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Initial Particle Distributions for Simulated Plasma

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A simple method is proposed for distributing charged particles in space so that they have a thermal energy spectrum. The ions and electrons are taken in pairs which are placed randomly over the mesh but the relative position within each pair is chosen to fit the Debye distribution. Hardly any more time is needed to set up the particles properly in this way than is needed for purely random positioning.

1. INTRODUCTION

In the computer simulation of plasmas, the ions and electrons are placed in phase space according to some prescription and are allowed to interact through the electric field computed from the charge distribution. The development of various waves and instabilities can then be studied. The most commonly used prescription is to place the particles in completely random positions but this is unrealistic, as it leaves too much energy in the longer wavelength modes. Sometimes this is avoided by going to the other extreme of positioning on a regular spatial lattice [1] or even [2] uniform also in velocity space but then the fluctuations are subthermal. This quiet start has the advantage that the behaviour of single modes is not obscured by the thermal noise but on the other hand the nonlinear interaction between modes is not represented correctly.

So far there has been no way of starting off the particles from equilibrium but we show here that this can, in fact, be done very easily. The computer experiment then accurately simulates a plasma having the corresponding value of N_D (the number of particles in a Debye sphere). If we are interested in plasmas with a larger N_D than we can afford to use, we can either extrapolate from the results of small N_D experiments or use the quiet start to keep the fluctuations down. The choice lies between the known random errors in the one case versus the possibility of systematic errors during the drift towards equilibrium in the other.

2. Random Positioning

As two-dimensional experiments are of most current interest, we express our results in this form. The Fourier transform of the density is

$$\rho_{\mathbf{k}} = \sum_{j=1}^{n} q_j \exp(i\mathbf{k} \cdot \mathbf{x}_j),$$

where the j-th particle has charge q_j per unit length ($\pm e$ on a rod of length ℓ) and is situated at $\mathbf{x}_j$. The sum is taken over all particles in the experiment and periodic boundary conditions are assumed. The density correlation function is

$$\langle \rho_k \rho_{-k} \rangle = \sum_j q_j^2 + \sum_j \sum_{i \neq j} q_j q_i \exp[i\mathbf{k} \cdot (\mathbf{x}_j - \mathbf{x}_i)]$$

which, when all particles are put in completely randomly, reduces to ne^2/ℓ^2. The energy spectrum

$$\mathscr{E}_{\mathbf{k}} = \frac{\ell}{8\pi} \langle E_{\mathbf{k}} E_{-\mathbf{k}} \rangle = \frac{2\pi\ell}{k^2} \langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle$$

then suffers an infrared catastrophe whereas, in thermal equilibrium, it should be proportional to $(1 + k^2\lambda^2)^{-1}$ where λ is the Debye length [3].

3. Thermal Positioning

In order to modify $\langle E_{\mathbf{k}} E_{-\mathbf{k}} \rangle$, we must alter the binary correlations within the plasma. The effect of an ion at $\mathbf{r} = 0$ is described by Poisson's equation

$$\nabla^2 \phi = \frac{4\pi e}{\ell} (-\delta(\mathbf{r}) + n_- - n_+),$$

where the charge densities induced by the ion are

$$n_\pm(\mathbf{r}) = \tfrac{1}{2} n \exp(\mp e\phi/\kappa T) \simeq \tfrac{1}{2} n \mp \tfrac{1}{2} ne\phi/\kappa T$$

in the conventional approximation. The equation

$$\nabla^2 \phi = \frac{-4\pi e}{\ell} \delta(r) + \frac{\phi}{\lambda^2},$$

where $\lambda^2 = \kappa T\ell/4\pi ne^2$, is linear; so the principle of superposition can be applied. By solving this equation we find that the net excess charge in the vicinity of the ion is $-e$, that is to say there is in effect one extra electron near it. The correct

charge density is achieved if we let there be an actual electron near the ion with probability density $f(r)$ given by

$$\nabla^2 f = f/\lambda^2.$$

The solution of this equation in two dimensions is

$$f(r, \theta) = \frac{1}{2\pi\lambda^2} K_0(r/\lambda),$$

where K_0 is a modified Bessel function of the second kind.

Thus, the recipe we propose is: put the ions in completely random positions and to each ion place one electron such that its probability density is f, independently of all other ions and electrons. The particle velocities are selected independently from a Maxwellian distribution in the usual way [4]. This method is symmetrical between ions and electrons and it ignores correlations between like particles but compensates for this by doubling the unlike particle correlations. The density spectrum now has $\frac{1}{2}n$ statistically independent terms each of the form $2e^2\ell^{-2}(1 - \cos \mathbf{k} \cdot \mathbf{x})$; hence

$$\langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle = \frac{ne^2}{\ell^2} \langle 1 - \cos \mathbf{k} \cdot \mathbf{x} \rangle$$

$$= \frac{ne^2}{\ell^2} \left(1 - \frac{1}{1 + k^2\lambda^2}\right).$$

The energy spectrum then has the form appropriate to thermal equilibrium

$$\mathscr{E}_{\mathbf{k}} = \frac{\frac{1}{2}\kappa T}{1 + k^2\lambda^2}.$$

Within the Debye sphere surrounding an ion, in any decent plasma, there are many charged particles [5]. This number is subject to large statistical fluctuations (of the form $N_D \pm \sqrt{N_D}$) but on the average there is half an electron more and half an ion less than in a randomly chosen region of the same volume. The likelihood of being able to detect the difference between this situation and our proposal, in which the sphere contains one extra electron, is remote. We have an excess density near every particle, but the overlap of spheres of influence means that no observable effect is produced. The total number of particles is predetermined; so the mean particle density cannot rise simultaneously all over the plasma. Only if N_D were of the order unity would the unwanted boson-like property show itself.

This simple recipe is in fact better than some variants which at first sight might appear to be improvements upon it. For example, the ions might still be put in

randomly but the electrons could be assigned randomly to the ions rather than one to each of them. Each electron would then have a chance $(\frac{1}{2}n)^{-1}$ of being near a given ion but there are $\frac{1}{2}n$ electrons altogether. This would still give the correct mean negative charge near an ion but some electrons would cluster about the same ion and would therefore find themselves positively correlated in position. The simple method of setting up the particles avoids this.

4. Approximation of the Debye Distribution

The usual way [4] of producing random variables with any desired probability distribution $f(z)$ starting with random numbers ξ having a uniform distribution in the range 0 to 1, is to solve

$$F(z) = \int_{-\infty}^{z} f(z')\, dz' = \xi$$

for z. The angular coordinate θ can be chosen easily but the radial variable $z = r/\lambda$ must be obtained from

$$zK_1(z) = \xi.$$

This equation could be solved by Newton's method but the evaluation of the modified Bessel function is a slow process and it is preferable to find an approximation $z(\xi)$ to $F^{-1}(\xi)$ which inverts this equation directly with sufficient accuracy.

The probability distribution obtained from the trial function $z(\xi)$ was matched to the desired distribution $f(z)$ by adjusting the parameters in $z(\xi)$ so as to minimise the goodness of fit parameter χ^2. The best approximation so far discovered is

$$z(\xi) = \frac{1.0721q + .6601q^2 + .0697q^3}{1 + .0867q - .1840 \ln q},$$

where $q^2 = -\ln \xi$. Here over fifty million pairs of particles would be needed before the deviations from the true Debye distribution equalled the purely statistical fluctuations. Putting it another way, 99.95% of the electrons are placed within 0.001 λ of their correct position and less than one electron in 10^{12} is to be found misplaced by more than 0.01 λ.

5. Results

The energy spectrum has been computed under conditions similar to those used in experiments [6] carried out with the GALAXY code [7]. An ensemble of 38 trials with 16384 particles in each trial gave the mean and standard deviation

shown by the vertical lines in Fig. 1. The size of the mesh was 64×64 and λ was $4/\pi$ times the mesh interval δ. The χ^2 test showed that the values agree (20% significance level) with the desired theoretical curve. This curve allows for the distortion caused by nearest-grid-point weighting, typically 5% under these conditions. The calculated spectrum for $\mathbf{k}$ parallel to one of the axes is

$$\mathscr{E}_{\mathbf{k}} = \frac{\frac{1}{2}\kappa T}{k^2\lambda\delta} \frac{2 \sin^2 \frac{1}{2}k\delta \sinh \delta/\lambda}{\cosh \delta/\lambda - \cos k\delta}.$$

This was derived by first finding the probability that the electron and ion should be separated by m mesh intervals given that the ion is at x, and then taking the average over x. For comparison we show the theoretical curve for purely random positioning—here the energy content of the modes keeps on rising as k falls.

Figure 1 has shown that the plasma is apparently in thermal equilibrium at time $t = 0$ but it could be that this is just a fluke and that the spectrum would

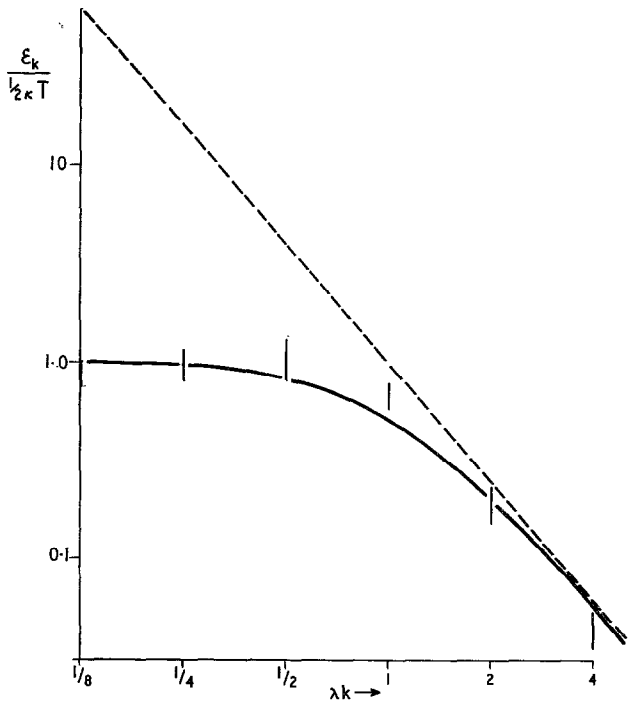

FIG. 1. Energy spectrum as a function of k. The solid curve is the theoretical spectrum and the bars show the measured values with their standard deviations. The broken line is the spectrum for purely random positioning.

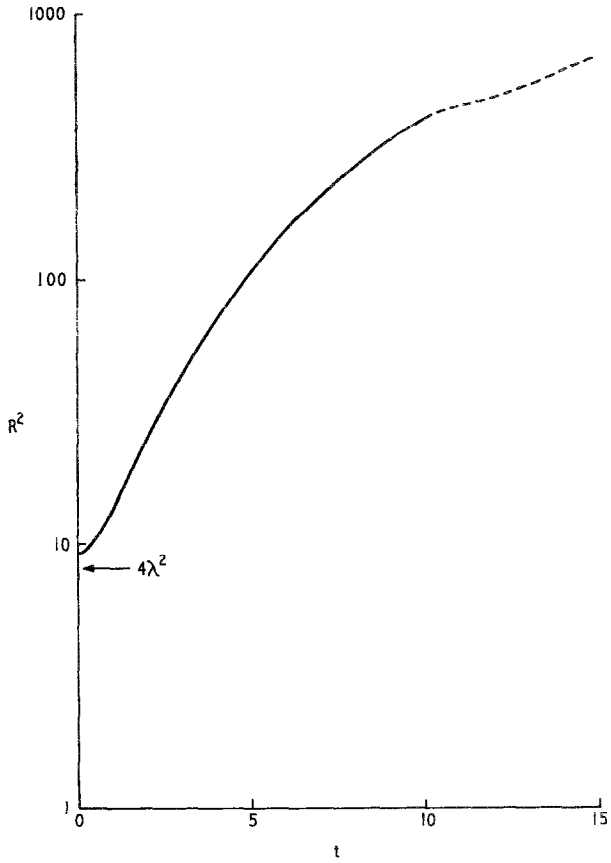

FIG. 2. The dispersal of initially correlated particles. R^2 is the mean square displacement as a function of time.

deteriorate as the plasma evolves. This possibility has been investigated using the GALAXY code. Initially each particle is correlated with only one other; if the spectrum is still alright when these initial correlations have disappeared, then the correlations *must* have been shared around among the other $\frac{1}{2}n^2$ pairs of particles. Once this has happened, the plasma is indeed very close to being really in equilibrium. A useful criterion for assessing the decay of the initial correlations is the mean square displacement R^2 within the original pairs. This starts off at $4\lambda^2$ and it can be followed until it begins to be limited by the periodic lattice. Figure 2 shows R^2, sampled over 16 pairs, as a function of time with unit of length δ and unit thermal velocity. These experiments had 4096 electrons and 4096 positrons and λ was 2. By about $t = 5$, R^2 has increased so much that the initial pairs of particles can be considered to be broken.

Figure 3 compares the direction averaged spectra initially ($t = 0$) and after the plasma has evolved (average $t = 34$). The points represent an ensemble average over 5 plasmas with thermal starts having $\lambda = 2$ and the solid curves give theoretical spectra. It is clear that both sets of points are consistent with the expected deviations marked on the theoretical $\lambda = 2$ curve and so we conclude that the spectrum maintains itself happily as the plasma evolves.

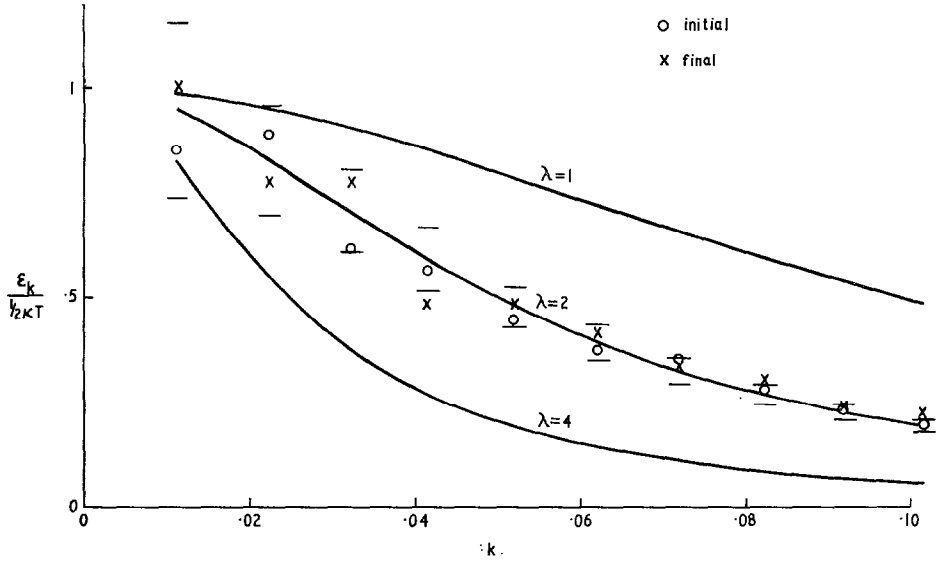

FIG. 3. Initial and final spectra for the thermally started plasma compared with the theoretical spectra for $\lambda = 1, 2$ and 4. The horizontal lines denote the theoretical standard deviation.

6. COMPARISON WITH OTHER METHODS

The thermally started plasma has been shown to stay in equilibrium but it might be that the random or uniform starts relax quickly into thermal equilibrium. This is investigated in Fig. 4 where the sum of the energy in the lowest 220 modes is plotted for each of the three cases. The energy following the thermal start remains steady long after the initial correlations have dispersed. The initially random distribution is markedly inferior as it displays large persistent oscillations instead of getting much closer to equilibrium. Morse [1] has stated that the uniform start evolves into thermal equilibrium in about one plasma period, and, as far as $\sum \mathscr{E}_k$ is concerned, this is true. However, we can apply a more sophisticated statistical test because we know from the central limit theorem that E_k, being

the superposition of a very large number of random vectors, has a two-dimensional Gaussian distribution in the complex plane. Hence the energy in mode **k** relative to the thermal energy, $\eta = \mathscr{E}_{\mathbf{k}}/\mathscr{E}_{\mathbf{k}(\text{thermal})}$, has an exponential distribution,

$$f(\eta) = e^{-\eta}.$$

The largest η among the 220 modes under investigation then has as its probability distribution

$$f(\eta_{\max}) = 220(1 - \exp[-\eta_{\max}])^{219} \exp[-\eta_{\max}].$$

The values of $\eta_{\max}$ following the thermal start were quite consistent with this distribution as 71 fell in the range 4.5 to 7.5 times thermal compared with the theoretical expectation of 70.4. The largest $\eta_{\max}$ observed throughout the 88 time steps was 9.85 times thermal, which is reasonable because we deduce from $f(\eta_{\max})$ that this value will be exceeded in two out of three equilibrium plasmas. The

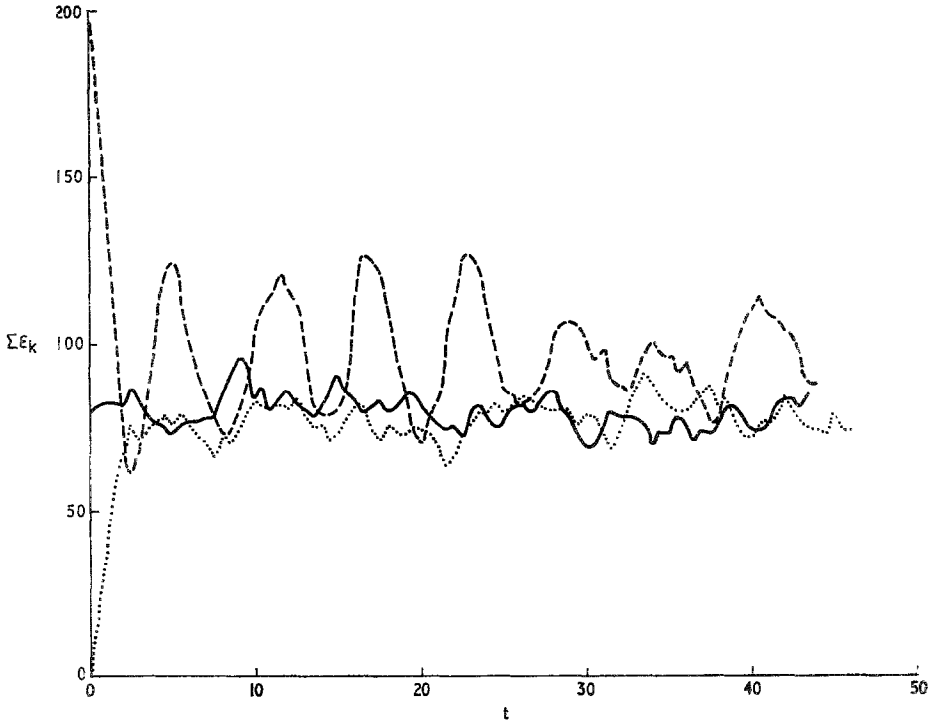

FIG. 4. Total energy in the lowest modes as a function of time for the thermal start (solid line) compared with the random start (broken line) and uniform start (dotted line). In equilibrium $\Sigma\mathscr{E}_k$ should be 75.

uniform start gave most of its η_{max} in the right range, but η_{max} shot up to 14.08 times thermal at $t = 10$. We state, with a 99.8 % chance of being correct, that this proves that the plasma is not in equilibrium, belying the assumption from Fig. 4 that the uniformly started plasma had reached equilibrium by about $t = 2$. Therefore, such plasmas should be viewed with suspicion—they might not be as quiescent as they look.

7. Generalization

Because the mass of the particles does not enter into the equation for the electric field, the recipe applies equally well when massive ions are present. An experiment with $M/m = 2048$ confirmed that the spectrum remains thermal when the ions are still essentially in their original positions but the electrons have moved away. This can be generalised as follows: a subgroup of particles, sensing a thermal field, will move so as to maintain this field. Therefore the ions, who see the thermal field of the rapidly moving electrons, will on their own time scale move so that the field remains thermal.

We have seen how an equilibrium distribution can be set up; by a generalisation of the linear superposition argument we can easily add any desired deviations from equilibrium. Suppose for instance that we require a 10 times thermal content in mode $\mathbf{k}$. This can be achieved by putting $3n^{1/2}$ particles in according to the charge probability distribution $\cos \mathbf{k} \cdot \mathbf{x}$, electrons in the negative half cycles and ions in the positive, with the remainder of the particles in thermal equilibrium.

8. Conclusion

The computing time needed to set up the thermal distribution in four-dimensional phase space is increased by 45 per cent when the Debye correlations are taken into account. This increase, being equivalent to one time step, is negligible compared with the duration of the whole experiment. The comparative runs with the GALAXY code have shown that the random and uniform starts take much more than one time step to reach equilibrium. It is not claimed that our method is a complete solution to the problem; it can only reproduce the main features of the binary correlations. However, these correlations are the ones commonly used as the test for thermal equilibrium and it is well worth including them when it can be done so easily by this method.

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