new particle located at a point $\vec{r}_{j,\text{new}}$ chosen at random within the spherical shell $r_j(t_i)\leq r_{j,\text{new}}\leq R$. This new particle will have the same velocity $\vec{v}_j$ unless $\vec{v}_j\cdot\vec{r}_{j,\text{new}}>0$, in which case $\vec{v}_j$ is replaced by $-\vec{v}_j$. This procedure for reinjecting particles which have left the sphere is slightly different from the "periodic boundary conditions" employed in the usual "molecular-dynamics" approach (p. 47 of Ref. 8); in the latter, the new particle enters the sphere from the opposite side, i.e., $\vec{r}_{j,\text{new}}=-\vec{r}_j(t_{i+1})$ with exactly the same velocity vector $\vec{v}_j$. The problem with "periodic boundary conditions" is that each particle is continually crossing and recrossing the sphere every R/v_j seconds; this means that autocorrelation functions such as $\langle\vec{\epsilon}(t)\cdot\vec{\epsilon}(0)\rangle$ will exhibit periodic increases in correlation every R/v seconds. Even in models where collisions alter the trajectories, the use of periodic boundary conditions produces spurious contributions to correlation after R/v_{avg} seconds (p. 48 of Ref. 8) and, for a model with no collisions such as ours, this can produce very serious errors.

With our method of reinjecting particles, there is no correlation between $\vec{r}_j(0)$ and $\vec{r}_j(t)$ after the jth particle exits the sphere, and this of course underestimates the true correlation. That is, the contribution to the autocorrelation function from the jth ion, $\vec{\epsilon}_j(0)\cdot\vec{\epsilon}_j(t)$, drops suddenly to zero when the particle exits the sphere. However, since we have required that R be much larger than λ_D, the true contribution $\vec{\epsilon}_j(0)\cdot\vec{\epsilon}_j(t)$ will be very small because $\epsilon_j(t)$ is very small when $r_j(t)\geq R$. We thus expect our reinjection method to be accurate for calculating autocorrelation functions such as $\langle\vec{\epsilon}(t)\cdot\vec{\epsilon}(0)\rangle$ which are important in spectral line broadening; this will be discussed in more detail below.

To study the dynamic properties of our model, we have performed calculations of the electric field autocorrelation function and compared them with the theoretical expression[9] which is known from the work of Rosenbluth and Rostoker:[10]

$$c(t)=\langle\vec{\beta}(t)\cdot\vec{\beta}(0)\rangle$$
$$=\frac{3}{\sqrt{\pi}}\left[\frac{r_0}{\lambda_D}\right]\frac{1}{\tau}[1+\tau^2-\sqrt{\pi}\tau(\tau^2+\tfrac{3}{2})e^{-\tau^2}\operatorname{erfc}(\tau)]\,, \tag{3.1}$$

where $\tau=t\omega_p/\sqrt{2}$ and $\omega_p=\sqrt{4\pi ne^2/m}$ is the plasma frequency for particles of mass m. Equation (3.1) diverges as $1/t$ due to the fact that $\langle\epsilon^2\rangle$ is infinite unless small values of r_j [see Eq. (2.2)] are excluded. In our computer simulation, we have excluded the region $r_j<9a_0$, where $a_0=5.29\times 10^{-9}$ cm is the Bohr radius; this cutoff corresponds to field $\beta>788$ and results in $\langle\beta^2\rangle=79$. If one were interested in studying fields stronger than $\beta=788$, it would be better to replace Eq. (2.2) by a function derived from an effective potential[11] which takes account of the quantum effects that soften the interaction for small r. For line broadening, a simple

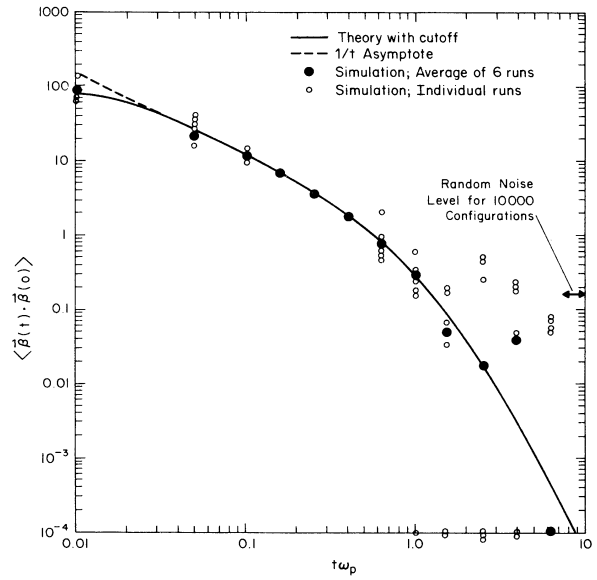

FIG. 3. Electric field autocorrelation function obtained from theory [Eq. (3.1) plus a cutoff at small r] compared with six different computer simulation runs (open circles) for 125 ions and 10000 configurations each. The solid circles denote the average of these six runs. Open points plotted on or below the baseline, $c(t)=10^{-4}$, denote values which are small but negative. The normalized electric field β was discussed in Sec. II.

cutoff in r_j is sufficient to represent these quantum effects because one is interested only in the Fourier transform of functions like $c(t)$ and the region $t\omega_p \lesssim 10^{-2}$, where this cutoff has an effect, makes a negligible contribution to the integral of $c(t)$. This should not be confused with the so-called strong collision cutoff employed in theories which use an S matrix (see Sec. II of this paper and pp. 236 and 237 of Ref. 12). As noted above, the effect of our cutoff at $r_j=9a_0$ is to restrict $\langle \vec{\beta}(t)\cdot\vec{\beta}(0)\rangle$ to values less than $\langle \beta^2\rangle=79$ (see also Sec. 2.2 and Fig. 1 of Ref. 9).

In Fig. 3 we have compared the theoretical expression, Eq. (3.1), with six different computer simulation calculations each having 125 ions and 10000 configurations. The solid points are the averages of these six calculations (equivalent to a single run with 60000 configurations) and the open circles represent the individual calculations themselves. This was done to illustrate the noise level corresponding to 10000 configurations. Where the noise level is low, $0.1 \le t\omega_p \le 1.0$, some of the individual data points are obscured by the average value point. For large t where $\langle \vec{\beta}(t)\cdot\vec{\beta}(0)\rangle \to 0$, some of the data points are negative and could not be correctly plotted; these data points were simply plotted at the bottom of the graph to give an indication of the noise. For $t\omega_p \ge 10$, the average value is essentially zero but the simulation produced values in the range ± 0.17, which, as explained below, is denoted as the random noise level in Fig. 3. This random noise level is due to the fact that, as t increases, more and more ions are leaving the sphere and these ions are being replaced by new ions at randomly chosen points within the shell from which they left (as discussed above); these new ions have no correlation with the initial position, $\vec{r}_j(0)$, of the ion which they replaced, hence they should produce contributions to $\vec{\beta}(t)\cdot\vec{\beta}(0)$ which sum to zero. In fact, this sum will be zero only when the number of configurations is very large; for 10000 configurations there will be some noise and the actual observed values of $\langle \vec{\beta}(t)\cdot\vec{\beta}(0)\rangle$ may be either positive or negative as $t\to\infty$. To calculate this noise level, we took the fields $\vec{\beta}_1$ and $\vec{\beta}_2$ for two completely independent randomly chosen groups of 125 ions and we averaged the product $\vec{\beta}_1\cdot\vec{\beta}_2$ over 10000 of these randomly chosen groups. This procedure was repeated twenty times in order to roughly estimate a variance, σ^2, for these averages; by this method we obtained $\sigma=\pm 0.17$ which is the random noise level for 10000 configurations indicated in Fig. 3.

The slight increase in noise as $t\to 0$ is due to the relatively poor statistics for strong fields. That is, the probability of finding an ion inside a thin shell of mean radius r_j which gives rise to large ϵ_j, is proportional to $4\pi r_j^2$ and this decreases as $r_j\to 0$ or $\epsilon_j\to\infty$. Consequently there are very few configurations which start out with large electric fields and the noise level tends to be larger for any quantity which is sensitive to strong fields. Now, recalling that $\langle \vec{\beta}(t)\cdot\vec{\beta}(0)\rangle \to \langle \beta^2\rangle$ as $t\to 0$ and $\langle \beta^2\rangle$ is determined primarily by strong fields, it is not surprising that the noise level increases slightly as $t\to 0$.

For a model with 125 ions, at $T=10^4$ K and $n=10^{17}$ cm^{-3}, we have $R=3\lambda_d$ so the average time which elapses before an ion leaves the sphere is $R/v_{\text{avg}} \cong 3/\omega_p$. The results of the simulation clearly agree with the theoretical $c(t)$ for t up to about $3/\omega_p$, but after this point, the noise level is too large to draw any conclusions about the error introduced by our method for reinjecting those ions which leave the sphere. It would be possible to reduce the noise by increasing the number of configurations and thereby study the region $t > 3/\omega_p$, where we expect our simulation to underestimate $c(t)$. However, this is such a small effect that it would be very costly in terms of computer time to reduce the noise sufficiently to study it and, for spectral line broadening, this region of $c(t)$ is unimportant in any case. For the sake of discussion, we also note that in our early work[4] we actually did use periodic boundary conditions and it was found that this produced a correlation function $c(t)$ which was definitely too large for $t\omega_p > 2$; it was this result which prompted us to look for an improved procedure.

The stationarity of our model was also checked by calculating the static probability distribution $P(\beta)$ at several different times up to $t\omega_p=10$. For calculations with periodic boundary conditions, $P(\beta)$ did not remain constant in time due to the rather large increments in t_i which we used. With our new method for reinjecting the ions which leave the sphere, $P(\beta)$ remained stationary in time regardless of the increments in t_i. We thus conclude that, for a model with noninteracting particles such as ours, our method of reinjecting the ions is more accurate and less costly than the usual periodic boundary conditions employed in the molecular dynamics methods.

Finally, we note in passing that, in the usual molecular-dynamics method, $c(t)=\langle \vec{\beta}(t)\cdot\vec{\beta}(0)\rangle$ would be

evaluated by calculating $\vec{\beta}(t+s)\cdot\vec{\beta}(s)$ for a single configuration and averaging over s (see p. 210 of Ref. 8). In our calculations, we evaluate $\vec{\beta}(t)\cdot\vec{\beta}(0)$ for each of N_c configurations and take an average over these configurations. Obviously, there should be no difference between these methods of averaging as long as the systems are stationary.

IV. CONCLUSIONS

We have tested a computer simulation model for a gas of statistically independent ions which move on straight paths and interact with an atom through static Debye shielded fields. We find that 125 ions contained in a spherical volume will satisfactorily reproduce the known electric microfield distribution function $P(\beta)$ as well as the known electric field autocorrelation function $\langle \vec{\epsilon}(t)\cdot\vec{\epsilon}(0)\rangle$. The dynamic properties of this system were treated by reinjecting those ions which exit the sphere at randomly chosen points within the shell from which they left. This reinjection procedure differs from the periodic boundary conditions employed by the usual molecular-dynamics method and we found that it gave improved results for both the correlation function $c(t)$ and the stationarity of the system.

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