Numerical Simulation of Ultracold Plasmas: How Rapid Intrinsic Heating Limits the Development of Correlation

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In recent experiments, ultracold plasmas were produced by photoionizing small clouds of laser-cooled atoms. It has been suggested that the low initial temperature of these novel plasmas leads directly to strong correlation and order. In contrast, we argue that rapid intrinsic heating raises the electron temperature to the point where strong correlation cannot develop. The argument is corroborated by a molecular-dynamics simulation of the early-time plasma evolution.

In recent experiments, ultracold neutral plasmas were produced by rapidly photoionizing small laser cooled clouds of atoms [1–3]. The energy (or frequency) of the ionizing photons was adjusted to barely exceed the ionization energy of the atoms.

These novel plasmas present interesting challenges to theory. For example, it has been suggested that the low initial temperature leads to strong correlation and order [1]. In contrast, we argue that rapid intrinsic heating raises the electron temperature to the point where strong correlation cannot develop.

The basic idea is easy to understand physically. For a plasma in thermal equilibrium, the strength of correlation is determined by the coupling parameter $\Gamma = e^2/akT$, where a is the Wigner-Seitz radius (i.e., $4\pi a^3 n/3 = 1$) [4]. For the maximum density and lowest electron and ion temperatures reported in the experiments [i.e., $n \simeq 2 \times 10^9$ cm^{-3}, $T_e \simeq 0.1$ K, and $T_i = 10$ μK], the electron coupling parameter has the value $\Gamma_e \simeq 30$, and the ion coupling parameter is much larger. Thus, one might expect the low temperatures to lead to strong correlation.

However, the plasma is not created in a state of thermal equilibrium. Before photoionization, the neutral atoms are uncorrelated, so immediately after photoionization ion-ion and electron-electron correlations are negligible. There may be some electron-ion correlation that remains as an artifact of the ionization process, but this is not a thermal equilibrium correlation. For example, there is no long range order. The temperatures reported are measures of particle kinetic energy, but do not imply the degree of correlation that would exist for a true thermal equilibrium.

Thermal equilibrium correlations can develop only through the action of Coulomb interactions as the plasma evolves. However, as the correlations begin to develop, the correlation energy is released to the electron plasma as heat, and this limits the strength of correlation reached. To reach a correlation strength corresponding to $\Gamma_e \simeq 1$, each electron picks up thermal energy $kT_e \simeq e^2/a$. At this point the coupling parameter has the value

$$\Gamma_e = e^2/akT_e \simeq (e^2/a)/(e^2/a) = 1,$$

so further development of correlation ceases. Even if the initial electron temperature were zero, corresponding formally to infinite Γ_e, strong correlation would not develop.

Heating associated with the liberation of correlation energy also was considered by Murillo [5]. However, he treats the electrons only as a dielectric fluid that Debye shields the interaction between the ions. His analysis focuses on the liberation of correlation energy for a system of Debye shielded ions. Unfortunately, this approach misses the electron heating that dominates the early stages of evolution, and the electron temperature determines the degree of shielding.

Another way to understand the electron heating is to note that electrons are born in a spatially varying potential, and immediately begin to move downhill. A typical electron picks up kinetic energy e^2/a while moving an interparticle spacing, a. The time scale for this initial heating is approximately $a/\sqrt{e^2/am_e} \sim \omega_p^{-1}$, where ω_p is the plasma frequency.

This heating is the beginning of the collisional process by which the plasma approaches a state of thermal equilibrium. For the low temperatures of these plasmas the thermal equilibrium state is a recombined neutral gas. The collisional cascade of electrons to deeper and deeper binding in the Coulomb wells of ions is called three-body recombination [6]. In this process, the recombination energy is carried off by a second electron (rather than a photon) and enters the plasma as heat. For these plasmas, three-body recombination is very rapid — much faster than radiative recombination. Although three-body recombination is not the focus of this paper, our simulation must include this physics since the heating is a byproduct of the recombination. The initial recombination is into weakly bound (high n Rydberg states), so a classical molecular dynamics simulation captures the essential physics.

The simulation is challenging because the time scale for an electron bound in one of these Rydberg states is much shorter than the time scale for a typical electron. In plasma simulations of this kind some authors have used two time

scales: one for particles with near neighbors and another for the remaining particles [7]. Another variant is to use piecewise analytic solutions for Kepler orbits. We prefer a treatment that doesn't make special assumptions about particles with near neighbors, but seamlessly encompasses the continuum of time scales required.

Fortunately, such a treatment was developed previously in computational studies of binary star formation in globular clusters. The binary stars are the analog of the high n Rydberg atoms, and the cluster is the analog of the plasma cloud. We have adapted a code developed originally by Aarseth [8] for the study of binary star formation.

The code is a molecular dynamics simulation in the sense that the force on a given particle from each of the other particles is calculated directly. Time integration is effected with a predictor-corrector scheme using a fourth-order polynomial fit to the orbit. The crucial feature is that the time step for each particle is adjusted independently depending on such factors as the rate of change of the acceleration. Thus, a bound electron can have a much shorter time step than a typical electron without slowing down the whole simulation. To keep all of the particles moving in near synchrony, the code advances next the time step for the particle that is furthest behind in absolute time. To evaluate the force on this particle, the other particle positions are extrapolated back in time to exact synchrony using the polynomial fit to the orbits.

As one would expect, there are interesting parallels between the dynamics of these plasmas and the dynamics of globular clusters. Indeed, the heating that occurs as a byproduct of three-body recombination is similar to the heating of clusters that accompanies the "hardening" of binary stars. Through collisional interactions the binary stars become more deeply bound, and the liberated gravitational energy enters the cluster as heat. This heating mechanism is thought to be crucial in the support of clusters against gravothermal contraction and core collapse [9].

Simulation Results.—By using properly scaled length and time, the number of parameters that define a simulation is reduced to a minimum. Here length is scaled by the Wigner-Seitz radius a and time by the inverse of the plasma frequency ω_p^{-1}. With these scalings, the equations of motion and initial conditions are specified by four parameters: the mass ratio m_i/m_e, the number of electrons (which is equal to the number of ions) N, the initial value of the coupling parameter Γ_e, and a rounding parameter ε for the Coulomb potential.

To avoid singularities, the Coulomb potential is rounded to the form

$$1/\sqrt{|\mathbf{r}_1 - \mathbf{r}_2|^2/a^2 + \varepsilon^2},$$

where $\varepsilon \ll 1$. For this simulation ε is chosen to have the value $1/31$, and this value is small enough that the rounded potential is a good approximation to the Coulomb potential for the vast majority of particles. For a few deeply bound

pairs, the approximation is marginal (e.g., $1/\varepsilon = 31$ and $\max[E_{\text{binding}}/(e^2/a)] \simeq 25$), but these deeply bound pairs are not the focus of this investigation.

To give correlations the maximum opportunity to develop, the initial electron and ion temperatures (or more precisely, kinetic energies) are taken to be zero, corresponding formally to $\Gamma_e(t = 0) = \infty$ and $\Gamma_i(t = 0) = \infty$.

The mass ratio is chosen to have the value $m_i/m_e = 100$. This relatively low value insures that the ions have time to participate in the correlation dynamics during the course of the simulation. The electron-electron correlation function relaxes to a steady-state form in a few scaled time units, and the ion-ion correlation function in a time that is longer by $\sqrt{m_i/m_e} = 10$. The simulation runs for $t_{\max}\omega_p = 70.9$ scaled time units and energy is conserved to an accuracy of 0.1%.

So that the correlation function takes the simple form $G(\mathbf{r}_1, \mathbf{r}_2) = G(|\mathbf{r}_1 - \mathbf{r}_2|)$, we arrange the initial and boundary conditions to insure uniform plasma density. Specifically, 4096 electrons and 4096 ions are distributed randomly inside a spherical volume bounded by a reflecting wall. The correlation measurements are made well away from the wall. In scaled units, the radius of the sphere is determined by the number of electrons, $(r_s/a)^3 = N$.

The initial density profiles for the experimentally produced plasma clouds were Gaussian [1–3]. One should think of the uniform density spherical plasmas as a small central section of a larger Gaussian cloud.

Figure 1 shows a plot of the scaled electron temperature [i.e., $1/\Gamma_e(t) = kT_e(t)/(e^2/a)$] versus the scaled time $t\omega_p$. To obtain this plot, histograms of electron kinetic energies are made (excluding tightly bound electrons) and matched to Maxwellians. Rapid heating to $\Gamma_e \simeq 1$ is clearly visible. The longer-term slower heating is associated with three-body recombination.

Figure 2 shows the electron-electron correlation function averaged over the time interval $t\omega_p = 3.5$ to 7.1. The correlation function starts out flat, corresponding to randomly distributed electrons, but quickly relaxes to the form shown in Fig. 2 and retains this form. The only change
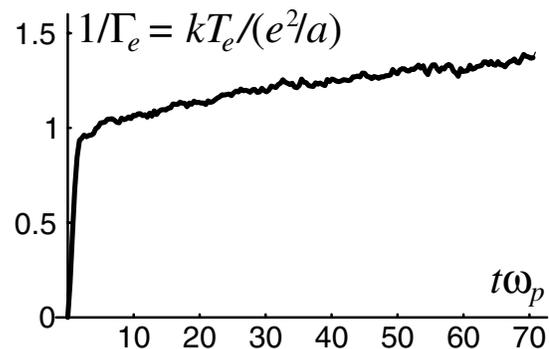

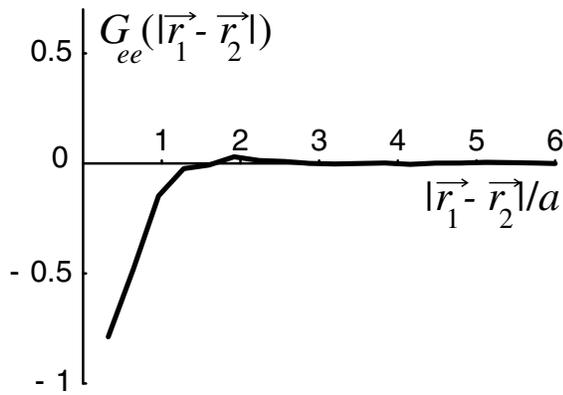FIG. 1.   Scaled temperature versus scaled time.

FIG. 2.   Electron-electron correlation function, averaged from $t\omega_p = 3.5$ to $t\omega_p = 7.1$.

with increasing time is in the width of the region near $|\mathbf{r}_1 - \mathbf{r}_2| = 0$ where $G_{ee} \simeq -1$. This value for G_{ee} reflects the fact that it is energetically unfavorable for two electrons to be at the same location, and the width of the region is of the order of $|\mathbf{r}_1 - \mathbf{r}_2| \simeq e^2/kT_e$. In measurements of G_{ee} at later times the width is observed to decrease as the plasma temperature slowly increases.

For comparison, Fig. 3 shows the correlation function for a one component plasma in thermal equilibrium at correlation strengths $\Gamma = 1, 10, 20,$ and 40 [10]. As expected, the correlation curve in Fig. 2 corresponds in shape to the $\Gamma = 1$ curve in Fig. 3. The curves in Fig. 3 for $\Gamma = 10$, 20, and 40 exhibit oscillations indicating the presence of local order, that is, of a local lattice. The lack of these oscillations in Fig. 2 shows that such order is missing in the electron distribution for the ultracold plasma.

Figure 4 shows the ion-ion correlation function averaged over the time interval $t\omega_p = 67.4$ to 70.9. Again the correlation function starts out flat and relaxes to the form shown, although the relaxation time is longer than for the electrons. The absence of oscillations shows that local order is missing, and comparison to Fig. 3 indicates a correlation strength of order $\Gamma_i \sim 1$.
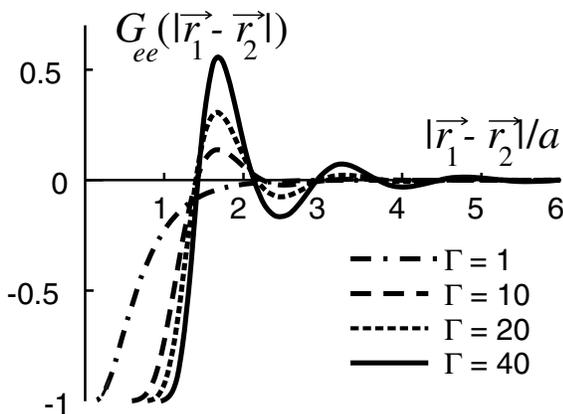
Figure 5 shows the electron-ion correlation function averaged over the time interval $t\omega_p = 3.5$ to 7.1. In this case, G_{ei} is positive near $|\mathbf{r}_1 - \mathbf{r}_2| = 0$, since it is energetically favorable for an electron to be near an ion. However, this positive electron-ion correlation is not an indication of the local order characteristic of strong correlation; rather it reflects the beginning of recombination.

From the simulation results, we see that intrinsic rapid heating prevents the development of strong correlation (order) even though the initial electron and ion temperatures are zero [i.e., $\Gamma_e(0) = \Gamma_i(0) = \infty$]. However, one might worry that the result is a consequence of the low mass ratio or of the reflecting wall boundary conditions. After all, electron evaporation from an unbounded cloud is a cooling mechanism. Consequently, we carried out an extensive simulation for 4096 electrons and 4096 ions in an unbounded cloud with a Gaussian initial density distribution and a realistic mass ratio (for Xe ions). Again, we observed the rapid initial heating to $\Gamma_e \simeq 1$ followed by slower heating due to three-body recombination. The evaporative cooling could not compete with the heating.

One important caveat is that the simulations follow only the early time evolution of the plasma. Later, the plasma undergoes expansion, and this can be a strong cooling mechanism that reduces the temperature. Our studies imply only that the initial low temperatures do not directly lead to strong correlation and order during early times.

Also, in accord with the experiments, we assumed that the atoms were uncorrelated before photoionization. If as suggested by Murillo [5] correlations were imposed on the atoms before photoionization, that correlation structure would be inherited by the ions. This assumes that the ionization process is nearly complete. Further, if the correlation structure closely mimicked that of the Coulomb system, the ion-ion correlation energy would not be released to heat the ions and the correlations would persist for some time. The time would be limited by three-body recombination and by electron collisional heating of the cold ions.

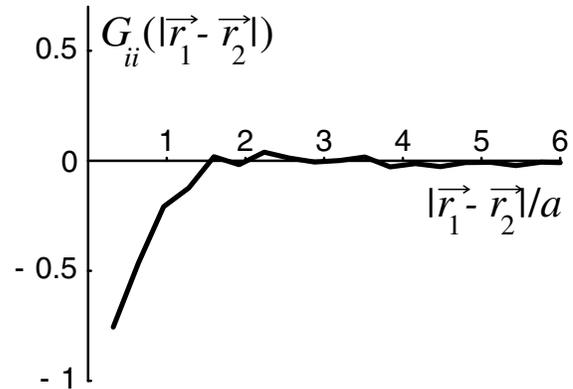FIG. 3.   Correlation function for one component plasma.

FIG. 4.   Ion-ion correlation function averaged over the time interval $t\omega_p = 67.4$ to $t\omega_p = 70.9$.
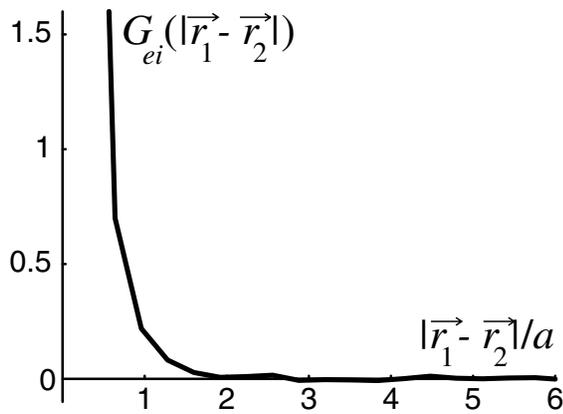
FIG. 5. Electron-ion correlation function averaged over the time interval $t\omega_p = 3.5$ to 7.1.

Finally, we note that the experiments themselves provide some evidence against early strong correlation. The plasma expansion is driven by the electron pressure, but the effective pressure becomes negative for a strongly correlated plasma. This effect is well known from the theory of one component plasmas [11], and is easy to understand physically. Because of correlations, the electrostatic forces of interaction bind the plasma together giving rise to an effective pressure that is negative. If there were no intrinsic heating and the cloud were strongly correlated, the pressure would be negative and the cloud would not expand. Alternatively, one can rule out expansion on energetic grounds. The correlation energy is negative [i.e., $U_{corr} \sim -N(e^2/a)$], so plasma expansion can occur only by supplying positive kinetic energy [i.e., $(3/2)NkT_e$]. However, in the limit of strong correlation, $\Gamma_e = e^2/akT_e \gg 1$, there isn't enough kinetic energy to drive the expansion.

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