Influence of electron–ion collisions on Coulomb crystallization of ultracold neutral plasmas

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Abstract

While ion heating by elastic electron–ion collisions may be neglected for a description of the evolution of freely expanding ultracold neutral plasmas, the situation is different in scenarios where the ions are laser-cooled during the system evolution. We show that electron–ion collisions in laser-cooled plasmas influence the ionic temperature, decreasing the degree of correlation obtainable in such systems. However, taking into account the collisions increases the ion temperature much less than what would be estimated based on static plasma clouds neglecting the plasma expansion. The latter leads to both adiabatic cooling of the ions as well as, more importantly, a rapid decrease of the collisional heating rate.

Recently, the field of ultracold ($T \ll 1$ K) neutral plasmas and Rydberg gases has attracted attention both experimentally [1–3] and theoretically [4–9]. One of the motivations of the experiments [1, 10] is the creation of a so-called strongly coupled plasma, where the Coulomb coupling parameter $\Gamma_1 = e^2/(a k_B T_i)$ is much larger than unity (where $a = (4 \pi \rho_i/3)^{-1/3}$ is the Wigner–Seitz radius and $T_i$ is the temperature of the ions). In such a case, interesting ordering effects such as Coulomb crystallization into cubic or shell-structure lattices can be observed. In the experiments [1] strongly coupled ions cannot be observed since the temperature of the initially cold ions rises quickly on the timescale of the inverse ionic plasma frequency $\omega_{p,i}^{-1} = \sqrt{m_i/(4 \pi e^2 \rho_i)}$ due to disorder-induced heating [4, 6, 7]. Different ways to overcome this heating effect have been proposed [4, 11–15]. In [12, 13], e.g., it was suggested that continuous laser cooling during the plasma expansion may considerably increase the achievable Coulomb coupling parameter of the ions.

Using a hybrid molecular dynamics approach [16], we have predicted that Coulomb crystallization in an unconfined ultracold neutral plasma can indeed be obtained if the plasma ions are laser-cooled during the evolution of the system [14]. In this theoretical approach, the electronic component of the plasma is treated as a fluid while ions and recombined atoms...
are described on a full molecular dynamics level. More precisely, an adiabatic approximation is made for the electrons, which are assumed to be distributed according to the mean-field potential generated by ions and electrons, calculated in a self-consistent way. Their velocity distribution is assumed to be of Michie–King-type [17] which takes into account deviations of the quasi-equilibrium state from a Maxwell–Boltzmann distribution due to the finite depth of the potential well generated by the ions. The latter leads to an evaporation of a fraction of the electrons in the initial stage immediately after the plasma formation, which is taken into account using the results of [1]. The ions, on the other hand, are propagated under the influence of all other ions and the electronic mean-field. Finally, inelastic collisions, i.e. three-body recombination, electron-impact ionization and electron-impact (de)excitation, are included on the basis of a Monte Carlo treatment. 

Elastic electron–ion collisions, however, are neglected in this approach, as in other approaches for the description of ultracold plasmas [18].

This neglect of elastic electron–ion collisions in the dynamics is well justified for the description of freely expanding ultracold plasmas as created in [1] because of a clear separation of timescales. Due to the large mass ratio between ions and electrons, the time necessary for equilibration of the electron and ion temperature is typically of the order of a few milliseconds, while the plasma expansion takes place on a microsecond timescale. Hence, elastic electron–ion collisions only increase the ion temperature by some milli-Kelvin during the experimental observation time [1]. This amount of heating is negligible compared to the initial temperature increase due to disorder-induced heating, which raises the ion temperature to about one Kelvin. Hence, the time evolution of the ion temperature which enters $\Gamma_i$ and determines the degree of coupling of the ions is mainly determined by this disorder-induced heating.

However, this situation changes in the scenario of [14], where additional laser cooling of the ions compensates the disorder-induced heating and keeps the ionic temperature on a milli-Kelvin level. In this case, the ion temperature is not only increased by electron–ion collisions, but is also driven to the Doppler temperature, i.e. the limiting temperature $T_c$ for laser cooling, due to the coupling to the radiation field. The final ion temperature is now determined by the balance between the collisional heating rate and the laser-cooling rate [12, 13]. Since $T_c$ is typically of the order of one milli-Kelvin, i.e. of the same order of magnitude as the amount of collisional heating, the ion temperature may considerably increase through electron–ion collisions. Thus, electron–ion collisions could significantly decrease the Coulomb coupling parameter achievable by laser-cooling of expanding ultracold neutral plasmas. In the following, the influence of such collisions on the onset of Coulomb crystallization during the plasma expansion is critically reassessed.

The system under study is the same as that of [14], namely an unconfined, ultracold neutral plasma under the additional influence of a cooling laser. The plasma is treated on the basis of the hybrid-MD method outlined above and described in detail in [16]. Laser cooling is modelled by adding a Langevin force, $F_{\text{cool}} = -m_i \beta v_i + \sqrt{2 \beta k_B T_c m_i} \xi$, to the ion equation of motion, where $v_i$ is the ion velocity, $\xi$ is a stochastic variable with $\langle \xi \rangle = 0$, $\langle \xi(t) \xi(t + \tau) \rangle = 3 \delta(\tau)$ and the cooling rate $\beta$ and the corresponding Doppler temperature $T_c$ are determined by the properties of the cooling laser [19]. The weak electron coupling, which justifies our hybrid treatment of the plasma dynamics, also allows us to describe electron–ion collisions with a Boltzmann-type collision operator, as we shall discuss below. The implementation of electron–ion collisions is very similar to the treatment of electron–electron collisions used in [18] and has been introduced before in [20]. For an ion at position $\mathbf{r}_i$ with velocity $\mathbf{v}_i$, the rate of electron–ion collisions is

$$K_{\text{eic}} = \int d\mathbf{v}_e d\Theta \sin \Theta \left( \frac{d\sigma}{d\Theta} \right)_{\text{eff}} |\mathbf{v}_i - \mathbf{v}_e| f_e(\mathbf{r}_i, \mathbf{p}_e).$$

(1)
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Hence, \( P_{\text{eic}} = \Delta t K_{\text{eic}} \) is the probability that a collision will occur during a timestep \( \Delta t \). Numerically, the integration over the electronic velocity distribution in equation (1) is done via a Monte Carlo procedure. At each timestep, an electronic velocity \( v_e \) is chosen randomly according to a Maxwell–Boltzmann distribution with temperature \( T_e \). The probability for an electron–ion collision is then given by

\[
P_{\text{eic}}(v_e) = \Delta t \, \rho_e(r_i) v_e \int_{-1}^{1} \left( \frac{d\sigma}{d\Theta} \right)_\text{eff} \, d(\cos \Theta) = \Delta t \, \rho_e(r_i) v_e \frac{\pi \epsilon^4}{m_e v_e} (\Lambda - 1),
\]

with \( \ln \Lambda = \ln \left( \sqrt{3}/\Gamma_e^{3/2} \right) \) the so-called Coulomb logarithm and

\[
\left( \frac{d\sigma}{d\Theta} \right)_\text{eff} = \left\{ \begin{array}{ll}
\left( \frac{d\sigma}{d\Theta} \right)_\text{Coul} & \Theta \geq \Theta_{\text{min}} \\
0 & \Theta < \Theta_{\text{min}},
\end{array} \right.
\]

where \( \left( \frac{d\sigma}{d\Theta} \right)_\text{Coul} \) is the Rutherford cross section for Coulomb scattering [21] and \( \Theta_{\text{min}} = 2 \arcsin \Lambda^{-1/2} \) [22]. In the derivation of equation (2), the approximation \( m_e/m_i \to 0, v_i \to 0 \) has been made (see below).

In the Monte Carlo treatment outlined above, an electron–ion collision takes place with a probability \( P_{\text{eic}}(v_e) \). In this case, a scattering angle \( \Theta \) is determined according to the probability measure \( P(\Theta) \propto \left( \frac{d\sigma}{d\Theta} \right)_\text{eff} \), leading to the prescription

\[
\cos \Theta = \frac{\zeta(\Lambda - 1) - 1}{\zeta(\Lambda - 1) + 1},
\]

where \( \zeta \) is a random number distributed uniformly in \([0, 1]\). With this, the change of ionic momentum is given by \( \Delta p_i = m_e v_e (1 - \cos \Theta) \hat{\mathbf{j}} \), where \( \hat{\mathbf{j}} \) is a vector denoting the random direction of the momentum transfer chosen uniformly on the unit sphere. Finally, energy conservation is restored by adjusting the electronic temperature \( T_e \).

As mentioned above, the derivation of equation (2) implies the limit \( m_e/m_i \to 0 \). In this case, individual collision events satisfy momentum conservation, but energy conservation is violated and has to be corrected manually by adjusting the electron temperature. The error introduced by this approximation can be shown to be of the order of the temperature ratio \( T_i/T_e \) [23]. Hence, as long as the ionic temperature is small compared to the electronic temperature, which is the case over the whole time of the experiments under consideration, the corresponding corrections can be neglected. The method described above thus allows for an efficient simulation of electron–ion collisions without the need for time-consuming transformations between laboratory and centre-of-mass coordinate systems.

In order to check the influence of elastic electron–ion collisions on the plasma dynamics, we have simulated the expansion of a plasma with an initial electronic Coulomb coupling parameter of \( \Gamma_e(t = 0) = \Gamma_{e0} = 0.05 \), consisting of 20\,000 Be ions at a density of \( \rho_i(t = 0) = \rho_0 = 2.3 \times 10^8 \text{ cm}^{-3} \), cooled with a damping rate of \( \beta = 0.10 \nu_{pi}, (t = 0) \) and a Doppler temperature of 1 mK. As can be seen in figure 1, the inclusion of elastic electron–ion collisions significantly reduces the ionic coupling parameter which can be achieved in this case. However, the value \( \Gamma_i \) obtained after several \( \mu \)s is still considerably larger than the critical value \( \Gamma_{i,c} = 174 \) [24] for crystallization. The good agreement found between the distribution of interionic distances, calculated as described in [14], and the pair-correlation function of a one-component plasma at \( \Gamma_i = 400 \) [25] also confirms that the system evolves well into the strongly coupled regime (figure 2). We note here that Debye shielding of the ion–ion interaction, which is not included in the present considerations, tends to increase the crystallization limit. However, as shown in [26], even for a comparably large electron coupling of \( \Gamma_e = 0.2 \) the crystallization limit is increased to \( \Gamma_{i,c} \approx 198 \) only, hence the inclusion of Debye screening does not significantly alter the results obtained with the present model.
Figure 1. Time evolution of the ionic Coulomb coupling parameter with (solid line) and without (dashed line) the inclusion of ion heating by electron–ion collisions for a plasma of 20 000 Be ions with $\rho_{i0} = 2.3 \times 10^8$ cm$^{-3}$, $\Gamma_{i0} = 0.05$, $\beta = 0.10 \omega_{pe}$, $\Gamma_{i}(t = 0)$ and $T_c = 1$ mK.

Figure 2. Distribution of scaled interionic distances after a time of $t = 40 \mu$s, compared to the calculated pair–correlation function of an OCP at $\Gamma_{i} = 400$. The initial-state parameters are the same as in figure 1.

In fact, the simulation results show that the final $\Gamma_{i}$ is much larger than what one would expect from a static estimate by equating the heating $\gamma_{eic} T_e$ resulting from electron–ion collisions to the cooling $2 \beta (T_i - T_e)$ of the laser cooling as done in [12, 13]. From the procedure described above, $\gamma_{eic}$ is obtained as

$$\gamma_{eic} = \frac{2}{3k_B} \int d\mathbf{v}_e d\Theta \sin \Theta \frac{m_e v_e^2}{2} (1 - \cos \Theta)^2 \left( \frac{d\sigma}{d\Theta} \right)_{eff} v_e f_e(r_i, p_e),$$

leading to the Landau–Spitzer expression for the average heating rate [27]

$$\gamma_{eic} = \sqrt{\frac{2}{3\pi}} \frac{m_e}{m_i} \Gamma_i^{3/2} \omega_{pe} \ln \Lambda,$$

where $\omega_{pe}$ is the electronic plasma frequency. The validity and extensions of the Landau–Spitzer formula, which was originally derived for weakly coupled plasmas, have been discussed.

$^1$ Again, this implies the limit $T_i/T_e \rightarrow 0$ which is well-fulfilled over the whole timescale of the experiments as described above.
in several publications [27–30]. In [27], ion heating by binary collisions has been studied without employing the cutoff-procedure equation (3). For $\Gamma_i < 0.25$, their numerical results are reproduced by equation (6) to within 10%. Moreover, collective effects, which largely decrease the relaxation rate at strong coupling [29], were found to be negligible even for arbitrarily strong ion–ion coupling, as long as the electron–ion coupling is weak and the resonance of the ion excitation spectrum lies far below that of the electrons [30]. Therefore, under the present conditions, which correspond to the parameter regime studied in [30], the Monte Carlo treatment described above yields an adequate description of the electron–ion temperature relaxation process.

Balancing collisional heating with the laser cooling one might expect a quasi-equilibrium state with a final ion temperature of

$$T_i = \frac{\gamma_{\text{eic}}}{2\beta} T_e + T_c,$$

leading to a Coulomb coupling parameter

$$\Gamma_i = \sqrt{\frac{6\pi m_i}{\Gamma_e m_e}} (\ln A)^{-1} \frac{\beta}{\omega_{\text{pe}}},$$

in the optimal limit that $T_c \rightarrow 0$. For the parameters used in figure 1, equation (8) predicts a final $\Gamma_i \approx 50$, which is much smaller than what is observed in the simulation.

In order to trace the origin of this discrepancy, we have performed a second set of simulations. In one simulation, we have set the Doppler temperature $T_c$ equal to zero and have turned off the initial correlation-induced heating of the ions by propagating them in the framework of a particle-in-cell method [18], i.e. on a mean-field level, rather than by a full MD simulation. By doing this, only the competition between the laser cooling, the heating by electron–ion collisions and the adiabatic expansion determines the evolution of the ion temperature. In the second type of simulation, $T_c$ is also set to zero and all particle interactions except the binary electron–ion collisions causing the ion heating are neglected, which results in a basically static ionic density.

The resulting time evolution of the ionic temperature for a plasma of 100,000 ions with $\rho_{i0} = 2 \times 10^7 \text{ cm}^{-3}$, $\Gamma_{i0} = 0.08$ and $\beta = 0.15 \omega_{\text{pe}}$ ($t = 0$) is shown in figure 3. In the static case (dashed line in figure 3), the temperature shows an initial linear rise with a slope corresponding to the collisional heating rate $\gamma_{\text{eic}} T_e$ and then quickly saturates to a value which is well described by equation (7) (marked by the arrow in the figure). However, in the case of an expanding plasma (solid line in figure 3) the temperature is drastically reduced. While the initial rise of the ion temperature stays the same, the temperature starts to drop already at a relatively early time, which at this stage is mainly caused by adiabatic cooling of the ions due to the plasma expansion. At later times, the ion temperature is driven to its steady-state value given by the balance between the collisional heating and the laser cooling (equation (7)). The long-time behaviour of the ionic temperature can be estimated from the plasma dynamics discussed in [14], where it was found that laser cooling strongly alters the expansion behaviour, leading to an increase of the plasma width $\sigma$ according to $\sigma \propto t^{1/4}$. It was also shown there that the adiabatic law for the selfsimilar plasma expansion, $\sigma^2 T_e = \text{const.}$, still holds, which gives together with equation (7) for $T_e \rightarrow 0$

$$T_i \propto \frac{1}{\sigma^{1/2} T_e^{1/2}} \propto \sigma^{-2} \propto t^{-1/2},$$

The slow diffusion of the ion distribution due to the finite ion temperature is negligible during the time of the simulation.
Figure 3. Time evolution of the ionic temperature for a plasma of 100,000 ions with $\rho_0 = 2 \times 10^7$ cm$^{-3}$, $\Gamma_{ei} = 0.08$ and $\beta = 0.15\alpha_{ei}(t = 0)$, using different levels of approximation (see text). The arrow shows the static estimate equation (7) for the final ion temperature, the dotted line in the inset equation (9).

Figure 4. Radial density of a plasma of 50,000 ions with initial-state parameters $\rho_0 = 2 \times 10^7$ cm$^{-3}$, $\Gamma_{ei} = 0.08$, $\beta = 0.17\alpha_{ei}(t = 0)$ and $T_c = 0.8$ mK after $t = 175$ $\mu$s, demonstrating the radial ordering in the inner plasma region.

while the ionic Coulomb coupling parameter increases according to $\Gamma_i \propto 1/\sigma T_e \propto t^{1/4}$. As can be seen in the inset of figure 3, equation (9) is well-reproduced by the numerical simulation. Hence, it is indeed this adiabatic cooling of the expanding plasma together with a decreasing collisional heating rate $\gamma_{ei} T_e$ which leads to much lower temperatures and consequently to much larger Coulomb coupling parameters than those predicted by a static estimate.

The simulations described above demonstrate that electron–ion collisions do not prohibit achieving ionic Coulomb coupling parameters above the crystallization limit. However, for a given set of initial-state parameters, $\Gamma_i$ can be significantly reduced by collisional heating during the plasma evolution, leading to an additional restriction of the initial-state parameters for which strongly coupled states can be achieved. Since it was found that the degree of spatial order in the system sensitively depends on initial conditions such as the number of ions, electron temperature etc, one may wonder whether the long-range ordering into shell structures described in [14] is still observable in simulations taking into account the electron–ion collisions. This is demonstrated in figure 4 for a plasma of 50,000 ions with a density of
$\rho_{i0} = 2 \times 10^7 \text{ cm}^{-3}$ and $\Gamma_{i0} = 0.08$, cooled with a damping rate of $0.17 \alpha_{p,1} (t = 0)$ and a limiting temperature of $T_c = 0.8$ mK. The ordering into concentric shells is clearly visible in the radial density after a time of $t = 175 \mu$s.

In summary, we have presented simulations for laser-cooled ultracold neutral plasmas including elastic electron–ion collisions. It is found that these collisions can have a significant influence on the final ionic temperature, and hence the degree of correlation, achievable under given experimental conditions. Yet, with a proper choice of initial conditions rather large Coulomb coupling parameters can still be achieved. As we have shown, this is due to the fact that the expansion of the plasma drastically reduces the ion temperature, due to adiabatic cooling of the ions as well as a decreasing heating rate during the course of the plasma evolution. Therefore, the resulting Coulomb coupling parameters are much larger than one would expect from static estimates as in [12, 13]. We thus conclude that our predictions made in [14] about the possibility of observing Coulomb crystallization in such a system remain valid. In particular, we have shown here that the electron–ion collisions do not preclude the build-up of long-range order and the formation of the shell structures predicted in [14]. The experimental realizability of the discussed scheme has been demonstrated recently in [10]. There, the ion temperature of an ultracold strontium plasma was measured by driving the core transition of the plasma ions during the gas expansion. Since the same transition which allowed for Doppler imaging can be used to cool the ions, these experiments provide the first step towards a realization of strongly coupled ultracold plasmas in the laboratory.

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References

[1] Killian T C, Kulin S, Bergeson S D, Orozco L A, Orzel C and Rolston S L 1999 Phys. Rev. Lett. 83 4776
[2] Robinson M P, Tolra B L, Noel M W, Gallagher T F and Pillet P 2000 Phys. Rev. Lett. 85 4466
[3] Dutta S K, Feldbaum D, Walz-Flannigan A, Guest J R and Raithel G 2001 Phys. Rev. Lett. 86 3993
[4] Murillo M S 2001 Phys. Rev. Lett. 87 115003
[5] Robicheaux F and Hanson J D 2002 Phys. Rev. Lett. 88 055002
[6] Kuzmin S G and O’Neil T M 2002 Phys. Rev. Lett. 88 065003
[7] Mazevet S, Collins L A and Kress J D 2002 Phys. Rev. Lett. 88 055001
[8] Tkachev A N and Yakovlenko S I 2001 Quantum Electron. 31 1084
[9] Pohl T, Pattard T and Rost J M 2003 Phys. Rev. A 68 010703(R)
[10] Simien C E, Chen Y C, Gupta P, Laha S, Martinez Y N, Mickelson P G, Nagel S B and Killian T C 2004 Phys. Rev. Lett. 92 143001
[11] Gericke D O and Murillo M S 2003 Contrib. Plasma Phys. 43 298
[12] Kuzmin S G and O’Neil T M 2002 Phys. Plasmas 9 3743
[13] Killian T C, Ashoka V S, Gupta P, Laha S, Nagel S B, Simien C E, Kulin S, Rolston S L and Bergeson S D 2003 J. Phys. A: Math. Gen. 36 6077
[14] Pohl T, Pattard T and Rost J M 2004 Phys. Rev. Lett. 92 155003
[15] Pohl T, Pattard T and Rost J M 2004 J. Phys. B: At. Mol. Opt. Phys. 37 L183
[16] Pohl T, Pattard T and Rost J M 2004 Preprint physics/0405125 (Phys. Rev. A at press)
[17] King I R 1966 Astron. J. 71 64
[18] Robicheaux F and Hanson J D 2003 Phys. Plasmas 10 2217
[19] Metcalf H J and van der Straten P 1999 Laser Cooling and Trapping (New York: Springer)
[20] Nanbu K 1980 J. Phys. Soc. Japan 49 2042
[21] Friedrich H 1998 Theoretical Atomic Physics (Berlin: Springer)
[22] Li D 2001 Nucl. Fusion 41 631
[23] Pohl T 2004 PhD Thesis T U Dresden, Germany (in preparation)
[24] Dubin D H E and O’Neil T M 1999 Rev. Mod. Phys. 71 87
[25] Ng K C 1974 J. Chem. Phys. 61 2680
[26] Hamaguchi S, Farouki R T and Dubin D H E 1996 J. Chem. Phys. 105 7641
[27] Gericke D O, Murillo M S and Schlanges M 2002 Phys. Rev. E 65 036418
[28] Lee Y T and More R M 1984 Phys. Fluids 27 1273
[29] Dharma-wardana M W C and Perrot F 1998 Phys. Rev. E 58 3705
  Dharma-wardana M W C and Perrot F 2001 Phys. Rev. E 63 069901 (erratum)
[30] Hazak G, Zinamon Z, Rosenfeld Y and Dharma-wardana M W C 2001 Phys. Rev. E 64 066411