Simulation of the Expansion of an Ultracold Neutral Plasma

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We report the results of simulations that explain many properties of ultracold neutral plasmas. We find that three-body recombination is important at very low temperatures since it is a heating mechanism for the electron gas and it preferentially removes the slow ions from the plasma. We also find that collisions between cold electrons and Rydberg atoms are an important source of electron heating and deexcitation of atoms formed in the plasma. Simulations show that the Coulomb coupling constant does not become larger than $\sim 1/5$ for the reported experiments.

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Several recent experiments have investigated the behavior of ultracold plasmas that are nearly neutral but have a nonuniform spatial distribution [1–5]. In experiments at NIST [1–3], a cold plasma was produced by photoionizing Xe atoms held in a magneto-optical trap. The Xe^+ ions initially have the energy of the Xe atoms in the trap ($\sim 10~\mu$K) and the initial electron energy, E_e ($\sim 1-1000$ K), is controlled by tuning the laser that ionizes the Xe atom. The electron thermal pressure causes the plasma to expand. In these experiments, the plasma expands faster than expected at the lowest temperatures [2]. This has been related to enhanced electron-ion recombination at low temperatures; however, the mechanism controlling the recombination and the explanation for the observed distribution of electron binding energies are not known [3]. In other experiments [4,5], the excitation laser is tuned to highly excite, but not ionize, the atoms. The highly excited atoms then evolve into a plasma.

Ultracold plasmas are interesting systems for several reasons. The plasmas have very well-characterized initial conditions (E_e, size, etc.) that can be accurately controlled. The very low ion and electron temperatures are beyond the range of other neutral plasma experiments. The plasma parameters in some experiments are apparently in a range where the electron component of the plasma has a Coulomb coupling parameter larger than 1. The Coulomb coupling parameter [6] is the ratio of the electrostatic energy to the thermal energy: $\Gamma_e = (e^2/4\pi\varepsilon_0 a)/k_B T_e$ with $a = (3/4\pi n)^{1/3}$. If the Coulomb coupling parameter is larger than 1, then interesting plasma physics effects (such as Wigner crystals) could occur. Also, important atomic physics processes (namely electron-ion recombination) need to be reevaluated when $\Gamma_e \sim 1$.

In this paper, we present results from our simulations of ultracold plasmas. These simulations include basic processes in both plasma physics and atomic physics; without accurate treatment of both plasma and atomic processes, we find that the simulations produce nonphysical results. We have performed simulations at three levels of approximation for the electron dynamics: an electrostatic particle code with a Monte Carlo model of Coulomb collisions,

an isothermal fluid code, and an aggregated rate equation code. Most of the discussion in this paper will focus on the simplest model since it contains the relevant physics in the clearest form.

In the NIST experiments [1–3], a spherical cloud of essentially stationary atoms ($r_{\rm rms} \sim 340~\mu$m [7]) are photoionized using a laser pulse with a width of ~ 10 ns. Some electrons promptly leave the plasma [1]. This prompt loss occurs on a rapid time scale, $\sim r_{\rm rms}/v_e \sim 6$ ns for electrons with 100 K of kinetic energy. The prompt losses proceed until sufficient space charge builds to trap low energy electrons. Since the electrons are generated with a narrow band laser, they start with a nonthermal energy distribution. The electron thermalization time [8] can be estimated from $\tau_{ee} \sim 1.2 \times 10^{-6}~{\rm s}^4\,{\rm m}^{-6}\,v_e^3/n_e \ln(\Lambda)$ where $\Lambda = 4\pi\epsilon_0 3 k_B T_e \lambda_D/e^2$, λ_D is the Debye length, and e is the electron charge. For 100 K electrons with a density $n_e = 10^{15}~{\rm m}^{-3}$, $\ln(\Lambda) = 6.0$ and the thermalization time $\tau_{ee} \sim 64$ ns. While the electrons thermalize, some high energy electrons boil away, which reduces the electron number and temperature [1].

After the electrons thermalize, the plasma as a whole expands [2]. The characteristic expansion velocity is $v_{\rm exp} \propto \sqrt{k_B T_e/M_i}$ as is typical for ambipolar loss and plasma expansion into a vacuum [9]. The plasma expansion is a much slower process than the electron thermalization and can take up to 50 μs [2]. The expansion of the plasma is from the thermal pressure of the electrons and gives the ions a radially directed velocity; the ions gain very little thermal energy from the electrons since the ion-to-electron mass ratio is $\sim 2 \times 10^5$. During the plasma expansion, some of the electrons recombine with ions [3]. The mechanism for recombination is not known. Three-body recombination [(TBR), $e + e + A^+ \rightarrow A^* + e$] seems to be ruled out since it gives atoms with a binding energy of $E_b \sim 2k_B T_e$ nearly independent of the electron density [10]. The experiments measure distributions of binding energies that depend strongly on density and that, counterintuitively, extend to deeper binding energies as E_e decreases [3]. Another difficulty with TBR as the recombination mechanism is that the size of the resulting atom,

$R \sim e^2/4\pi\epsilon_0 E_b$, can be larger than the distance between ions. The ratio of the recombined atom's size to the distance between ions is $R/a \sim \Gamma_e/2$. Thus, TBR is not a simple process if the Coulomb coupling parameter becomes comparable to 1.

The most sophisticated theoretical treatment of ultracold plasmas is through a molecular-dynamics simulation of the electron and ion motion [11]. These simulations showed substantial recombination at the lowest temperatures but were restricted to times short compared to the ion expansion time. We performed simulations of the expansion of these small, ultracold plasmas at three levels of approximation in order to ensure that all relevant physics were included. In all simulations, the ions were treated as a zero temperature fluid since the ion thermal energy remains small compared to the radial kinetic energy from the plasma expansion.

Our most sophisticated treatment of the electrons used particles moving in a macroscopic radial electric field. The electric field is determined self-consistently from the electron and ion densities. We use a Monte Carlo method to model the effect of the Coulomb collisions of electrons with electrons and with ions [12]. The main result from these calculations is the number and temperature of the electrons that remain after the prompt loss and evaporation from the plasma. We also find that the electrons thermalize very rapidly on the time scale of the ion expansion for $E_e < 200$ K, as expected from the estimate given above [13].

We used the results from the Monte Carlo simulation to obtain the initial parameters for an isothermal fluid model. We assume that the ions have spherical spatial distribution and no pressure. The fluid equations for the ion density, $n_i(r, t)$, and the ion velocity, $\mathbf{v}_i(r, t) = \hat{r}v_i(r, t)$, are

$$\frac{\partial n_i}{\partial t} + \frac{1}{r^2}\frac{\partial r^2 v_i n_i}{\partial r} = 0,$$

$$\frac{\partial v_i}{\partial t} + v_i \frac{\partial v_i}{\partial r} = a, \qquad (1)$$

$$a(r, t) = \frac{e^2}{\epsilon_0 M_i r^2}\int_0^r [n_i(\bar{r}, t) - n_e(\bar{r}, t)]\bar{r}^2 \, d\bar{r},$$

where M_i is the ion mass, and a is the radial acceleration and the electron distribution, $n_e \propto \exp[-U(r)/k_B T_e]$. We take $v_i = 0$ and $n_i = N_i(\beta/\pi)^{3/2}\exp(-\beta r^2)$ as the initial conditions; N_i is the number of ions. The parameters, β, T_e, and N_e, are taken from the Monte Carlo simulation of the plasma using experimental initial conditions.

At each time step the electron potential energy, U, the electron density, n_e, and the electron temperature, T_e, must be found self-consistently with respect to three conditions: (i) the electrons are in thermal equilibrium, (ii) the number of electrons is conserved, and (iii) the total energy is conserved. We used a variation of the Poisson solver described in Ref. [9].

In Fig. 1, we graph the scaled radial acceleration as a function of the scaled radial distance from the center of the plasma for three different temperatures. It is apparent from this figure that for most of the ions the acceleration is proportional to the temperature and to the radial distance from the plasma center. The acceleration is proportional to $r \cdot T_e$ because the electron distribution must be proportional to $\exp(-U/k_B T_e)$ to be in thermal equilibrium *and* it must be nearly equal to the ion distribution, $\propto \exp(-\beta r^2)$, since $N_i - N_e \ll N_i$. This means $U = -(\beta k_B T_e)r^2 + $ const which gives an ion acceleration of $a = r2\beta k_B T_e/M_i$. An acceleration linear in r gives a velocity linear in r which preserves a Gaussian spatial distribution.

Since most of the ions experience an acceleration proportional to r, this leads us to our simplest model for the plasma dynamics: set $n_i(r, t) = N_i[\beta(t)/\pi]^{3/2} \times \exp[-\beta(t)r^2]$, $v_i(r, t) = \gamma(t)r$, and $a(r, t) = r2\beta(t) \times k_B T_e(t)/M_i$. Substituting this ansatz into Eq. (1) gives the following ordinary differential equations:

$$\frac{d\gamma}{dt} + \gamma^2 = 2k_B T_e(t)\beta(t)/M_i,$$

$$\beta(t) = \beta(0)\exp\left[-2\int_0^t \gamma(\bar{t})\,d\bar{t}\right], \qquad (2)$$

$$\frac{3}{2}k_B T_e(0) = \frac{3}{2}k_B T_e(t) + \frac{3}{4}M_i \frac{\gamma^2(t)}{\beta(t)},$$

where $\gamma(0) = 0$ and the last relationship is simply the conservation of energy: thermal electron energy plus the kinetic energy of the ions is constant. At the low temperatures of this paper the energy in the macroscopic electric fields are a small fraction of those in Eq. (2).

In Fig. 2, we show the experimentally measured asymptotic expansion velocity versus the initial energy per created ion. At high energies ($E_e > 40-50$ K), the asymptotic velocity simply arises from the conservation
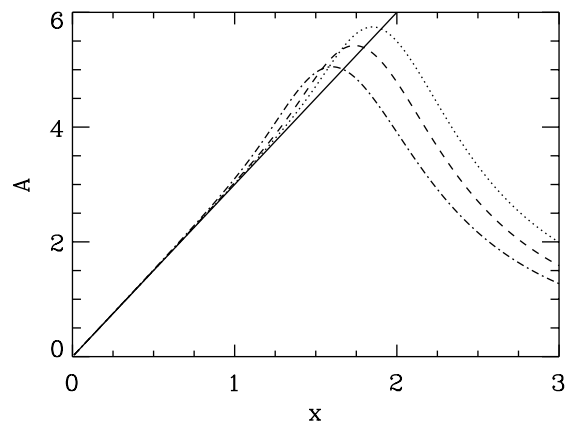

FIG. 1. The scaled acceleration, $A = a(r)M_i\sqrt{\langle r^2 \rangle}/k_B T_e$, versus the scaled radial distance $x = r/\sqrt{\langle r^2 \rangle}$ for electron temperatures of 15 K (dotted line), 30 K (dashed line), and 75 K (dot-dashed line). The solid line is the model result from $a = (2\beta k_B T_e/M_i)r$ which is equivalent to $A = 3x$.
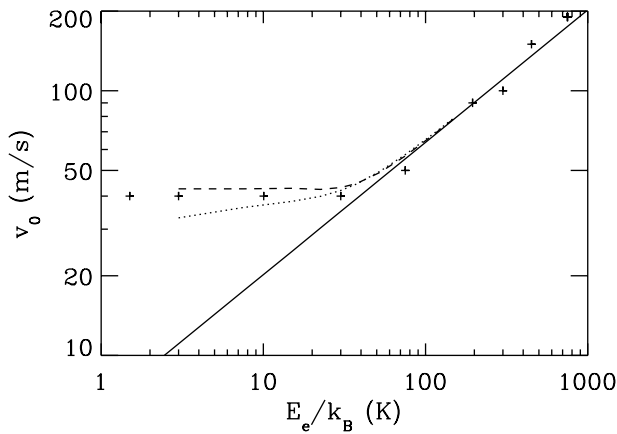
FIG. 2. Asymptotic expansion velocity, v_0, as defined in Ref. [2] as a function of the initial energy per ion. The crosses indicate representative experimental results [2]. The solid line is with no three-body recombination. The dotted line is with three-body recombination but no electron-Rydberg atom scattering. The dashed line is with three-body recombination and electron-Rydberg scattering. The calculations are for the initial average density of $n_e = 10^{15}$ m^{-3}.

of energy [2]. At lower energies, the plasma expands much faster than expected. In Ref. [3], the presence of Rydberg atoms was detected after the plasma expanded. At low temperatures there is substantial formation of Rydberg atoms. When a Rydberg atom forms, an electron goes to negative energy and thus (by conservation of energy) the remaining electrons must increase in energy. Recombination acts as a source of energy which causes the plasma to expand faster than expected.

Although the discussion above argues that a new recombination method is needed, the rest of this paper shows that a proper treatment of three-body recombination *and* of the subsequent behavior of the Rydberg atoms can explain all of the observed features of expanding, ultra-cold plasmas. In the simulations presented below, three-body recombination is included as usual: the number of recombinations during a time interval, δt, is given by $N_r = \delta t C T_e^{-9/2} \int n_e^2 n_i \, dV$, where the constant C is well known [14] and the energy given to the "plasma" is $\Delta E = 2k_B T_e N_r$ [10]. Interestingly, the recombination preferentially occurs where the density is highest which is the region where the ions are slowest; by removing the slowest ions, the average ion energy increases.

If we only include three-body recombination, we get an asymptotic expansion velocity which is in somewhat better agreement with experiments (dotted line in Fig. 2) but there still exist serious discrepancies. At the lower temperatures, we find that a substantial fraction of the ions recombine with electrons (e.g., one-third recombine for the 15 K case and one-half recombine for the 7.5 K case). This large a fraction of recombination was not observed. The distribution of binding energy of the Rydberg atoms does not agree with experiment: higher E_e gives larger binding energies in the simulation, whereas the opposite trend was observed [3].

The missing mechanism is electron scattering from the resulting Rydberg atoms [15]. We account for the electron-Rydberg scattering using the collision kernel in Ref. [14]. This includes deexcitation, excitation, and ionization: deexcitation heats the electron plasma, excitation cools the electron plasma, and ionization cools the electron plasma and increases the electron density. All three types of collision are important to correctly describe the evolution of the Rydberg population and the free electron temperature. A crude estimate of the importance of the electron-Rydberg atom scattering can be obtained from the geometrical size of the atom $R = e^2/4\pi\epsilon_0 E_b$ and the velocity of the electron $v = \sqrt{3k_B T_e/m_e}$; the collision rate is $\Gamma_{e-\mathrm{Ryd}} \sim \pi R^2 v n_e$. An atom with a 20 K binding energy has a size $R \sim 0.8$ μm; an electron at 10 K has a velocity of $v \sim 2 \times 10^4$ m/s; this gives a rate of 4×10^7 Hz (a collision every 25 ns) at an electron density of 10^{15} m^{-3}. Our results did not depend strongly on the exact form for the electron-Rydberg cross section because a successful deexcitation increases the binding energy and thus reduces subsequent scattering (the geometrical cross section is proportional to E_b^{-2}).

The results from including electron-Rydberg scattering are plotted in Fig. 2 using the dashed line. The simulation now reproduces all of the major features of the experiments without adjustable parameters. The asymptotic expansion velocity of the ions now plateaus for energies less than $\sim$40 K. We find that the distribution of binding energies is not very sensitive to E_e in the plateau region <40 K. At the higher E_e, we find that the recombined electrons are less deeply bound than at the lower input energies: the higher E_e plasmas expand faster which reduces the number of electron-Rydberg deexcitation collisions. We also find that the binding energy increases with the electron density for a fixed input energy because the higher electron density increases the number of electron-Rydberg atom deexcitation collisions.

Although the simulation reproduces all the main features of the experiments, we must check that the calculations are self-consistent. In particular, if the Coulomb coupling parameter becomes comparable to 1 then the electrons can not be described by a simple density in thermal equilibrium, and the three-body recombination does not make sense when $\Gamma_e \sim 1$ since that means the resulting atoms are comparable in size to the distance between ions. In Fig. 3 we plot the Coulomb coupling parameter versus time for two different initial input energies. It is clear that the plasma coupling constant only increases with time if three-body recombination is not included in the simulation; eventually, the plasma becomes strongly coupled and the fluid equations would break down. The reason for the increase is that the temperature of the plasma falls more rapidly than the size of the plasma increases; from Eq. (2), the plasma temperature must decrease to balance the kinetic energy given to the ions.

If three-body recombination is included in the simulation, the Coulomb coupling parameter behaves in a more
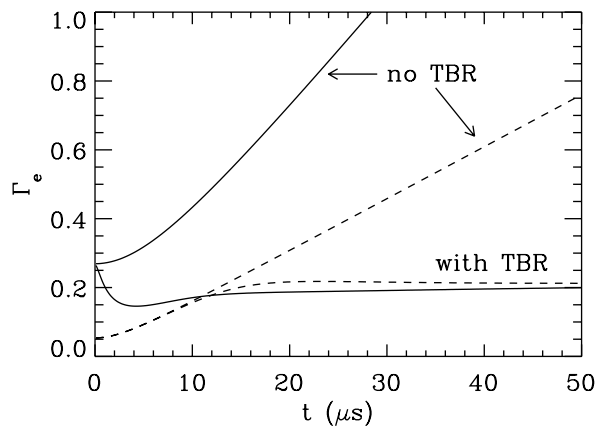
FIG. 3. Coulomb coupling constant, Γ_e, versus time for two initial energies: $E_e/k_b = 15$ K (solid lines) and 75 K (dashed lines). For each energy, one simulation does not include three-body recombination (TBR) and one simulation includes TBR and electron-Rydberg scattering. Note that including three-body recombination keeps Γ_e less than $\sim 1/5$. The calculations are for initial average density of $n_e = 10^{15}$ m^{-3}.

interesting way. For the higher temperatures (when Γ_e is initially less than $\sim 1/5$), the Coulomb coupling parameter initially increases (because T_e is decreasing) but then plateaus at a value of $\sim 1/5$. For lower temperatures (when Γ_e is initially larger than $\sim 1/5$), the Coulomb coupling parameter decreases rapidly until it plateaus at a value of $\sim 1/5$. This shows that our simulation of the plasma is self-consistent. The Coulomb coupling parameter is much less than 1 during the main part of the expansion which means the plasma can be described by the simple fluid equations used here. Also, the recombination occurs in atoms whose size ($\sim \Gamma_e/2$) is one-tenth of the distance between the ions which means we do not need to invoke new atomic physics mechanisms to describe the recombination.

The behavior of the Coulomb coupling parameter when including three-body recombination can be understood through qualitative arguments. The three-body recombination rate is proportional to $n_e^2 T_e^{-9/2}$ which means the rate increases rapidly as the temperature drops. Three-body recombination tends to turn itself off because every recombination decreases the density and increases the temperature of the remaining electrons. If the ions were frozen in space, $\Gamma_e \propto n_e^{1/3}/T_e$ only decreases. If the ions move, Γ_e tends to increase as discussed above. The interplay of these two tendencies gives the plateau in Fig. 3. We find that the plateau value of the Coulomb coupling parameter is not very sensitive to the plasma parameters because the three-body recombination increases very rapidly with decreasing temperature.

In conclusion, our simulations show that the recent experiments on ultracold plasmas [1–3] can be explained through a proper treatment of both the plasma and atomic physics. The simulations are robust and self-consistent: recombination is into states smaller than one-tenth the average distance between ions, and the Coulomb coupling parameter does not become larger than $\sim 1/5$. We find that

the counterintuitive distribution of binding energies can be explained by electron-Rydberg atom scattering: the binding energies are larger at higher densities because there are more deexcitations, and the binding energy is smaller at higher temperatures because the hotter plasmas expand faster which reduces the number of electron-Rydberg collisions.

There are several predictions that follow from these simulations that can, in principle, be tested experimentally. (i) *All* plasma dynamics should vary smoothly with initial electron energy if all other plasma parameters (density, size, etc.) are fixed; in particular, the behavior will not vary strongly even as the initial electron energy is reduced to 0 K. (ii) The expansion velocity of a Rydberg atom depends on the ion velocity at the time the recombination occurs; this time can be roughly related to the binding energy, and thus trends in the expansion velocity of a Rydberg atom versus binding energy should be observable. (iii) For spherical plasmas, the temperature of the plasma will either rapidly decrease or increase to reach $\Gamma_e \sim 1/5$; this condition gives an estimated temperature given by $k_B T_e \sim 5e^2/4\pi\epsilon_0 a$.

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