Equilibration rates and negative absolute temperatures for ultracold atoms in optical lattices

Akos Rapp, Stephan Mandt, and Achim Rosch
Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany
(Dated: November 29, 2010)

As highly tunable interacting systems, cold atoms in optical lattices are ideal to realize and observe negative absolute temperatures, \( T < 0 \). We show theoretically that by reversing the confining potential, stable superfluid condensates at finite momentum and \( T < 0 \) can be created with low entropy production for attractive bosons. They may serve as “smoking gun” signatures of equilibrated \( T < 0 \). For fermions, we analyze the time scales needed to equilibrate to \( T < 0 \). For moderate interactions, the equilibration time is proportional to the square of the radius of the cloud and grows with increasing interaction strengths as atoms and energy are transported by diffusive processes.

PACS numbers: 05.30.Fk,05.30.Jp,05.60.Gg,05.70.Ln,03.75.Nt
are exponentially suppressed and negligible.

Negative $T$ in equilibrium is only possible for Hamiltonians bounded from above. Thus, for the models (112), $V_0 < 0$ and for bosons also $U < 0$ is required. Nevertheless, ultracold atoms have to be prepared with some $V_0 > 0$ initially, and we shall discuss how $T < 0$ can be reached from such conditions (preparation of high-energy states in spin-systems is discussed in Ref. [11]).

To get some intuition on negative $T$, note that the equilibrium density matrix, $e^{-\hat{H}/k_B T}$, for a Hamiltonian $\hat{H}$ at $T < 0$ is identical to the density matrix for reversed temperature $\hat{T} = -T$ and a Hamiltonian $\hat{H} = -\hat{H}$. For the models (112) therefore considering $T < 0$ is equivalent to $\hat{T} > 0$ with parameters $-V_0$, $-U$, and most importantly, $-J$. As for a cubic lattice with lattice constant $a$ the sign of $J$ can be absorbed into a shift of all momenta, $k \rightarrow k + Q$ with $Q = (\pi/a, \pi/a, \pi/a)$ [using (11) that $-J \cos(ka) = J \cos(ka + \pi)$], the phase diagram of the negative-$U$ Hubbard models for $T < 0$ are identical to that of the positive-$U$ Hubbard models if the momenta are shifted in all observables. Most dramatically, bosons will therefore condense at momenta $(\pm \pi/a, \pm \pi/a, \pm \pi/a)$, i.e., in the maxima of the band structure, for $U < 0, T < 0$ [see Fig. 1(b)]. Note that $T < 0$ bosonic condensates are stable for attractive and unstable for repulsive $U$. For fermions superfluidity can also be reached for $T < 0, U > 0$ but in this case the fermionic pairs condense at zero momentum as $\sum_k f_{k_1}^+ f_{-k_1}^+ = \sum_k f_{k+Q_1}^+ f_{-k-Q_1}^+$. We remark that it has been shown [12] that for $U \gg J$ one can nevertheless induce a condensate at momentum $Q$ even for fermions in a different nonequilibrium situation. To summarize, the momentum distribution of a Bose-Einstein condensate is probably the best way to detect $T < 0$ due to the qualitative difference to the $T > 0$ system, and we will quantitatively estimate under what conditions such a state can be reached.

In principle, it is possible to reach $T < 0$ without any entropy production by first adiabatically decreasing $J$ until $J = 0$, then switching suddenly $U \rightarrow -U$ and $V_0 \rightarrow -V_0$, followed by an adiabatic increase of $J$ until the desired value is reached. In practice this is not a good choice as the timescales for equilibration diverge for $J \rightarrow 0$. Therefore one needs a faster scheme where $J$ remains finite but as little entropy as possible is produced. As a reversal of $V_0, U$ and $T$ is formally equivalent to a sudden quench $J \rightarrow -J$ without inverting $T$ (see above), the basic idea is to start from an initial state where $J$ is finite but the kinetic energy is very small, i.e., a Mott or a band insulator.

For bosons we propose the following. The system is (I) prepared in a Mott-insulating state. (II) $J$ is switched off suddenly by increasing the intensity of the optical lattice. This freezes all density-density correlation functions. One waits (III) for a time $t_w$ during which the potential and the interaction are reversed slowly, $V_0 \rightarrow -V_0$ and $U \rightarrow -U$. (IV) $J$ is switched suddenly back to its initial value and (V) the system equilibrates. Finally, (VI) the negative trapping potential and/or the interaction strength $U$ is weakened adiabatically with the goal to reach a superfluid condensate at $T < 0$. For fermions, parts of this scheme have been implemented in Ref. [11], where, however, $V_0$ was not reversed but set to 0.

The waiting time $t_w$ allows us to reverse $V_0$ and $U$ slowly (manipulation of $U$ requires “slow” changes of magnetic fields in some experimental setups), and more importantly, it leads to a complete dephasing of the kinetic energy, $E_{\text{kin}}$, as has been argued in Ref. [11]. During $t_W$ each site in the lattice collects a different phase due to $V_0$. Effectively, therefore $E_{\text{kin}} \propto \sum_{ij}(a_i^+ a_j)$ averages to zero for $t_W \gg 1/\Delta V$, where $\Delta V$ is the potential difference between neighboring sites. Note that for a Mott insulator $E_{\text{kin}}$ vanishes in the center of the trap but is sizable in the outer parts of the cloud where $\Delta V$ is large. Estimates using the parameters of Ref. [6] show that waiting times $t_w \gtrsim 10$ ms are sufficient for a complete dephasing.

For a quantitative estimate of the entropy generated during this sequence, one first needs to know the total energy $E_{\text{tot}}$ after step (V), i.e., before the final equilibration stage. As the kinetic energy is zero after dephasing and the initial density distributions are fully preserved, we obtain $E_{\text{tot}} = -(E_{\text{int}} + E_{\text{pot}})$, where $E_{\text{int}}$ and $E_{\text{pot}}$ are the initial interaction and potential energies, respectively. We obtain these variationally using the Gutzwiller wave function for bosons [13] assuming a low-$T$ initial state for a given strength of the confining potential characterized by the dimensionless compression $V_0 N^{2/3}/6J$, where $N$ is the number of atoms. This combination appears naturally [8] as the thermodynamic limit in a trap is given by $N \rightarrow \infty$ with $V_0 N^{2/3} = \text{const}$.

Energy conservation allows us to determine the state after equilibration. The corresponding temperature will be negative and large. We therefore used a high-temperature expansion [14] to obtain the thermodynamic potential in the presence of the trap. We found that an expansion up to 4th order in $\beta J$ gives accurate results. For simplicity, we locally approximated the system by a homogeneous one. Corrections to this so-called local-density approximation [13] vanish with $1/N^{1/3}$ and are therefore tiny for typical atom numbers, $N \sim 10^5$. Finally, the (negative) temperature was determined by setting $\langle H_b \rangle = E_{\text{tot}}$ and then the entropy was computed from the high-$T$ expansion.

In Fig. 2 the entropy per boson is shown as a function of the initial compression $V_0 N^{2/3}$ of the cloud for several values of $U$. We also calculated the result without dephasing (dashed lines), obtained in the limit $t_W \rightarrow 0$, corresponding to the scheme originally proposed by Mosk [9]. Entropies and $|T|$ are about 40% higher in this case.

The entropy per boson drops for increasing $|V_0|$ as
Ref. [11] we have determined the scattering rate such that energy and particle number are conserved. In relaxation time approximation, from a band insulating, rather than a Mott-insulating initial state for low densities, \( \tau \ll |U|/T < 1 \) one can reach a regime, where scattering is rare. In Ref. [11] the numerics was also compared to experiments.

We first consider an instantaneous quench, \( V_0 \rightarrow V_{0f} = -0.05V_0 \) for \( U = 2J \), parameters which reflect approximately the experimental conditions of Ref. [11]. Temperature and density profiles (and parameters) are displayed in Fig. 3. Here \( T(r, t) \) is defined as the temperature of a homogeneous reference ensemble in equilibrium with the same energy and particle density.

Because of energy conservation and the upper bound on the kinetic energy, the atomic cloud cannot expand to arbitrary size but equilibrates for \( t \rightarrow \infty \). The initial \( T > 0 \) becomes rapidly negative and slowly obtains a homogeneous value (which can be calculated from energy conservation in an independent way). It takes longer to equilibrate in the tails of the cloud, where scattering rates are small and strong Bloch oscillations occur.

Two time scales determine the relaxation mainly. First, \( \tau(n, e) \) determines locally the equilibration rate according to Eq. (4) but local interactions do not change the local energy and particle density. Therefore a second time scale describes how long it takes to redistribute particles and energy across the cloud. For not too weak interactions, see below, this transport will be diffusive and not convective as momentum is not conserved and can be efficiently transferred to the optical lattice by umklapp scattering for the relatively high \( |U| \) considered here. The corresponding diffusion time is estimated as

\[
\tau_D \sim \frac{r^2}{D} \sim \frac{U^2 N}{J^3}
\]
(energy) diffusion in $d = 2$. Figure 4 also shows the time $t_{90}(U)$ needed to reach $J\beta_0 = -0.469$ (90% of the inverse temperature for $t \to \infty, U \to 0$). For larger $U$ one gets $t_{90} \sim \tau_D \propto U^2$, but for small $U$, $t_{90}$ diverges due to the divergence of the local relaxation time, $\tau \propto 1/U^2$. In all cases, relaxation is not very fast, $t_{90} > 300/J$. The fastest relaxation to equilibrium occurs for relatively weak interactions when $U$ is a fraction of the full bandwidth $8J$.

FIG. 5: (color online). The inverse temperature $\beta(r=0,t)$ in the center of the trap as a function of rescaled $t/\Delta t$ for various $U$ and system sizes (solid: $N = 3000$, dashed: $N = 6000$, dotted: $N = 12000$). Dash-dotted line: $J\beta_0 = -0.469$.

In order to reach $T < 0$ with small $|T|$, it is useful to decrease $|V_0|$ slowly to reduce entropy generation and to see whether adiabatic conditions can be realized. We therefore use the protocol shown in the inset of Fig. 5 after a sudden quench at $t = 0$, $V_{0i} \to -V_{0i}$, $-V_0$ is reduced linearly, $V_0(t) = -V_0 + (V_{0f} + V_{0i})t/\Delta t$ for $t < \Delta t$ and $V_0(t) = V_{0f} < 0$ for $t > \Delta t$. As shown in Fig. 5, upon increasing $\Delta t$, considerably lower values of $\beta < 0$ can be obtained and one approaches the adiabatic limit. Only due to the high entropy assumed for the initial state $(S/N = 1.2k_B$, implying $J\beta = 1.47$ for $V_{0i} \to V_{0f}$ adiabatically), $|T|$ remains relatively high even for $\Delta t \to \infty$ where $J\beta \approx -1.21$. The overall entropy production for $\Delta t \to \infty$ is tiny, $\Delta S/N \approx 0.12k_B$, i.e. the bosonic case, $\text{Fig. 2}$ as for the large initial $T$, kinetic energies were small. Note that even for $\Delta t = 1600/J$ deviations from the adiabatic behavior are considerable, which shows how difficult it is to reach truly adiabatic conditions. Nevertheless, it is possible to reach $T \approx -2J$ within a time $200/J \approx 100$ ms for typical parameters $[11]$.

In our opinion the observation of finite momentum superfluidity, Fig. 1B, is probably the best “smoking gun” signature of $T < 0$ in equilibrium. To reach it, it is, however, necessary to switch the interaction $U \to -U$ using a Feshbach resonance for bosons. We expect that the associated loss processes by three-particle scattering can efficiently be reduced in an optical lattice. An important issue are the time scales needed for local equilibration and – most importantly – redistribution of energy and particles across the system. For fermions we find that relaxation is most efficient for relatively weak interactions. More generally, the long equilibration times arising from the necessity to redistribute energy and particles should be important for all equilibration processes and quenches in inhomogeneous systems both for positive and negative $T$. Here we expect that the equilibration properties of low-$|T|$ bosons differ qualitatively from high-$|T|$ fermions due to the suppression of umklapp scattering for bosons and due to the onset of superfluidity.

We acknowledge discussions with I. Bloch, D. Rasch, E. Demler, and U. Schneider, and financial support by the SFB 608 and SFB/TR 12 of the DFG and the Studienstiftung des deutschen Volkes (S.M.).

[1] E.M. Purcell and R.V. Pound, Phys. Rev. 81, 279 (1951).
[2] P. J. Hakonen, et. al., Phys. Rev. Lett. 63, 365 (1992).
[3] A.S. Oja and O.V. Lounasmaa, Rev. Mod. Phys. 69, 1 (1997).
[4] N.F. Ramsey, Phys. Rev. 103, 20 (1956).
[5] D. Jaksch, et. al., Phys. Rev. Lett. 81, 3108 (1998).
[6] M. Greiner, et. al., Nature 415, 39 (2002).
[7] R. Jördens, et. al., Nature 455, 204-207 (2008).
[8] U. Schneider, et. al., Science 322, 1520-1525 (2008).
[9] A.P. Mosk, Phys. Rev. Lett. 95, 040403 (2005).
[10] A.S. Sorensen, et. al., preprint, arXiv:0906.2567.
[11] U. Schneider, et. al., preprint, arXiv:1005.3545.
[12] A. Rosch, et. al., Phys. Rev. Lett. 101, 265301 (2008).
[13] W. Krauth, M. Caffarel, and J.-P. Bouchaud, Phys. Rev. B 45, 3137-3140 (1992).
[14] J. Oitmaa, C. Hamer, and W. Zheng: *Series expansion methods for strongly interacting lattice models* (2006, Cambridge University Press, Cambridge, England, 2006).
[15] I. Bloch, J. Dalibard, W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).