

Atomic Gases at Negative Kinetic Temperature

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We show that thermalization of the motion of atoms at negative temperature is possible in an optical lattice, for conditions that are feasible in current experiments. We present a method for reversibly inverting the temperature of a trapped gas. Moreover, a negative-temperature ensemble can be cooled (reducing $|T|$) by evaporation of the lowest-energy particles. This enables the attainment of the Bose-Einstein condensation phase transition at negative temperature.

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Amplification of a macroscopic degree of freedom, such as a laser or maser field, or the motion of an object, is a phenomenon of enormous technological and scientific importance. In classical thermodynamics, amplification is not possible in thermal equilibrium at positive temperature. In contrast, due to the fluctuation-dissipation theorems [1,2], amplification is a natural phenomenon, and fully consistent with the second law of thermodynamics, in a negative-temperature heat bath [3–6]. Negative temperatures were introduced by Purcell and Pound [7] to describe spin systems, and further generalized theoretically by Ramsey and Klein [8,9]. Useful introductions to thermodynamics at negative temperature are given by Landau and Lifshitz [10] and by Kittel and Kroemer [11]. Negative temperatures are used to describe distributions where the occupation probability of a quantum state increases with the energy of the state. The prerequisite for a negative-temperature ensemble to be in internal equilibrium is that it occupies a part of phase space where the entropy decreases with internal energy. An ensemble in this part of phase space cannot be in thermal equilibrium with any positive-temperature system. An increasing occupation number (and a decreasing entropy) can only exist up to a certain maximum energy. Unlike the magnetic energy of spins, kinetic energy is not bounded from above in free space, which apparently rules out a negative kinetic temperature. Here, we show that the band structure of a moderately deep optical lattice defines an upper bound to the kinetic energy of atoms in the first band. Therefore, atoms in an optical lattice form a simple system in which thermalization of the kinetic energy is possible at negative temperatures.

Optical lattices, which are periodic potentials created through optical standing waves [12], impose a band structure on the motion of ultracold atoms. The kinetic energy of atoms in the lattice depends on their effective mass or band mass, which, in analogy to the case of electrons in a semiconductor, can be strongly different from the normal rest mass. The effective mass can even become negative, as has been demonstrated in one-dimensional optical lattices [13,14]. An isotropic negative-effective mass can be real-

ized in the vicinity of a band gap in a three-dimensional (3D) optical lattice. The band gap is an energy range inside which no single-particle eigenstates exist. If the atoms are constrained to energies just below the band gap the effective mass will be negative in all directions and the entropy of the ensemble will decrease with energy. This is the condition for existence of a thermal ensemble with negative temperature [8].

For thermalization to take place, the characteristic time scale for exchange of energy between particles must be shorter than time scales associated to heating and loss. In other terms, we need a high rate of intraband scattering, with negligible interband scattering. Interband scattering is a collision process between two atoms in the first (“valence”) band which causes one atom to be promoted to the second (“conduction”) band while the valence band atom loses energy. Additional losses may be caused by interband tunneling, a one-body process in which an atom tunnels through a classically forbidden region, to reappear in a different band.

In this Letter, we show that all the requirements for thermalization at negative temperature can be met in a 3D optical lattice. First, we show that an optical lattice can have a 3D band gap for atoms, at experimentally feasible lattice intensities. Moreover, interband scattering can be completely suppressed, and confinement of the negative-mass atoms can be easily accomplished using a magnetic trap for *high-field seeking* states. We calculate rates of interband tunneling and find they can be made negligible. Finally, we show how a trapped gas at positive temperature can be reversibly converted to a negative temperature.

The motion of atoms in a simple cubic 3D optical lattice with a harmonic confining potential is described by the Schrödinger equation (See, e.g., [12,15]),

$$E\Psi = \left[\frac{-\hbar^2}{2m} \nabla^2 + U_{\text{lat}} + \alpha(x^2 + y^2 + z^2) \right] \Psi \quad (1)$$

with $U_{\text{lat}} = U_0(\cos^2 kx + \cos^2 ky + \cos^2 kz)$.

Here m is the bare atomic mass, α is the strength of the harmonic potential, U_0 is the depth of the standing wave potentials that form the lattice, and $k = 2\pi/\lambda$, where λ is the wavelength of the lattice light. The above Schrödinger equation is trivially separable by setting $E = E_x + E_y + E_z$. We now transform the equation to dimensionless units,

$$\tilde{x}, \tilde{y}, \tilde{z} = kx, ky, kz, \quad (2)$$

$$\tilde{\alpha} = \alpha/(E_r k^2), \quad (3)$$

$$a_x = \left(E_x - \frac{1}{2}U_0\right)/E_r, \quad (4)$$

$$q = U_0/4E_r, \quad (5)$$

with the lattice recoil energy $E_r = \hbar^2 k^2/2m$. The one-dimensional equation of motion takes the shape of a modified Mathieu equation,

$$\frac{d^2\Psi}{d\tilde{x}^2} + (a_x - 2q \cos 2\tilde{x})\Psi + \tilde{\alpha}\tilde{x}^2\Psi = 0. \quad (6)$$

In the absence of a parabolic potential ($\tilde{\alpha} = 0$), Eq. (6) is exactly the Mathieu equation. Its solutions are the Mathieu functions, which are propagating Bloch-Flouquet waves for values of a and q in the bands, and evanescent functions in the band gaps. The relevant bands are depicted in Fig. 1. Adopting the usual convention [16] we designate the eigenvalues corresponding to the band bottoms by $a_0(q)$, $a_1(q)$, etc., and the band tops by $b_1(q)$, etc., (see Fig. 1). If $0 < |\tilde{\alpha}| \ll q/\tilde{x}$, the lattice is locally only weakly perturbed by the parabolic potential, and the band structure will remain essentially intact. The energy positions of the bands become position dependent, in the same way as in a semiconductor in an applied electric field. A negative value of $\tilde{\alpha}$ corresponds to a confining potential for negative-effective mass atoms, see Fig. 2. The area under the valence band in Fig. 2 is classically forbidden as the kinetic energy of the atoms in this region is less than zero. The area

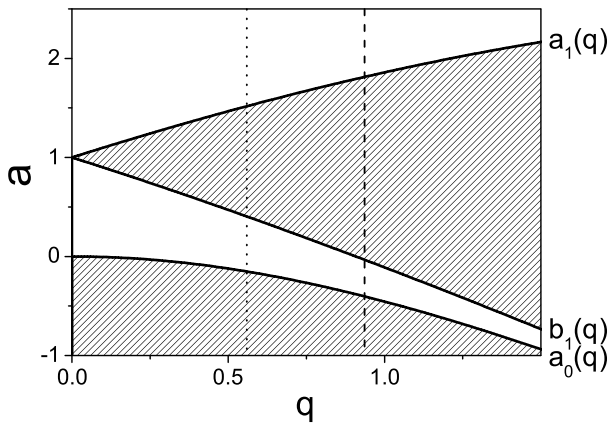


FIG. 1. Band structure of the one-dimensional Mathieu equation. White area: Bands, gray area: gaps. Dotted line: $q = 0.559$, dashed line: $q = 0.936$; see text.

between the bands is Bragg forbidden; i.e., no propagating modes can exist here due to interference.

For the negative-temperature phase to be metastable, there must be a band gap between the top of the valence band, where the negative-mass states exist, and the bottom of the conduction band, where the effective mass is positive. In a 1D system (with the motion in the other two directions confined) this band gap exists for $|q| > 0$. However, in a 3D optical lattice, the bands may overlap. The maximum energy an atom in the valence band of a 3D lattice can have is $3b_1(q)$, whereas the minimum energy in the conduction band is $2a_0(q) + a_1(q)$. The criterion for the existence of a band gap is $3b_1(q) < 2a_0(q) + a_1(q)$, which is fulfilled for $q > 0.559$.

If the 3D band gap is narrow, collisions between two valence band atoms can promote an atom to the conduction band, where it has positive effective mass. This interband scattering will not only lead to loss of atoms, but also to loss of energy, which is equivalent to heating (increasing $|T|$). We show now that interband scattering becomes energetically forbidden in two-body processes at high enough q . The maximum energy of the initial state, consisting of two valence band atoms, is $6b_1(q)$. The minimum energy of the final state, consisting of one valence and one conduction band atom, is $[3a_0(q)] + [2a_0(q) + a_1(q)]$. The interband scattering process is energetically forbidden if $6b_1(q) < 5a_0(q) + a_1(q)$, which is the case if $q > 0.936$. This value of q corresponds to a lattice depth almost an order of magnitude less than the depth employed to create a Mott-insulator phase [17]. In such a moderately deep lattice, thermalization rates and inelastic collision rates are all of the same order of magnitude as the respective rates at positive temperature in the absence of a lattice [15]. Through elastic collisions, the ensemble will always relax to a distribution with the highest possible entropy at its given energy, in this case a negative-temperature distribution.

To investigate how the gas thermalizes in the negative-temperature phase space, it is useful to consider the semi-

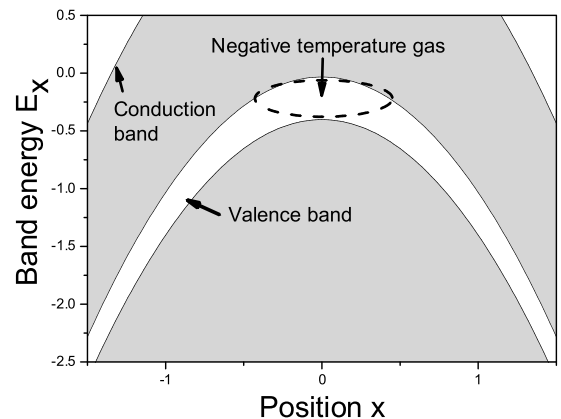


FIG. 2. Valence and conduction bands of a 1D optical lattice at $q = 0.936$. Grey area: Gaps, white area: Bands.

classical density of states (DOS). The DOS can usually be found by taking the energy derivative of the Wentzel-Kramers-Brillouin (WKB) phase integral, a procedure recently applied to a one-dimensional optical lattice with harmonic confinement (positive α) [18]. For negative α the WKB method cannot be used straightforwardly to calculate wave functions, as the ‘‘Bragg reflection’’ boundary condition at the outer turning points behaves differently from classical turning points. The WKB formula for the DOS does not depend on the boundary conditions and can be straightforwardly calculated in the one-band model of [18]. Within the one-band and WKB approximations, the DOS ρ_α at negative α is related to the DOS calculated for positive α by

$$\rho_\alpha(E) = \rho_{-\alpha}(-E), \quad (7)$$

where in the case of negative α , the top of the valence band is taken as the energy zero. The 3D DOS crosses over smoothly from a quadratic behavior at small negative energy to approximately square-root behavior at larger negative energy, as shown in Fig. 3. The DOS is nonzero for any energy lower than the band edge at the trap center, so in principle the negative temperatures are *not bounded* in an infinite lattice. In fact, this asymmetric behavior of the DOS makes thermal equilibrium at a positive temperature impossible, which is in contrast to spin systems [7], where thermal equilibrium at positive and negative temperature can be studied in the same field configuration.

We now examine the escape of the atoms through inter-band (Zener) tunneling. The trapped negative-mass valence band states are mixed with antitrapped conduction band states at the same energy, as the evanescent tails of these states extend through the Bragg forbidden region. The Zener tunneling rate Γ_{Zener} may be estimated using [19]

$$\Gamma_{\text{Zener}} \approx \omega_A \exp\left[-2 \int_0^\infty \text{Im}[k_{\text{Bloch}}(x)] dx\right], \quad (8)$$

where $k_{\text{Bloch}}(x)$ is the Bloch wave vector of the Mathieu equation corresponding to the energy $E - \alpha x^2$, and ω_A is

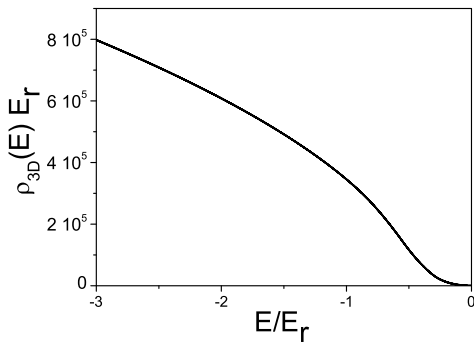


FIG. 3. Density of states $\rho(E)$ in a three-dimensional lattice with $\tilde{\alpha} = -10^{-3}$. The energy E is taken with respect to the top of the first (valence) band.

an attempt frequency of the order of the trap oscillation frequency (typically < 1 kHz). The resulting tunneling time constant is of order 10^5 seconds at $\tilde{\alpha} = 10^{-3}$. For $10^{-4} < \tilde{\alpha} < 10^{-2}$ we checked Eq. (8) numerically by high-precision quadrature of Eq. (6), and found agreement within an order of magnitude.

The conditions for existence of a negative-mass Bose-Einstein condensate (BEC) were recently studied by Pu and coworkers [15]; they also investigated the possibility of creating such a condensate by phase imprinting, and found this likely to be an inefficient mechanism as many atoms are transferred to other bands. Other mechanisms, such as accelerating the atoms uniformly to complete one-half Bloch oscillation, may be more efficient, especially since in a BEC nonlinearity due to the interactions counteracts dephasing [20,21]. Using these methods, the negative-mass BEC can be created in a mechanically unstable state as the interatomic scattering length a_{sc} remains positive [15].

We propose a radically different mechanism for the production of negative-temperature gases, based on the reversible creation of a Mott-insulator phase from a BEC [17]. The idea is to ‘‘freeze’’ a positive-temperature gas into a Mott insulator, by turning on a strong optical lattice. The Mott phase is then ‘‘molten’’ in a different trap configuration and with different interatomic interactions, to produce a negative-temperature gas. The procedure is outlined in Fig. 4, we will describe it here for a pure BEC but there is no *a priori* reason why it would not work when some thermal excitations are present. We start with a trapped BEC at $\alpha > 0$ and $a_{\text{sc}} > 0$ 4(a), and turn on a strong optical lattice, as is done in [17]. A Mott-insulator phase will form in which the atoms are confined to their local potential wells 4(b). We assume one atom is present per lattice site. Now we remove the trap 4(c), which can be

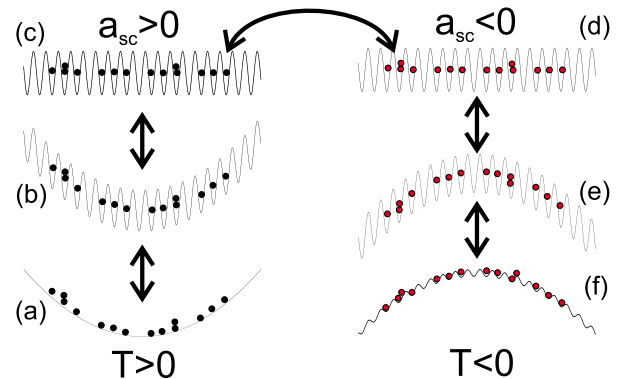


FIG. 4 (color online). Method for reversibly transforming a positive-temperature gas (a) into a negative-temperature gas (f). Each step is reversible; see text. (a) trapped gas at positive T , (b) a strong optical lattice, (c) a strong optical lattice without trap, (d) a strong optical lattice with changed a_{sc} , (e) a strong optical lattice with negative trap, (f) an optical lattice at $q = 0.936$ with a negative-temperature gas.

done rapidly without creation of entropy, as the atoms are tightly bound to their respective lattice sites. Then we change the sign of a_{sc} 4(c) and 4(d), for example, by tuning the magnetic bias field near a Feshbach resonance (See, e.g., [22]). Since the atoms are at different lattice sites and do not interact, this can be done rapidly without causing losses. The system passes through the point where both a_{sc} and α are zero, here the temperature of the Mott phase is not defined, but the entropy is. This passage transforms the Mott insulator from the lowest-energy many-particle state to the highest energy in the valence band. The confining potential is reconfigured to change the sign of α 4(e). This can be done either by changing the confinement field, or by changing the internal state of the atoms. A magnetic field minimum will trap negative-mass atoms in their lowest Zeeman state [15]. No change in the spatial distribution of atoms will take place due to the extremely low tunneling rate in the Mott insulator, so this step can proceed rapidly. When the lattice is slowly reduced in strength 4(f), the Mott insulator will melt into high energy states in the valence band, i.e., a negative-mass, negative-temperature gas. This approach seems practicable for all ultracold bosonic atoms which have suitably broad Feshbach resonances, such as ^7Li , ^{23}Na , ^{85}Rb , and ^{133}Cs . A detailed analysis of the reversibility criteria for each step will be published elsewhere.

The atomic gas can be cooled by forced evaporation. In the case of a magnetic trap, the evaporation can proceed through radio frequency (rf) induced spin flips to an untrapped (magnetic quantum number $m = 0$) state. One should tune the rf to selectively remove atoms with lower-than-average energy, so that the average energy per atom will increase. This leads to an increase of T , and a reduction of the entropy per particle S/N . A reduction of the entropy per particle is equivalent to an increase of the phase space density. Therefore we use the term *cooling* for any process that lowers $|T|$. At low enough $|T|$ the system can be described by a (negative) power law density of states, and the theory of evaporative cooling in a power law density of states [23] can be applied. (One should take care to reverse the signs of m , E , and T in Ref. [23] wherever applicable.) The condition for BEC in a 3D system is $n\Lambda^3 = 2.61$, where n is the number density of atoms and $\Lambda^2 = 2\pi\hbar^2 m_{\text{eff}}^{-1} k_B^{-1} T^{-1}$, where k_B is Boltzmann's constant. Since both the effective mass m_{eff} and T are negative, Λ is a real number. Achieving the BEC phase transition at negative temperature seems possible, either by heating (extracting energy), starting from a pure BEC, or by cooling, starting from a negative-thermal gas.

The negative value of a_{sc} , which is necessary to create the negative-mass BEC from a Mott insulator, is also a condition of stability for the negative-mass BEC.

In fact, the negative-mass BEC is likely to collapse if a_{sc} is positive [15]. It is very interesting to consider the possibility of superfluidity at negative a_{sc} in a negative-temperature system. One expects the superfluid phase to allow for dissipationless motion of objects, unless a critical velocity is exceeded, in which case negative dissipation sets in. Further properties of negative-temperature superfluidity are hitherto unexplored theoretically as well as experimentally.

In conclusion, in an optical lattice combined with a parabolic potential, a large phase space in which atoms can thermalize to negative kinetic temperatures is open for exploration.

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