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Temperature estimates for quantum systems after an ionization induced rapid switch of the spin statistics

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Abstract

It has recently become possible to create ultracold plasmas in the microkelvin temperature regime. Unfortunately, these plasmas are created in a disordered state and the build up of Coulomb correlations leads to rapid electron and ion heating that can be understood in terms of energy conservation. We explore this disorder–induced heating for the ionization of degenerate gases. In particular, we consider the ionization of fermionic gases, which are partially ordered by the Pauli exclusion principle, and the subsequent heating of the bosonic ions. The introduction of fermionic correlations mitigates the heating of the ions. However, we find from energy conservation that the final state for typical experimental situations is a classical plasma where the bosonic character of the particles is negligible.

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1. Introduction

In the recent years impressive progress has been made on the experimental techniques to create and diagnose dilute, ultracold many-body systems. For very low temperatures, clear signatures of quantum degeneracy effects have been observed. For instance, Bose–Einstein condensates (BEC) [1–3] and degenerate Fermi systems [4, 5] have been created in systems of trapped atoms. Due to the weak atom–atom interactions and the large interatomic distance, such systems behave almost as ideal gases.

Furthermore, ultracold plasmas, i.e. systems of charged particles have been created by laser ionization of ultracold gases [6, 7] and spontaneous ionization of Rydberg atoms [8]. In the plasma case, the interparticle potentials are much stronger than for the neutral phase leading to a build up of correlation energy shortly after the ionization process, which drives a rapid increase of the electron and ion temperatures [9, 10]. It has been suggested that an introduction of initial correlation by ionizing a degenerate gas of fermionic atoms can reduce this heating [9].

Moreover, the ionization process establishes a sudden switch of the statistics the particles obey since the fermionic atoms become bosonic ions plus electrons. Therefore, the question arises if the switch of statistics further reduces the ion heating. If heating could be avoided or the final temperature could be at least held below a few microkelvins, novel systems ranging from BEC consisting of charged particles to Coulomb crystals could be created.

We introduce here an approach that estimates the temperature achieved after a change of the statistics. We emphasize again that this is related to a switch of the interactions from a weak atom–atom to a screened Coulomb potential. Our calculations are only based on the conservation of total energy which requires estimates for the correlation, exchange and kinetic energy of a degenerate system. First we consider ideal quantum and correlated classical systems as limiting cases. The results indicate that an ideal treatment is only possible for weakly interacting atomic systems. In particular, we demonstrate that the correlations have to be included for ionic systems since, otherwise, energy conservation cannot be achieved while switching from Fermi to Bose statistics. Finally, we give the results for the final temperature of a plasma created by ionizing a degenerate Fermi gas.

2. Connection between final temperature and initial conditions

We consider an ultracold, degenerate atomic gas in a trap. These atoms are ionized by a short-pulse laser at $t = 0$. Due to the large mass ratio of ions and electrons, the latter pick up almost the entire laser energy. For the same reason, the time for energy equilibration between electrons and ions is much longer than the relaxation of the ion system. We, therefore, neglect energy transfer between the species and treat the electrons adiabatically. We also consider situations where the ionization process is much faster than any relaxation process in the ion subsystem. Therefore, we can describe the ionization as a sudden switch of interactions and statistics. Due to the sudden change, the momentum and the pair distributions of the ions directly after the ionization, i.e. at $t = 0^+$, are still the ones of the atoms. However, the interactions are now given by the much stronger screened Coulomb potential. To calculate the final temperature, we employ energy conservation

$$
\begin{aligned}
E_{\mathrm{total}}(0^+) &\equiv E_{\mathrm{kin}}(0^+) + E_{\mathrm{ex}}(0^+) + E_{\mathrm{corr}}(0^+) \\
&= E_{\mathrm{kin}}(\infty) + E_{\mathrm{ex}}(\infty) + E_{\mathrm{corr}}(\infty) \\
&\equiv E_{\mathrm{total}}(\infty)
\end{aligned}
\tag{1}
$$

where $E(\infty)$ denotes the quasi-equilibrium energies achieved after the relaxation of the ion subsystem, but for shorter times than the equilibration between electron and ions. The initial kinetic energy $E_{\mathrm{kin}}(t = 0^+)$ is given by the atoms; the exchange $E_{\mathrm{ex}}(t = 0^+)$ and correlation $E_{\mathrm{corr}}(t = 0^+)$ energies have to be calculated with the pair distribution of the atoms and the new screened Coulomb potential. The final energies depend on the final temperature, which has to be chosen in a way that ensures energy conservation (1).

3. Energy contributions for weakly correlated systems

Let us first consider the energy of an ideal quantum system consisting of one component with mass m. In this case, the equilibrium momentum distribution is known to be a Fermi/Bose function

$$
f^{\mathrm{F/B}}(p, \sigma) = \left[\exp\left(\frac{p^2/2m - \mu}{\mathrm{k_B}T}\right) \mp 1\right]^{-1}
\tag{2}
$$

where the chemical potential μ depends on density n, temperature T and the spin of the particles σ. The upper and lower signs refer to the Bose and fermion cases, respectively. The average kinetic energy of the system is then given by

$$E_{\mathrm{kin}} = \frac{1}{n}\sum_{\sigma}\int \frac{\mathrm{d}\mathbf{p}}{(2\pi\hbar)^3}\frac{p^2}{2m} f^{\mathrm{F/B}}(p,\sigma) \tag{3}$$

which is smaller than classical result $\frac{3}{2}k_{\mathrm{B}}T$ in the case of bosons and larger for fermions.

The potential energy (which is in this case the exchange energy) of the system can be easily calculated from the pair distribution $g(r,\sigma)$, namely

$$E_{\mathrm{ex}} = \frac{n}{2}\int \mathrm{d}\mathbf{r}\, V(r)[g^{\mathrm{ideal}}(r,\sigma) - 1] \tag{4}$$

where $V(r)$ is the pair interaction potential. For an ideal quantum system in equilibrium, the pair distribution can be calculated from the one-particle momentum distribution. For isotropic distribution, one obtains [11]

$$g^{\mathrm{ideal}}(r,\sigma) = 1 \pm \frac{1}{(2\sigma+1)}\left[\frac{4\pi\hbar}{nr}\sum_{\sigma}\int \frac{\mathrm{d}p}{(2\pi\hbar)^3}\, p\sin\left(\frac{pr}{\hbar}\right) f^{\mathrm{F/B}}(p,\sigma)\right]^2. \tag{5}$$

If the particles occupy a restricted number of spin states N_s (e.g., for spin polarized systems), the spin factor $2\sigma + 1$ has to be replaced by the number of occupied states N_s. It is worth mentioning that the exchange energy (4) with the pair distribution (5) is identical with the Fock energy defined by

$$E^{\mathrm{Fock}} = \pm\frac{(2\sigma+1)}{2n}\int \frac{\mathrm{d}\mathbf{p}_1}{(2\pi\hbar)^3}\frac{\mathrm{d}\mathbf{p}_2}{(2\pi\hbar)^3} V(\mathbf{p}_1 - \mathbf{p}_2) f(p_1,\sigma_1) f(p_2,\sigma_2). \tag{6}$$

From the last formula, one can easily see that the exchange energy of an ideal Fermi system is negative whereas that for an ideal Bose system is positive.

In figure 1, results for binary distribution assuming ideal behaviour are shown for a potassium gas. Clearly, there is more structure in the system for lower temperatures and for fewer spin degrees of freedom. Furthermore, it demonstrates the attractive/repulsive character of the exchange for bosons and fermions, respectively.

3.1. Exchange and total energy for weakly interacting Fermi and Bose systems

Let us now consider a weakly interacting atomic gas. Here, the interactions can be modelled by the Morse-type potential

$$V(r) = D_0[(1 - \mathrm{e}^{-\alpha(r-R_0)})^2 - 1]. \tag{7}$$

This empirical formula involves the binding energy of molecules D_0, the binding length R_0 and a parameter α which is connected with the vibrational frequency of the molecule. At low density this is a very weakly interacting system; therefore the pair distribution is dominated by exchange effects at very low temperatures.

We again consider a potassium gas to demonstrate quantum degeneracy effects on the energies (3) and (4). We estimate the exchange energy (4) using the ideal binary distribution (5) and the Morse-type potential (7). For potassium, the parameters of the Morse potential are $D_0 = 0.594$ eV, $R_0 = 3.91$ Å and $\alpha = 0.715$ Å $^{-1}$. Figure 2 shows results for total, kinetic and exchange energies calculated with the Morse potential. For temperatures down to $T = 5 \times 10^{-8}$ K, no signs of degeneracy effects can be found. Interestingly, degeneracy effects are first present in the exchange energy contribution, which slightly increases (lowers) the total energy for bosons (fermions) around $T = 10^{-8}$ K. The exchange contributions to

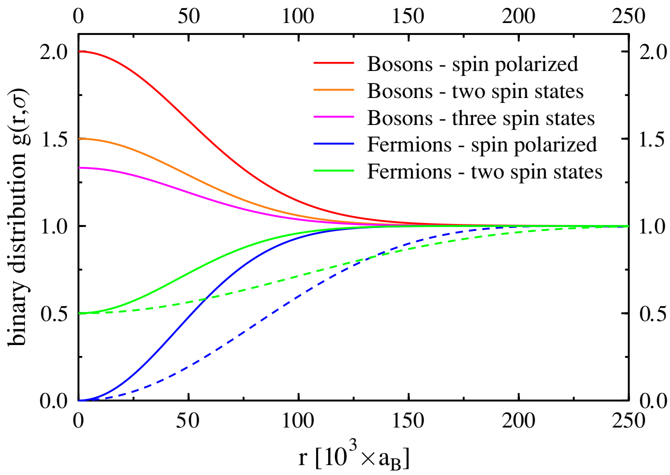

Figure 1. Binary distribution of an ideal quantum system of ^{40}K atoms (fermion case) and ^{39}K atoms (boson case) occupying a different number of spin states. The system temperature and density are $T = 10^{-9}$ K and $n = 10^{9}$ cm^{-3}, respectively. In addition, results for $T = 0$ (dashed lines) are shown for fermions.

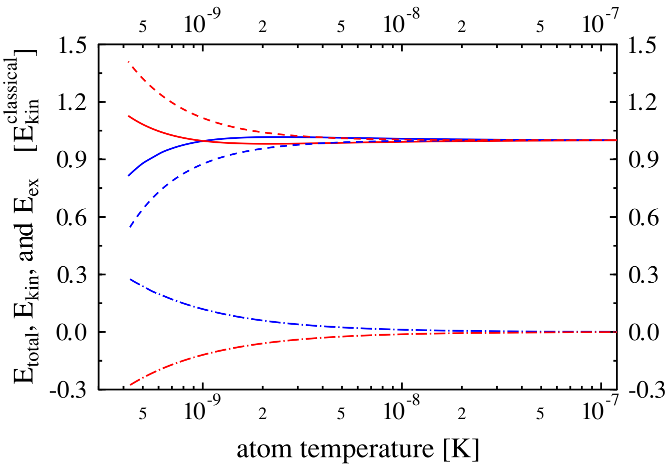

Figure 2. Total (solid), kinetic (dashed), and exchange (dash–dotted) energies of a potassium gas with $n = 10^{9}$ cm^{-3} normalized by the kinetic energy of the corresponding classical system. Interactions are modelled by the Morse potential (7). The blue and red lines correspond to bosonic (^{39}K) and fermionic (^{40}K) atoms, respectively.

the kinetic energy are dominant for lower temperatures, which gives rise to an increase of total and kinetic energy of a fermionic gas and a decrease for bosons. The kinetic energy of a fermionic system for such low temperatures is, of course, given by the Fermi energy that is much larger than the classical prediction.

It should be mentioned that the total energy is monotonically increasing with the system temperature for atomic systems. The small dips in the curves in figure 2 are overcompensated by the energy unit, i.e. $\frac{3}{2}k_{\mathrm{B}}T$, which is linearly increasing with temperature.

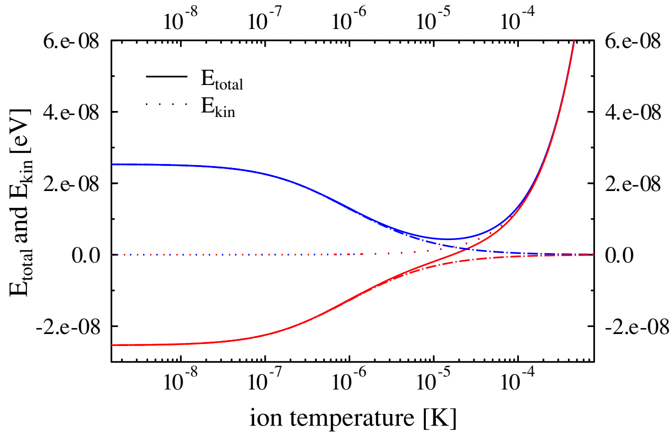

Figure 3. Total (solid), exchange (dashed–dotted), and kinetic (dotted) energies of potassium ions in a plasma. The interactions are modelled by a screened Coulomb potential (8) with an inverse screening length of $\kappa = 10^{-4} a_B^{-1}$. The blue (red) lines correspond to particles obeying Bose (Fermi) statistics.

3.2. Exchange and total energy for the initial plasma state

We will now demonstrate that the stronger interactions in a system of charged particles change the general behaviour of the total energy as a function of temperature. Again, we calculate the exchange energy using the binary distribution (5). We describe the interaction by a screened Coulomb potential

$$V(r) = \frac{Z^2 e^2}{r} \exp(-\kappa r) \tag{8}$$

where the inverse screening length κ is determined by the plasma electrons, and Z is the ion charge. Figure 3 shows the energies (3) and (4) for a system of K^+ ions in a system with a screening parameter of $\kappa = 10^{-4} a_B^{-1}$ (a_B is the Bohr radius). It clearly demonstrates that the total energy is dominated by the exchange contribution for low temperatures (here below $T < 10^{-5}$ K) if correlations are neglected.

Since the exchange energy of a fermion system becomes more negative with decreasing temperature, the total energy is monotonically decreasing. For bosons the behaviour is quite different due to the positive exchange energy. In the classical regime, the total energy decreases with temperature, but, when degeneracy becomes important, the total energy increases again since the positive exchange energy is the dominant contribution. This behaviour results in an unstable situation, because two system temperatures belong to one total energy. Furthermore, it demonstrates that, in principle, the statistics switch cannot be described by the ideal calculation. For example, the total energy of the system directly after the ionization, which is still characterized by fermionic distributions, is negative for $T < 10^{-5}$ K; since the bosonic total energy, where the system should relax to, is always positive, we cannot match the total energies for $t = 0^+$ and $t = \infty$.

Of course, this failure is due to the ideal description of an interacting system. The inclusion of correlations would include a negative energy contribution to the total energy, which makes in turn the total energy a unique function of the temperature and, therefore, allows for switching the statistics.

4. Energy of an interacting system of charged particles

For the kinetic energy of a classical system, we have the well-known result: $E_{\rm kin} = \frac{3}{2}k_{\rm B}T$. The potential (correlation) energy can be calculated in terms of the pair distribution by equation (4), but now $g(r)$ includes correlations and not exchange effects. We calculate the pair distribution by means of a hypernetted chain scheme

$$\begin{aligned} g(r) &= \exp[-V(r)/k_{\rm B}T + h(r) - c(r)] \\ h(r) &= c(r) + n \int {\rm d}\mathbf{r}' h(|\mathbf{r} - \mathbf{r}'|) c(r') \\ g(r) &= 1 + h(r) \end{aligned} \tag{9}$$

with a screened interaction potential. This scheme is known to show good agreement with molecular dynamics and Monte Carlo simulation results for the weakly and moderately coupled plasmas which should be considered here [12].

For systems as considered in figure 3, we should include correlations and degeneracy effects. Of course, a rigorous solution of this problem is quite complicated, and one needs to rely on techniques such as quantum Monte Carlo simulations.

Here, we first want to estimate how important both contributions are. The correlations, which are due to repulsive forces, are proportional to the strength of the screened Coulomb potential. To estimate the strength of exchange effects in a bosonic system, we go back to the ideal case where they can be exactly considered as the exchange potential

$$V_{\rm ex}(r) = -k_{\rm B}T \ln\left(1 + \exp\left(-\frac{2\pi r^2}{\lambda^2}\right)\right) \tag{10}$$

where $\lambda^2 = 2\pi\hbar^2/k_{\rm B}T$ is the thermal wavelength [13]. For bosons, this potential is attractive and, therefore, competes with the Coulomb repulsion.

To estimate which contribution, attractive exchange or Coulomb repulsion is more important, we compare the strength of both potentials. For an ultracold plasma, where the screening is typically large (in units of the interparticle distance), it turns out that the screened Coulomb potential is in the important regime with $r < \kappa^{-1}$ always much larger than the exchange potential (10). This means that the system is dominated by Coulomb repulsion. We, therefore, will use a classical calculation to obtain the total energy of a charged particle system.

5. Temperature estimates for systems long after the ionization

Now we can calculate the final temperature of the system after the ionization. The total energy at $t = 0^+$ is calculated with the distributions of the atomic system, but with the screened Coulomb potential (8). The final state is described by an interacting, classical system. The results will further justify such a treatment since degeneracy effects are negligible for the final temperatures. Since the total energy should be a unique function of the temperature, there can be no other solution for matching the initial and the final energy in the quantum regime.

Figure 4 gives results for different initial situations: different initial temperatures and different numbers of occupied spin states are considered. For comparison, results for a system without any initial correlation are shown also. Clearly, the introduction of initial correlations considerably reduces the amount of heating where lower final temperatures follow for more degenerate systems (colder and spin polarized). The results for $T_{\rm initial} = 0$ give the theoretical limit of possible initial correlations. However, $T_{\rm inital} = \frac{1}{4}T_F$ is the experimental limit so far,

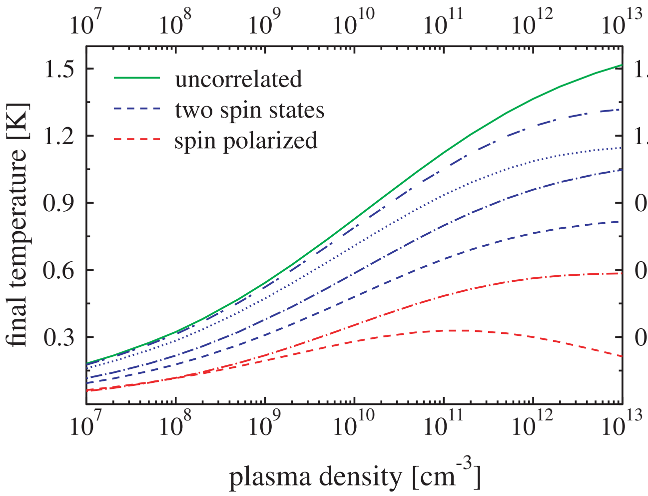

Figure 4. Final temperature of potassium ions in a plasma with an electron temperature of $T_e = 5$ K versus particle density. The screening length is calculated accordingly. The initial temperature of the Fermionic atoms is $T_{\text{initial}} = 0$ (dashed lines), $T_{\text{initial}} = \frac{1}{4}T_F$ (dash–dotted lines), and $T_{\text{initial}} = T_F$ (dotted line).

due to internal heating mechanisms in trapped gases [14]. Interestingly, degeneracy has only a small effect for plasma densities $n < 10^8$ cm^{-3}, even for $T_{\text{initial}} = 0$.

Reviewing the results in figure 4, we conclude that the heating due to the build up of correlation energy can be reduced by a factor of two to four for realistic situations. However, the inital temperatures considered are orders of magnitude lower than the final one. That is, the ion temperature still increases by several orders of magnitude; the final system is a moderately coupled, classical ion system. Therefore, additional laser cooling of the ions (see, e.g., [15]) may be needed should a strongly coupled ion system be created.

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