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Atom cooling by time-dependent potentials

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Using the concept of information entropy, it is shown that it is impossible to increase the phase-space density of atoms with time-dependent potentials or other time-dependent terms in the Hamiltonian, even if the motion is nonclassical.

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It has recently become possible to cool atoms to microkelvin temperatures by using laser cooling [1–3] or evaporative cooling [4,5]. With these cooling methods dense samples of ultracold atoms are obtained which allow high-resolution spectroscopy [6], the study of cold collisions [7], and hopefully in the future the observation of collective effects such as Bose-Einstein condensation.

The excitement about these techniques is due to the combination of low temperatures and high densities attained. Older techniques, like adiabatic expansion or selection of cold atoms out of a higher-temperature sample do not produce interesting densities. High-density samples of ultracold atoms can only be obtained if the decrease in temperature is accompanied by an increase in phase-space density ρ_Ω which is defined as the number of atoms N per volume V and volume V_p in momentum space, $\rho_\Omega = N/VV_p$.

The concept of phase-space density is useful because by Liouville's theorem it is a constant of the motion for conservative systems. A related quantity which is often used to characterize atomic beams is the brightness B which is the atom flux per unit area and unit solid angle $B=(N/V)v_\parallel(v_\parallel/v_\perp)^2$, where $v_\parallel$ and $v_\perp$ are the longitudinal and transverse velocity components, respectively. B is expressed in terms of ρ_Ω by introducing the speed ratio $s=v_\parallel/\Delta v$ and using $V_p = m^3 v_\perp^2 \Delta v$ (Δv is the spread in $v_\parallel$ and m the mass of the atom): $B=\rho_\Omega\, m^3 v_\parallel^4/s$. For two-dimensional atom optics (which leave the longitudinal velocity unaffected), Liouville's theorem is equivalent to constant brightness of an atom beam. This is similar to the theorem in light optics stating that an image cannot be brighter than the original object [8].

For many experiments such as atom interferometry or the achievement of Bose-Einstein condensation, an important figure of merit of an atomic sample is phase-space density or brightness. Fortunately (in contrast to conventional light optics) the phase-space density of a sample of atoms can be increased by violating the assumptions of Liouville's theorem using dissipation in the form of scattering of laser light and/or evaporation of particles. This is sometimes called "brightening" or more colloquially "real cooling" to distinguish it from lowering the temperature at constant phase-space density (e.g., adiabatic cooling).

Since Liouville's theorem is purely classical, the question remains if phase-space density can be enhanced by schemes relying on quantum-mechanical aspects of motion like quantum-mechanical wave packets, coherent superpositions of momentum states, or projection of quantum states by nonadiabatic switching of potentials. In this paper we use the concept of information entropy to show that brightening by time-dependent conservative forces is impossible even for nonclassical motion of the particles. Although it is very straightforward to obtain this result, our general proof seems to rule out recent suggestions of cooling schemes relying solely on conservative forces [9–11] (these suggestions were the stimulation for this work).

We begin with a review of the relevant definitions of quantum statistics. Although we mainly speak of atoms, our arguments apply also to ions or any other particles being cooled. Phase-space density is a classical quantity and cannot be readily used in quantum mechanics because of the noncommutativity of position and momentum operators. If one divides ρ_Ω by h^3, the phase-space volume of a quantum state, one obtains the number of atoms per quantum state, called quantum density or occupancy ratio. To obtain a related quantity for a system described by an arbitrary statistical operator (density matrix) ρ, one defines information entropy S' as [12,13].

$$S' = -k\langle \ln\rho \rangle \ , \tag{1a}$$

where the brackets $\langle A \rangle$ denote the average value $\langle A \rangle = \mathrm{Tr}(\rho A)$ of an operator A. Equation (1a) should, for the moment, only be regarded as a mathematical definition—the relation to the thermodynamic entropy will be discussed further below. Viewed in the basis which diagonalizes ρ, this becomes

$$S' = -k \sum_i p_i \ln(p_i) \ , \tag{1b}$$

where p_i are the eigenvalues of ρ. In the simplest case of n states with equal probability of occupation, one has $p_i = 1/n$ and obtains the familiar expression

$$S' = k \ln(n) \ . \tag{2}$$

The relation to information theory is obvious, $S'/k \ln 2$ being the number of bits to label n states. For N particles, n in Eq. (2) has to be interpreted as n_N, the number of populated N-particle states. For N indistinguishable noninteracting particles occupying n_1 one-particle states with occupation ratios much smaller than unity (i.e., negligible effects of quantum statistics) one can use $n_N = n_1^N / N!$ and Stirling's formula $\ln N! = N \ln N - N$ to obtain

$$S' = Nk[\ln(n_1/N) + 1] \ . \tag{3}$$

Thus S'/N is directly related to the quantum density N/n_1.

In thermal equilibrium at temperature T, ρ is a canonical distribution and S' is given by the (N-particle) partition function Z_N and energy E_N:

$$S' = k(\ln Z_N + \beta E_N) \ , \tag{4}$$

where $\beta = 1/kT$. For noninteracting particles and negligible effects of quantum statistics, Z_N and E_N can be expressed by the respective one-particle quantities $Z_N = Z_1^N / N!$ and $E_N = NE_1$. Equation (4) is then equivalent to Eqs. (2) and (3) because the effective number of populated states n_N is given by Z_N. The second term βE_N in Eq. (4) is in most cases an unimportant constant on the order of N. It is due to the use of a canonical distribution and represents the logarithm of the number of states of the heat reservoir.

If a classical phase-space volume ρ_Ω can be defined, the number of populated states is $(\rho_\Omega / h^3)^N / N!$ yielding

$$S' = Nk[\ln(\rho_\Omega / h^3 N) + \sigma_1] \ , \tag{5}$$

where σ_1 is constant.

Let us verify Eq. (5) for the important cases of particles confined to a volume V and bound by a harmonic potential. For noninteracting particles in volume V at a temperature T one has [14]

$$S' = Nk[\ln(V/N) + \tfrac{3}{2}\ln T + \sigma_0] \ , \tag{6}$$

with $\sigma_0 = \frac{3}{2}\ln(2\pi mk/h^2) + \frac{5}{2}$. The volume in momentum space is approximately a sphere with radius $p = \sqrt{2mkT}$ yielding Eq. (4) with $\sigma_1 = (\ln\pi)/2 - \ln(\frac{4}{3}) + \frac{5}{2}$.

For a three-dimensional harmonic oscillator with frequency ω the information entropy is

$$S' = Nk\left[3\eta \frac{1}{e^{\eta} - 1} - 3\ln(1 - e^{-\eta}) - \ln N + 1\right] ,$$

with $\eta = \hbar\omega / kT$. In the case of $kT \gg \hbar\omega$ one has

$$S' = k\{3N + \ln([kT/\hbar\omega]^3 / N!)\} \ . \tag{7}$$

The argument of the logarithm is the number of populated states. By introducing the mean momentum $p = \sqrt{2mkT}$ and amplitude $x = (2kT/m\omega^2)^{1/2}$ one can rewrite Eq. (7) in the form of Eq. (5) with $\sigma_1 = 4 + \ln(9\pi/16)$.

These examples show that for free or weakly bound particles in thermal equilibrium S' is related to phase-space density by Eq. (5).

The information entropy S' has two important properties. First, it is a constant of motion for conservative potentials. For an *arbitrary time-dependent* Hamiltonian $H(t)$ the time evolution of the statistical operator is given by the von Neumann equation [13]

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[H(t), \rho(t)] \ . \tag{8}$$

Because of this and the cyclic invariance of the trace, the expectation value $\langle f(\rho) \rangle$ of any operator that is a function of the statistical operator is constant in time; in particular $dS'(t)/dt = 0$ [13].

The physical reason for the time invariance of S' can be best understood by using the approximate relation with the number of occupied states [Eq. (2)]. Adiabatic changes do not alter occupation numbers; for example, a π pulse of resonance radiation simply swaps the population of states. For arbitrary changes of potentials there is still a unitary transformation between initial and final state. Therefore the number n of incoherently populated states remains the same.

The second important property of S' is the relation to the thermodynamic entropy S,

$$S = \max S'(\rho_i) \ . \tag{9}$$

The maximum is taken over all statistical operators ρ_i satisfying certain macroscopic conditions (i.e., N particles, volume V, energy E). It can be rigorously shown [12] that the canonical distribution has the largest information entropy of all statistical operators with the same average energy E.

It is now straightforward to show that it is impossible to increase phase-space density by time-dependent external fields: If at $t = 0$ the system is in thermal equilibrium, and described by a canonical distribution, one has

$$S'(0) = S(0) = Nk\{\ln[\rho_\Omega(0)/h^3 N] + \sigma_1\} \ . \tag{10}$$

$\rho(t)$ is generally not an equilibrium distribution. However, in all cases of brightening of atoms one ends up in a situation where at the final time τ, one can approximately assign a phase-space volume $\rho_\Omega(\tau)$ to the atoms by characterizing them by a confinement volume V and rms momentum p. Because of Eq. (9), $S'(\tau)$ is smaller than or equal to the thermodynamic entropy $S(\tau)$ of an equilibrium distribution confined to the same phase-space volume:

$$S(\tau) \geq S'(\tau) = S'(0) = S(0) \ , \tag{11}$$

which gives

$$\rho_\Omega(\tau) \geq \rho_\Omega(0) \ . \tag{12}$$

The argument above is analogous to the derivation of the increase of entropy S, which involves the step from the exact statistical operator to the coarse-grained operator of quasistatic equilibrium which is accompanied by loss of information [13].

We want to emphasize that there is no assumption on the classical or quantum-mechanical nature of the final state of the system. The above proof is indirect: the assumption that the final state has a higher phase-space density leads to a contradiction because this requires a smaller information entropy or (equivalently) a smaller number of incoherently populated states.

We have so far neglected the internal structure of atoms. In the simplest case of negligible correlation between internal and external degrees of freedom, $S'(t)$ can be decomposed in two terms $S'_{\text{ext}}+S'_{\text{int}}$ resulting in

$$S_{\text{ext}}(\tau)\geq S_{\text{ext}}(0)+[S'_{\text{int}}(0)-S'_{\text{int}}(\tau)] .$$

In this case, external phase-space density can be increased, but at most by a factor which is equal to the ratio of populated internal states at times $t=\tau$ and 0. Since the information entropy of the internal degrees of freedom increases, "dissipation" occurs in the internal variables.

One example of cooling by internal degrees of freedom is adiabatic demagnetization. The number of populated internal states is increased by a factor which is at most $2s+1$, s being the spin of the particles. Since at very low temperatures external degrees of freedom (lattice vibrations) contribute very little to the entropy, the temperature of the whole system can be decreased by several orders of magnitude.

However, in atom cooling, the external degrees of freedom are not frozen out and contribute to the entropy according to Eq. (6) or (7). If twice as many internal states are populated by an adiabatic process, the temperature drops only by at most a factor of $2^{2/3}$. Strong cooling can be achieved only if the initial population of internal states is restored (e.g., by optical pumping) and the system is cycled many times through these processes. This is similar to the idea of cyclic cooling which was proposed for atoms in a magnetic trap [15].

Collisions with other atoms in the system have so far been neglected. Their only role was to ensure equilibrium at $t=0$, e.g., by using an effusive atomic beam which is in thermal equilibrium due to the collisions inside the oven. In the general case of interacting particles, phase space is $6N$ dimensional (we assume for the moment a fixed atom number N and exclude evaporation where atoms are lost from the system). However, in the case of atom cooling, one starts and ends up in a situation where collisions are negligible except that they redistribute the atoms over all accessible states. One can therefore use one-particle wave functions and six-dimensional phase space at $t=0$ and τ implying that $S(0)$ and $S(\tau)$ are given by Eq. (5). Since information entropy is a constant of motion also for interacting particles, Eqs. (11) and (12) are unchanged.

We want to point out that the assumption of thermal equilibrium at $t=0$ [or equivalently $S'(0)=S(0)$] is essential. If this is not the case, the system has a lower information entropy than the thermodynamic entropy computed using the macroscopic boundary conditions. This can be used to change the boundary conditions and to achieve a higher phase-space density. For example, if one has N particles in a box and knows that, at some moment, there are no particles close to a wall element, one can move this part of the wall inward and confine the particles in a smaller volume. This is the principle of stochastic cooling, where dissipation occurs in the process of obtaining the additional information on the system. Stochastic cooling works well for charged particle beams; however, there is no suggestion so far as to how to apply it to cool neutral atoms.

Finally, we want to discuss cooling schemes using the selection of particles. This can be achieved by putting particles into a special internal state or by discarding particles. Since entropy is an extensive quantity, the quantities to be regarded are S'/N or quantum density. In the general case where the population is distributed over many states, the quantum density is the ratio of the particle number N and an effective number of states n_1 given by $\ln n_1=-\sum p_i\ln p_i$ (p_i are the eigenvalues of the *one-particle* statistical operator). S'/N contains a weighted average over the occupancy numbers Np_i: $S'/N =k[-\sum p_i\ln(Np_i)+1]$. If one discards particles in weakly populated states, S'/N decreases.

However, the more important quantity is the maximum occupation number $Np_{\max}$ in any quantum state where $p_{\max}=\max(p_i)$. The quantum density obtained by selecting particles in the most probable states is $Np_{\max}$. For noninteracting particles, $p_{\max}$ is a constant of motion because the time evolution of the statistical operator ρ is a unitary transformation leaving the eigenvalues invariant. It is therefore impossible to increase the maximum occupation number $Np_{\max}$ by any combination of selection processes and arbitrary time-dependent terms in the (one-particle) Hamiltonian.

This conclusion is not valid if one allows for collisions between the particles of the system. Such processes can increase or decrease $p_{\max}$ because $p_{\max}$ is a one-particle probability whereas the constant eigenvalues of the (N-particle) statistical operator are occupation numbers for N-particle states. For example, if the initial distribution is a truncated Boltzmann distribution, collisions will increase the occupation number in the states with the lowest energy. Although collisions do not change S' (as discussed above), they can change $p_{\max}$. This is exploited in evaporative cooling where the system is first cycled through selection processes (evaporation) which decrease S'/N but leave $Np_{\max}$ constant and then subjected to collision processes which increase $Np_{\max}$ but leave S'/N constant. The result is a sample of atoms with both decreased entropy S'/N and increased quantum density $Np_{\max}$.

Although not immediately obvious, information entropy and phase-space density are important quantities even for cooling a single particle (i.e., an ion in a trap). Usually, the particle is initially in some unknown state in a larger phase-space volume. The cooling process reduces the occupied phase-space volume. Information entropy has decreased because there are now fewer states populated with a correspondingly higher probability (increase of knowledge). If one had exact knowledge of the initial state of the particle, one could just transfer it into the lowest state by appropriate fields without any dissipation, leaving the information entropy unchanged. This emphasizes the one-to-one correspondence between brightening and increase of knowledge on the system.

In conclusion, we have used the well-established formalism of quantum statistics to show that "brightening" of atoms is impossible without dissipation or loss of atoms from the system. Cooling schemes which rely solely on resonance transitions or time-dependent potentials (both adiabatic and sudden changes) or on selection procedures do not increase phase-space density.

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