Using Fermi Statistics to Create Strongly Coupled Ion Plasmas in Atom Traps

M. S. Murillo
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 5 June 2001; published 24 August 2001)

We investigate the possibility of forming a strongly coupled ion plasma from a cold atomic gas. We show that rapid ion heating occurs as correlations develop from the initial disordered configuration. This heating severely reduces the Coulomb coupling of the final configuration, although the final Coulomb coupling can be maximized by introducing order into the initial atomic gas. We show that such order can be introduced into the initial state by employing a degenerate Fermi gas whereby the Pauli hole mimics the Coulomb hole. The corresponding initial state correlations can enhance the Coulomb coupling in the final state by orders of magnitude.

DOI: 10.1103/PhysRevLett.87.115003 PACS numbers: 52.27.Gr, 52.25.Kn, 52.65.Yy

It has recently become possible to create ultracold plasmas with electron and ion temperatures as low as $T_e \sim 100$ mK and $T_i \sim 10$ μK, respectively [1–3]. Such a novel nonequilibrium plasma allows for the possibility of both species being strongly coupled. Here strong coupling is defined in terms of the usual Coulomb coupling parameter $\Gamma_s = e^2/(aT_s)$, where T_s is the temperature (in energy units) of species s and $a = (3/4\pi n)^{1/3}$ is the Wigner-Seitz radius. For plasmas with a number density of $n \sim 10^9$ cm^{-3} this gives $\Gamma_e \sim 30$ and $\Gamma \equiv \Gamma_i \sim 3 \times 10^5$; for these conditions the electrons may form a strongly coupled fluid whereas the ions may form a Wigner crystal. Larger couplings are possible using higher density gases familiar from Bose-Einstein condensation and Fermi degeneracy experiments. Such plasmas should allow for detailed studies of the approach to nucleation [4] and the formation of a Coulomb glass [5]. In the strongly coupled fluid phase it may also be possible to measure properties of low-frequency fluid-phase shear modes [6] without the strong damping characteristic of colloidal plasmas.

Recent studies [1–3] have been directed toward the electron component of the ultracold plasma. The electrons form a classical gas since their temperature T_e is much larger than the Fermi temperature T_F by about $T_e/T_F \sim 10^3$. For conditions achieved so far in the experiments, no crystalline or quantal effects can be expected for the electron component.

For the ion component, however, which initially has a much lower temperature than the electrons, we expect that a Wigner crystal can be formed in principle. A glassy state may also be possible since the experimental procedure represents a deep, rapid quench from $\Gamma \sim 0$ to $\Gamma \sim 10^5$. Unfortunately, there are several factors that can prohibit the formation of such novel states. For example, in contrast to strongly coupled pure ion plasmas, electron screening will decrease the effective Coulomb coupling. Another important factor is the expansion of the plasma by ambipolar diffusion, which corresponds to an increasing a. This expansion, which occurs on hydrodynamic time scales $\tau_{\rm exp} \sim 1$ μs in typical experiments [2], also results in an inhomogenous plasma with spatially varying Γ_s. The effective density can also decrease as electrons recombine with the ions; however, there are indications that the recombination time $\tau_{\rm rec} > \tau_{\rm exp}$ may be enhanced in the experiments [1,7]. There is also an energy transfer from the electrons to the ions, which is slow due to the large electron-ion mass ratio. Recent theoretical calculations for dense plasmas indicate that this rate is also greatly suppressed in the strongly coupled regime [8]. Here disorder induced heating (DIH) is considered whereby potential energy associated with the initially disordered state is converted into kinetic energy and therefore a correspondingly higher ion temperature. This mechanism, which is faster than the others, is a result of the specific formation method of ultracold plasmas. It is shown that this heating can be mitigated by employing a Fermi degenerate gas which contains initial state correlations similar to those of a strongly coupled plasma.

In the experiments, atoms (e.g., xenon, cesium, rubidium) initially are laser cooled to a temperature of about $T_a \sim 10$ μK–4 mK before being photoionized. The atomic gas is a very weakly interacting system since the atoms are neutral and dilute ($n_a \sim 10^{10}$ cm^{-3}). The atoms are very disordered, although the atoms do not overlap, which sets a minimum distance σ between atoms of order atomic dimensions. Considered as a hard-sphere system, the atomic gas has a packing fraction of $\eta \equiv \pi n_a \sigma^3/6 \sim 10^{-13}$, which can be accurately modeled as a completely uncorrelated system. The electrons will rapidly equilibrate with themselves following the $\tau_{\rm ion} \sim 10$ ns ionization to approximately form a subsystem with temperature T_e. In a time of order the inverse electron plasma frequency $\tau_e = \omega_{pe}^{-1} = \sqrt{m_e/4\pi n e^2}$ the electrons will form screening clouds around the ions. Subsequently the ions, which no longer interact with the cooling lasers, will respond on a time scale given by the inverse ion plasma frequency $\tau_i = \omega_{pi}^{-1}$, for which $\tau_i/\tau_e = \sqrt{m_i/m_e} \sim 100$–1000.

The different time scales satisfy $\tau_{\rm ion} \sim \tau_e \ll \tau_i \ll \tau_{\rm exp} < \tau_{\rm rec}$, for typical experimental conditions. Thus, for considering the heavy ion dynamics, the electrons respond adiabatically. If the electrons are experimentally prepared at temperatures high enough that the electron-ion

coupling $\Gamma_{ei} \approx \Gamma_e$ is weak enough, then the electrons can be treated within a linear screening model [9]. These conditions correspond to what is commonly referred to as the Yukawa model in which the ions interact through the screened Coulomb interaction $u_Y(r) = e^2 \exp(-r/\lambda_e)/r$, where $\lambda_e = \sqrt{T_e/4\pi n e^2}$ is the electron (Debye) screening length. This model should apply between τ_e and $\tau_{\rm exp}$ everywhere except near the plasma boundary. The plasma can be described in terms of the two dimensionless Yukawa parameters Γ and $\kappa = a/\lambda_e$, where distances are measured in units of a. Screening can be quite strong in the experiments, typically $\kappa \leq 10$. The phase diagram of the Yukawa system is now well known [10], although not for κ values as large as this. To produce a crystal or a glass, it is advantageous to create a low-κ (hot electron) system for which the crystallization Γ_c is lower. For electron temperatures $T_e \sim 500$ mK, the screening parameter is $\kappa \sim 5$ and the crystallization boundary is near $\Gamma_c \sim 10^4$ [10] for the expected face-centered cubic crystal phase. For typical ion temperatures then we have $\Gamma/\Gamma_c \sim 30$ and the ion subsystem can—in principle—crystallize. However, just more than an order of magnitude heating would put the plasma into the fluid phase.

Current experiments begin to expand on a $\tau_{\rm exp} \sim 1$ μs time scale, depending on the initial electron temperature. Given that the ultracold plasma acts as a Yukawa system between τ_e and $\tau_{\rm exp}$, the nucleation time is known [4] to be roughly $\tau_{\rm nuc} \sim 1000\sqrt{(m/m_r)/(n/n_r)}$ μs, where the reference mass and density are $m_r = 100 m_p$ and $n_r = 10^9$ cm^{-3}, respectively, and m_p is the proton mass. A strongly coupled ion plasma therefore allows the dynamics of nucleating droplets that precede catastrophic nucleation to be studied, although we do not expect a well-formed crystal since $\tau_{\rm nuc} > \tau_{\rm exp}$. Such experiments may provide insights into the validity range of classical nucleation theory for Yukawa systems. It is therefore of interest to understand and attenuate the fastest heating mechanisms.

We can quantify DIH by computing the temperatures in the initial and final states, subject to energy conservation. The basic notion is that, in the initial state, ions may experience large forces from very close neighbors. In the equilibrated final state the ions are either in a crystal lattice or a liquid quasilattice with significant force cancellation. Clearly each ion will gain kinetic energy as it moves from a high force region to a low force region. More quantitatively, consider a homogeneous Yukawa system characterized by the Hamiltonian [9]

$$\mathcal{H} = \sum_n \frac{p_n^2}{2m_i} + \frac{1}{2\Omega} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{v(k)}{\epsilon(k)} [n(\mathbf{k})n(-\mathbf{k}) - N] + F_e - NT\Gamma \frac{\kappa}{2}, \quad (1)$$

where $v(k) = 4\pi e^2/k^2$ is the bare Coulomb interaction, Ω is volume, $\epsilon(k) = 1 + (k^2\lambda_e^2)^{-1}$ is the electron dielectric response, $n(\mathbf{k}) = \sum_m \exp(-i\mathbf{k}\cdot\mathbf{r}_m)$ is the (Fourier space) ion density, F_e is the Helmholtz free energy of a uniform electron gas, and the final term is the free energy associated with the screening clouds. Ion correlations can be described in terms of the static structure factor $S(k) = N^{-1}\langle n(\mathbf{k})n(-\mathbf{k})\rangle$, which allows the average energy to be written in terms of (1) as

$$\langle \mathcal{H} \rangle = \frac{3}{2} NT + \frac{N}{2\Omega} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{v(k)}{\epsilon(k)} [S(\mathbf{k}) - 1] + F_e - NT\Gamma \frac{\kappa}{2}. \quad (2)$$

The two final terms, which are related to the electron subsystem, are expected to be constant during the ion heating phase and can be neglected [7]. Since ultracold plasmas are not in contact with a heat bath following the ionization process, energy is a conserved quantity. From (2) one obtains a relation between T_i and T_f of

$$T_f = T_i + \frac{1}{3\Omega} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{v(k)}{\epsilon(k)} [S_i(\mathbf{k}, T_i) - S_f(\mathbf{k}, T_f)], \quad (3)$$

where $S_i(\mathbf{k}, T_i)$ and $S_f(\mathbf{k}, T_f)$ are the structure factors in the initial and final states, respectively. This indicates how the temperature of the ultracold plasma changes as a result of differing correlations in the initial and final states. In this expression we may take $S_i(\mathbf{k}, T_i) \approx 1$ since the atomic gas is very uncorrelated, which leads to the estimate

$$T_f \approx T_i - \frac{2}{3} T_f \Gamma_f U_{\rm ex}. \quad (4)$$

The excess energy $u/\Gamma = U_{\rm ex} - \kappa/2$ has been tabulated [10] based on molecular dynamics simulations, and $\frac{u}{\Gamma_f} + \frac{\kappa}{2}$ is always negative and nearly constant for a given κ; therefore, the final ion temperature is greater than the initial temperature when $S_i(\mathbf{k}, T_i) \approx 1$. The initial temperature is usually low enough that (4) can be written as $T_f \approx \frac{2}{3}\frac{e^2}{a}|\frac{u}{\Gamma_f} + \frac{\kappa}{2}|$, which indicates that denser systems, those with smaller a, have higher final temperatures independent of the initial temperature. For $\kappa = 4.5$ the final coupling from this estimate is about $\Gamma_f \approx 20$, which is in the strongly coupled *fluid* phase.

The detailed time development of the temperature is difficult to calculate analytically, and molecular dynamics simulations have been used for this. The ultracold plasma is again modeled as a homogeneous Yukawa system so that boundary effects do not obscure the study of intrinsic ion heating; thus, the calculations pertain to the central portion of the plasma before significant expansion has occurred. During the time interval between τ_e and $\tau_{\rm exp}$ the ions move according to the equations of motion

$$m_i \frac{d^2\mathbf{r}_n}{dt^2} = e^2 \sum_{m\neq n} \mathbf{r}_{nm} \frac{\exp(-r_{nm}/\lambda_e)}{r_{nm}^3} (1 + r_{nm}/\lambda_e), \quad (5)$$

where m_i is the ion mass and $\mathbf{r}_{nm} = \mathbf{r}_n - \mathbf{r}_m$ is the interparticle separation. Immediately following the plasma formation the ions are disordered in the sense that their positions are uncorrelated. This can be described in terms of the initial conditions such that each $\mathbf{r}_n$ is chosen randomly, but not within an atomic diameter of any other ion. The

ion velocities are chosen from a Maxwellian at the initial atom temperature. Equation (5) is then solved numerically subject to these initial conditions. These molecular dynamics simulations are nonequilibrium in the sense that, after setting the initial conditions, there is no reservoir (thermostat) to maintain any species temperatures: energy is a conserved quantity and the simulations are carried out in the microcanonical ensemble. During the simulations the kinetic temperature is measured, as *defined* by

$$T_{\rm ion}(t) = \frac{m_i}{2N}\sum_n v_n^2(t)\,. \tag{6}$$

Note that this definition does not assume a particular form for the velocity distribution. Periodic boundary conditions are used to mimic the homogeneous Yukawa system. Simulations were carried out with various numbers N of particles, and we obtained final results with $N = 6000$ particles. The time step in the simulations was chosen to guarantee energy conservation of about 0.03%.

The amount of initial disorder is determined in the following manner. Atoms are essentially at random positions before ionization, which we quantify by a hard-sphere radius σ. Different levels of disorder are achieved by randomly placing the ions within the simulation cell, but rejecting those positions for which the nearest neighbor distance is less than σ. For the dilute gases under consideration $\sigma \sim 0.0001$.

We performed simulations for the "typical" [1] case of xenon ions ($m_i = 130 m_p$) with an initial temperature and density of $T_i = 10\ \mu$K and $n_i \sim 10^9$ cm^{-3}, respectively. For this plasma the initial coupling parameter is $\Gamma \approx 3.4 \times 10^5$ and the ions are initially uncorrelated and classical. The electrons were taken to be at a temperature of $T_e = 500$ mK, which corresponds to a screening parameter of $\kappa \approx 4.5$. For this large κ value, face-centered cubic crystallization occurs near a coupling parameter of $\Gamma_c \approx 7900$. The temperatures (6) from the simulations are shown in Fig. 1 for densities of $n = 10^8$, 5×10^8, and 10^9 cm^{-3}. The heating is dramatic with a temperature increase of about 4 orders of magnitude for these cases. These results can be compared with the prediction of (4). For $\kappa \approx 4.5$, $u/\Gamma \approx -2.36$ [10] for the final fluid state. The final temperature is then $T_f = 140$ mK, which is in close agreement with the simulation results. The Coulomb coupling parameter Γ is shown in Fig. 2, along with the crystallization boundary for $\kappa = 4.5$ at $\Gamma_c = 7900$. Note that the densest case corresponds to both the hottest *and* most strongly coupled state.

The result (3) predicts that similar correlations in the initial and final states can reduce the final temperature. In the final state, for which there is strong Coulomb repulsion, ions will tend to be ordered such that no two ions are very close—this is the so-called "Coulomb hole." To maximize the final Γ it is imperative to introduce initial state correlations. Correlations can be quantified by the radial distribution function $g(r)$, which describes the likelihood of finding two ions at a separation of r, relative to an ideal

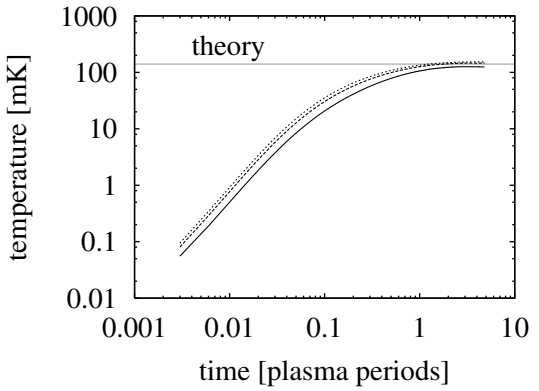

FIG. 1. Ion temperature versus time with no initial state correlations for various densities. The top (dotted) curve has $n = 10^9$ cm^{-3}; the middle (dashed) curve has $n = 5 \times 10^8$ cm^{-3}; the bottom (solid) curve has $n = 10^8$ cm^{-3}. The theoretical final temperature for $n = 1 \times 10^9$ cm^{-3} is shown as a horizontal line.

gas. The radial distribution function is connected with the structure factor through $S(k) - 1 = n\mathcal{F}[g(r) - 1)]$, where $\mathcal{F}[\cdots]$ denotes the Fourier transform. Typically $g(r)$ has the form of vanishing for $r \to 0$ and tending to unity for $r \to \infty$, with intermediate values determined by details of the correlations. For an ideal gas, such as exists in the initial atomic gas, $g(r) \approx 1$ for all $r > \sigma$. We propose to introduce structure into the initial ideal gas by cooling Fermionic atoms into a degenerate state. Such a gas, for which $T/T_F \sim 1$, has already been achieved experimentally [11] by cooling below 300 nK. Since $g(r)$ is a many-body quantity, *any* cause of correlations will tend to order the particles. For a completely degenerate ensemble of Fermions it is well known that $g_{\rm QM}(r) = 1 - [3j_1(k_F r)/(k_F r)]^2$, which qualitatively has a similar form to a strongly coupled plasma $g(r)$: the Pauli hole mimics the Coulomb hole. Here $j_1(x)$ is a spherical Bessel function

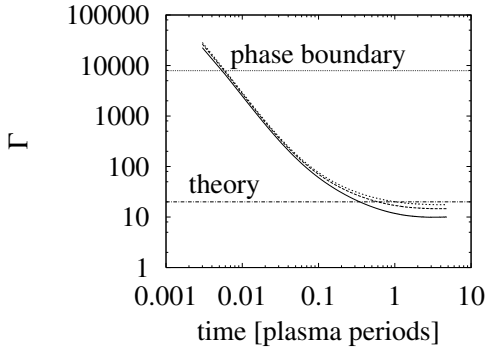

FIG. 2. Ion coupling parameter Γ versus time, again with no initial state correlations. The top (dotted) curve has $n = 10^9$ cm^{-3}; the middle (dashed) curve has $n = 5 \times 10^8$ cm^{-3}; the bottom (solid) curve has $n = 10^8$ cm^{-3}. The theoretical prediction of the final Γ for $n = 10^9$ cm^{-3} and the phase boundary for a $\kappa = 4.5$ system are shown as horizontal lines. Note that, although the densest case has the highest final temperature, it also has the highest final Γ. For these uncorrelated initial states, rapid heating to a weakly coupled state occurs.

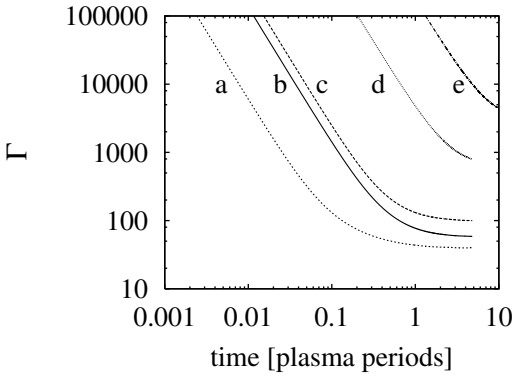

FIG. 3. Ion coupling parameter Γ versus time plasmas with Fermi correlated initial states. For $n = 1.1 \times 10^{11}$: (*a*) $\sigma_{\mathrm{QM}}^{\mathrm{eff}} = 0.01$; (*c*) $\sigma_{\mathrm{QM}}^{\mathrm{eff}} = 0.1$; (*d*) $\sigma_{\mathrm{QM}}^{\mathrm{eff}} = 0.5$; (*e*) $\sigma_{\mathrm{QM}}^{\mathrm{eff}} = 1.0$ (fully ionized); and for $n = 3.7 \times 10^{10}$: (*b*) $\sigma_{\mathrm{QM}}^{\mathrm{eff}} = 0.1$. Different values for $\sigma_{\mathrm{QM}}^{\mathrm{eff}}$ correspond to different levels of initial state correlations, which arise from varying degrees of ionization. Note that the heating is slower and less effective as the initial state correlations increase.

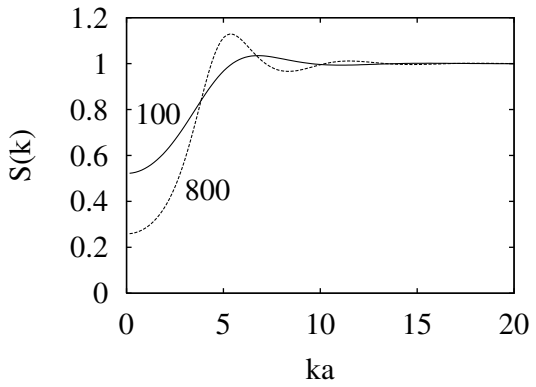

FIG. 4. Ion structure factors for $\Gamma = 100$ and $\Gamma = 800$ with $\kappa = 6.2$ from hypernetted chain calculations.

and $k_F = (6\pi^2 n)^{1/3}$ is the Fermi momentum. Correlations arise from the antisymmetric nature of the many-particle wave function that prohibits two ions from occupying the same physical space. An effective σ_{QM} can be obtained by noting that $g_{\mathrm{QM}}(r) \approx 0.5$ for $k_F r_\sigma \approx 2.4983$; thus, particles are less likely to be found with interparticle spacing below r_σ and vice versa, and r_σ plays the role that σ did for the classical case. We have $\sigma_{\mathrm{QM}} \sim r_\sigma/a = 1.0332$, which is obviously much larger than the $\sigma \sim 0.0001$ for the classical case.

The effective σ_{QM} is expected to be somewhat smaller than unity since the plasmas are usually partially ionized in the experiments. Partial ionization can be modeled by reducing σ_{QM} appropriately to account for the level of ionization. For 10% ionization the interparticle distance is reduced by about $10^{1/3} \approx 2.15$ and we take the effective σ to be $\sigma_{\mathrm{QM}}^{\mathrm{eff}} = 0.5$, which is still much larger than the ideal classical gas case. We performed several simulations to investigate Fermionic initial state correlations at the two (plasma) number densities $n = 3.7 \times 10^{10}$, 1.1×10^{11}. The ion mass was taken to be $m_i = 40 m_p$, which corresponds to the alkali potassium system, for which Fermi degeneracy has already been achieved [11]. Since the heating is extremely rapid, classical dynamics have been used in the evolution. This introduces a small error initially only for about $0.001\omega_p^{-1}$. The results are shown in Fig. 3. (Note the different scale on the ordinate.) For the lower density case, an ionization level corresponding to $\sigma_{\mathrm{QM}}^{\mathrm{eff}} = 0.1$ is shown. For the higher density case ionization levels corresponding to $\sigma_{\mathrm{QM}}^{\mathrm{eff}} = 0.01, 0.1, 0.5$, and 1.0 are shown. It is quite clear that introducing correlations into the initial state dramatically increases the final state Coulomb coupling. For the most correlated case the final Coulomb coupling is *orders of magnitude* higher than for the classical case. The structure factors $S(k)$, which can be measured in with light scattering, for cases (*b*) and (*d*) are shown in Fig. 4. This suggests a method by which the level of coupling can be experimentally measured.

In summary, it has been shown that significant heating of the ion component of an ultracold plasma occurs as correlations arising from strong Coulomb coupling develop. Heating occurs on a time scale of the order of the ion plasma frequency and is determined by the difference in correlations between the initial and final states. This has been confirmed by accurate nonequilibrium molecular dynamics simulations. Although this heating severely reduces the final level of coupling, we have shown that denser plasmas have higher levels of coupling in spite of greater heating. Moreover, we have shown that correlations can be introduced into the initial state, thereby maximizing the final coupling, by exploiting a Fermi degenerate atomic gas for which the Pauli hole mimics the Coulomb hole. Our results show that introducing initial state correlations yields coupling levels orders of magnitude larger. We also pointed out that this effect can be experimentally measured by laser scattering which yields the coupling dependent ion structure factor $S(k)$.

The author wishes to thank E. Timmermans for very useful discussions.

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