Intrinsic Heating and Cooling in Adiabatic Processes for Bosons in Optical Lattices

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We show that by raising the lattice ''adiabatically'' as in many current optical lattice experiments on bosons, even though the temperature may decrease initially, it will eventually rise linearly with lattice height, taking the system farther away from quantum degeneracy. This increase has nothing to do with the entropy of the bulk Mott phase and is caused by the *adiabatic compression* of the mobile atoms between Mott layers. Our studies show that one can *reverse* the temperature rise to reach quantum degeneracy by *adiabatic expansion*, which can be achieved by a variety of methods.

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At present, there is worldwide interest in emulating strongly correlated electronic systems using cold atoms in optical lattices. Should these efforts be successful, we shall have a whole host of new methods for studying strongly correlated systems which allows one to vary density, interaction, and dimensionality with ease. Typically, experiments are performed in the regime where the system is in a tight binding band. To reach the strongly correlated regime, the lattice gas must achieve quantum degeneracy in this narrow band [1]. This can be very challenging, as the temperature for quantum degeneracy can be several orders of magnitude lower than that in the bulk. The issue of temperature is also important for mapping out phase boundaries, deciding the proximity to a quantum phase transition, and studying quantum critical phenomena.

In current experiments on bosons, one typically starts with a magnetic trap and then turns on a lattice adiabatically. How temperature changes in this process is a question of great interest. While there are many studies [2,3], there is not yet analytic understanding of the cooling power of this process. For a noninteracting gas in a tight binding band, the only energy scale is the hopping integral t, which decreases exponentially with lattice height V_0. By dimensional analysis, the entropy density of a quantum gas in an infinite lattice must be a function of T/t [4], where T is the temperature. At first sight, this seems to suggest a powerful cooling scheme. As V_0 is turned on adiabatically, t will drop exponentially. This will force T to decrease as rapidly in order to keep the entropy constant. This, however, does not work in practice because of particle interactions. The entropy density is not only a function of T/t but also U/t, where U is the on-site repulsion energy. As both t and T decrease, U/t becomes so important that it overwhelms the T/t contribution. Note that the interaction effect is not only important in the Mott regime, but also in the superfluid phases close to the quantum critical point where the condensate is severely depleted. Thus, even on the superfluid side, the ratio T/t *cannot* be constant for sufficiently large V_0.

For an *infinite* lattice, the temperature of Bose gas *must rise* when it is brought deeper into the Mott regime. This is because the energy gap in the Mott phase is given by U, which increases with lattice height V_0 [5]. Raising the lattice will therefore make it harder to generate excitations. The only way to keep the entropy constant is then to raise the temperature to counter the rising excitation energy, which, unfortunately, drives the system away from quantum degeneracy.

The presence of a trap, however, has a profound effect on the adiabatic processes, to the point that the bulk effects mentioned above are completely irrelevant. In a trap, a lattice Bose gas will have a ''wedding cake'' structure consisting of concentric regions of Mott phases separated by a shell of mobile atoms (referred to as a ''conducting'' shell). Since the boson number fluctuates in these shells, they have much higher entropy density than the Mott regions at temperatures $T < U$, and are the sources of entropy at low temperatures. As we shall see, the adiabatic processes in current experiments produce an *adiabatic compression* on these conducting shells which causes the temperature of the system to increase. However, by understanding how entropy distributes in the system, it is possible to reverse this temperature increase and reach quantum degeneracy through *adiabatic expansion*.

(A). Relevant energy scales.— The potential of an infinite optical lattice is $V_L(\mathbf{x}) = V_0 \sum_{i=1,2,3} \sin^2(\pi x_i/d)$, where d is the lattice spacing. In deep lattices, bosons will reside in the lowest band and the system is described by the boson Hubbard model, $\mathcal{K} = \hat{H}_t + \hat{H}_U - \mu\hat{N} \equiv \mathcal{K}_o + \hat{H}_t$, where $H_t = -t\sum_{\langle \mathbf{R},\mathbf{R}'\rangle} a^\dagger_{\mathbf{R}} a_{\mathbf{R}'}$, $\hat{H}_U = \sum_{\mathbf{R}} U n_{\mathbf{R}}(n_{\mathbf{R}} - 1)/2$, $\mathcal{K}_o \equiv \mathcal{H}_U - \mu\hat{N}$, $a^\dagger_{\mathbf{R}}$ creates a boson at site $\mathbf{R}$, $n_{\mathbf{R}} = a^\dagger_{\mathbf{R}} a_{\mathbf{R}}$, and μ is the chemical potential. Both the hopping integral t and on-site energy U can be calculated from lattice height V_0 and recoil energy $E_R \equiv (\pi\hbar)^2/(2Md^2)$ [6]. In Table I, we show the values E_G, U, t, and t^2/U for ^{87}Rb (with scattering length $a_s = 5.45$ nm) in a lattice with $d = 425$ nm for various lattice heights, where E_G is the lowest band gap in the density of state, and t^2/U is the scale for virtual hopping. We see that for $V_0/E_R \geq 10$, we have $U \gg t \gg t^2/U$. Since the superfluid-insulator transition is estimated to be $V_0/E_R = 12 \sim 13$ for ^{87}Rb [7], the condition $U \gg t \gg t^2/U$ is well

TABLE I. Relevant energy scales of for lattice bosons.

V_0/E_R	3	5	10	15	20	30
E_G/E_R	0.58	1.91	4.42	6.23	7.63	9.79
E_G (nK)	90	294	678	956	1171	1503
U (nK)	15.5	24.2	44.6	63.7	82.0	117.2
t (nK)	17.9	10.4	3.01	1.03	0.39	0.073
t^2/U (nK)	20.66	4.45	0.20	0.0166	0.0019	0.00005

satisfied in this regime, and is strongly enforced at higher lattice heights. Table I shows the great challenge of reaching quantum degeneracy (i.e., $T \sim t$ [1]) even for V_0 as low as $15E_R$, and the enormous challenge of reaching temperatures $\sim t^2/U$.

(B). Adiabatic compression.— In current experiments, the optical lattices are constructed from red detuned lasers where atoms are sitting in the region where the laser intensity is high. The lattice is switched on adiabatically in a magnetic trap $V_m(\mathbf{r}) = M\omega_0^2 r^2/2$, with frequency ω_0. However, due to the Gaussian profile of the laser beam, the laser itself will also produce a confining harmonic potential. When these two potentials are properly aligned, the frequency ω of the total harmonic trap ($V(\mathbf{r}) = M\omega^2 r^2/2$) exceeds ω_0, and is given by [5]

$$\omega^2 = \omega_0^2 + 8V_0/(Mw^2), \tag{1}$$

where w is the waist of the laser beam. Thus, raising the lattice will provide an *adiabatic compression*. In fact, for strong lattices, the laser contribution can dominate over that of the magnetic trap. For example, for $V_0 = 12E_R$, $E_R = h \times 3.2$ kHz, $w = 130\ \mu$m, and $\omega_0 = 2\pi \times 15$ Hz, the second term in Eq. (1) is already 10 times larger than the first. As we shall see, this adiabatic compression is the cause of temperature increase in a trap.

(C). Density profile and entropy distribution.— We shall focus on the case $U \gg t$, and temperature range $U \gg T > 0$. (T has the dimension of energy.)

(C1) $T = 0$.—If t were zero, all sites are decoupled, and $\mathcal{K} = \mathcal{K}_0$. The eigenstates on each site are number states. When μ lies in the interval $(m-1)U < \mu < mU$, the ground state has $\langle n_{\mathbf{R}} \rangle = m$, ($m = 0, 1, 2, \dots$). In a trap, the density profile can be obtained using local density approximation (LDA) by replacing μ with $\mu(\mathbf{r}) = \mu - V(\mathbf{r})$. This leads to a wedding cake structure, (see Fig. 1), with sharp steps located at

$$R_m = \sqrt{2(\mu - mU)/(M\omega^2)}, \tag{2}$$

and μ is determined by the number constraint,

$$N = \int d\mathbf{r} n(\mathbf{r}) = \frac{4\pi}{3} \sum_m (R_m/d)^3, \tag{3}$$

with the m-sum restricted to $0 \le m < \mu/U$.

Since the energy difference (relative to μ) between the m to $(m+1)$ boson state is $\mathcal{E}_{m+1} - \mathcal{E}_m = mU - \mu$, the number states m and $m+1$ are degenerate at $\mu = mU$. This degeneracy will be lifted when $t \neq 0$, which introduces fluctuations between neighboring number states. As a result, the sharp steps in Fig. 1 are rounded off over a shell of width $(\Delta R_m)^{(0)} \sim (m+1)t/(M\omega^2 R_m)$.

It is important to note that the increase of V_0 will also makes the Bose gas more repulsive, since $U \sim (V/E_R)^{0.88} \sim V_0$ [6]. The number constraint, Eq. (3), then implies that μ must also increase with V_0 due to the increase of U. As a result, the radii R_m only has a weak V_0 dependence. In other words, trap tightening and increase of repulsion, both caused by the rising V_0, almost cancel each other. This effect can be verified numerically, and is important for our later discussions.

(C2) $U \gg T \gg t$.—In this case, the thermodynamics is again dominated by $\mathcal{K}_0$ with H_t as a perturbation. For $\mu \sim mU$, the number density $n(T, \mu) = \langle a^\dagger a \rangle / d^3$ is,

$$n(T, \mu) = d^{-3}[m + f] + (..), \tag{4}$$

where f stands for $f(mU - \mu)$, $f(x) = (e^{x/T} + 1)^{-1}$, and (..) denotes terms of order of $((t/T)^2, e^{-U/T})$ and higher.

The fact that the density profile of the step is a Fermi function with width T means that this width can be used as a temperature scale of the system. It is also simple to show that the entropy density is

$$s(T, \mu) = d^{-3}[-(1-f)\ln(1-f) - f\ln f] + (..). \tag{5}$$

Applying the Sommerfeld expansion on Eq. (5) shows that the relation between μ and N is still given by Eq. (3) with

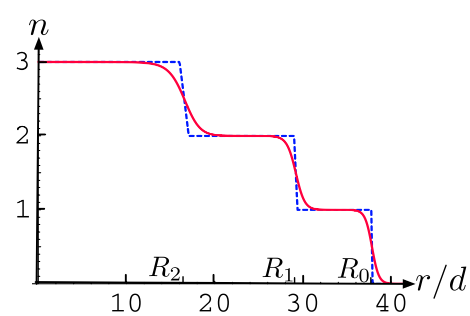

FIG. 1 (color online). Density distribution in a harmonic trap. The density profile of the steps at $T > t$ is described by the Fermi function in Eq. (4). The system considered has 3.5×10^5 ^{87}Rb bosons, in a magnetic trap with $\omega_o = 2\pi(15$ Hz), $V_0/E_R = 25$, $d = 425$ nm.

corrections $O(T/U)^2$. The width of the conducting layer ΔR_m is now given by $\Delta\mu(\mathbf{r}) \simeq T$, or

$$\Delta R_m \simeq T/(M\omega^2 R_m). \tag{6}$$

In Fig. 2, we have plotted the entropy density as a function of position. One sees that the entropy density $s(r)$ is concentrated in the conducting layers and is essentially zero ($\sim O(e^{-U/T})$) in the Mott region. The maximum value of entropy per site $s(\mathbf{r})d^3$ is $\ln 2 + O((t/T)^2)$. It occurs at R_m, reflecting the degeneracy of m and $m+1$ number states at $\mu = mU$. The total entropy of the wedding cake structure $S_{\rm cake} = 4\pi \int drr^2 s(T, \mu(\mathbf{r}))$ is then $\sim 4\pi \sum_m R_m^2 \Delta R_m \ln 2/d^3$, or $S_{\rm cake} \sim \sum_m T R_m/(m\omega^2 d^3)$. Using the Sommerfeld expansion, and with the $(t/T)^2$ correction, we have

$$S_{\rm cake}(T) = \frac{4\pi^3}{3}\frac{T}{M\omega^2 d^3}\sum_m R_m(1 + O[(t/T)^2, (T/U)^2]). \tag{7}$$

(C3) Heating by compression.— As the lattice height is raised adiabatically, ω^2 in Eq. (7) increases [see also Eq. (1)], and T must increase to keep the entropy constant. The simplest case is a single Mott region, which occurs when $U/2 > \mu > 0$. In this case, $R_0 = \sqrt{2\mu/(M\omega^2)}$, and $N = 4\pi R_0^3/(3d^3)$. The size of Mott regime (R_0) is independent of T and ω, and Eq. (5) becomes $S_{\rm cake}(T) = (\frac{4\pi^3}{3})\frac{T}{M\omega^2 d^2}(\frac{3N}{4\pi})^{1/3}$. In the limit of large V_0, Eq. (1) implies $S_{\rm cake} \propto T/V_0$. In general, there are several Mott steps. However, as we have discussed at the end of (C1), the sum $\sum_m R_m$ in Eq. (7) depends weakly on V_0. So we again have $S_{\rm cake} \propto T/V_0$; hence, the temperature increases with the lattice height.

(C4) Cooling by adiabatic expansion.— Having identified the source of heating, one can reverse the heating process by (i) adding a blue detuned laser to generate a repulsive trap (with negative curvature $-\omega_1^2$) of variable strength so that Eq. (1) becomes $\omega^2 = \omega_0^2 - \omega_1^2 + 8V_0/mw^2$. (ii) Turn on a (magnetic) antitrap which make the sign of ω_0^2 negative. This can be achieved by flipping the spin of the boson from low field seeking state to high field seeking. This process is adiabatic as the flipping of spin does not affect the number distribution of the system. (iii) Use a laser beam with large width w and reduce ω_0. The reduction of ω^2 will enable one to reach the lowest possible temperatures within the regime $U > T > t$. As $T \to t$, Eq. (7) is no longer valid, and the entropy has to be calculated differently. [See (C6)]. [8]

(C5) Condition for cooling.—Before discussing the case $T < t$, we first discuss how the initial temperature T_i of a Bose gas (in a magnetic trap without lattice) is related to the temperature T_f of the final wedding cake structure. The thermodynamics of a Bose gas in harmonic trap (no lattice) has been studied by Giorgini, *et al.* [9]. For initial temperature $T_i < \mu_0$, where μ_0 is the chemical potential in the center of the trap, their results imply the entropy is

$$S_i(T, N) = \frac{7A\zeta(3)}{5\sqrt{2}}\left(\frac{15a_s N}{\sigma}\right)^{1/5}\left(\frac{T}{\hbar\omega_o}\right)^{5/2}, \tag{8}$$

where $\sigma = \sqrt{\hbar/(M\omega_o)}$ and a_s is the s-wave scattering length, and $A = 10.6$.

The temperatures T_i and T_f are related as $S_i(T_i, N) = S_{\rm cake}(T_f, N; V_0)$, where $S_{\rm cake}(T, N; V_0)$ is obtained by inverting the number relation $N = \int n[T, \mu(r)] = N(T, \mu)$ for μ and substituting it into the relation $S_{\rm cake} = \int s[T, \mu(\mathbf{r})]$. In Fig. 3, we have represented S_i by a black

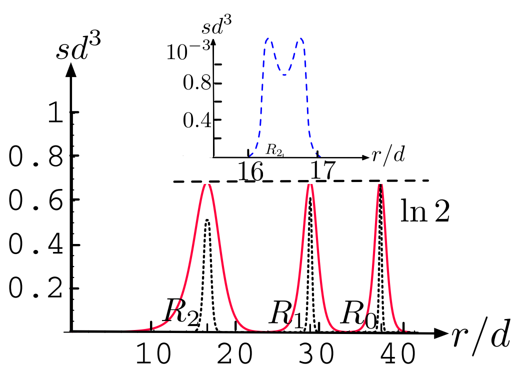

FIG. 2 (color online). Entropy density as a function of position with the same parameters as in Fig. 1. The solid and dotted curves are for $T = 5$ nK and $T = 1$ nK. The decrease of the peak value of s at smaller r is due to the $(t/T)^2$ and Sommerfeld expansion correction in Eq. (5). The inset is the entropy density at temperatures $T < t$ discussed in (C6).

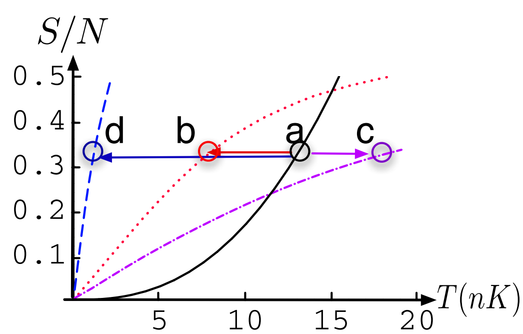

FIG. 3 (color online). Illustration of intrinsic heating and cooling: Solid curve is S_i. The dotted and dotted-dashed line are for $V_0/R_R = 15$ and 30 with the final overall trapping frequencies $\omega = 2\pi(53.7\ \text{Hz})$ and $\omega = 2\pi(74.5\ \text{Hz})$, respectively. The system has the same parameters as that in Fig. 1. Point (a) denotes the initial temperature T_i. The final temperature for $V_0/E_R = 15$ and 30 are denoted by point (b) and (c). The dashed curve with steepest slope is the total entropy for the adiabatic expansion process with $\omega = 2\pi(15\ \text{Hz})$, with T_f given by point (d). For $T_i > 15$ nK, considerable heating will occur when raising a red detuned laser lattice beyond $V_0 = 15E_R$. Adiabatic expansion, however, can cool the system considerably.

solid line for a system of 3.5×10^5 ^{87}Rb bosons, $\omega_o = 2\pi(15\ \mathrm{Hz})$, $a_s = 5.45$ nm. T_i is chosen to be 13 nK. The entropies S_{cake} of the final states obtained by raising a red laser lattice to $V_0/E_R = 15$ and 30 in the same magnetic trap are represented by a dotted and dotted-dash curve, respectively. At these lattice heights, the system has three Mott layers. The reason that S_{cake} deviates from the linear dependence on T when T increases is because of the corrections from Summerfeld expansion in Eq. (4) and (5). The dashed line with large slope is the entropy of a final state with low (total) trap frequency ($\omega = 2\pi(15)$ Hz), produced by the expansion schemes mentioned in (C3). In this case, the system has only one Mott layer.

In the entropy-temperature plot in Fig. 3, T_i and T_f are connected by a horizontal line. Heating (cooling) occurs if S_{cake} lies on the right- (left-) hand side of T_i. Temperature increase is reflected in the fact that the slope of $S_{\mathrm{cake}}(T, N; V_0)$ decreases with increasing V_0, and S_{cake} will eventually lie on the right-hand side of any T_i. For given T_i, the critical V_0 above which intrinsic heating occurs is given by $S_i(T_i, N) = S_{\mathrm{cake}}(T_i, N; V_0^*)$. For our example ($T_i \sim 13$ nK), we have $V_0^* \sim 25E_R$. If $T_i > 20$ nK, V_0^* will be much lower. Raising a red laser lattice will lead to a significant increase in temperature. (See also [9]). In contrast, adiabatic expansion can lead to an order of magnitude or more reduction in temperature.

(C6) $T < t$.—In this case, hopping cannot be treated as a perturbation. To find the entropy, we focus on mobile layer (where $\mu \sim mU$). Denoting the number states $m + 1$ and m on each site as a "pseudospin" $|1/2\rangle$ and $|-1/2\rangle$, we can write $a_{\mathbf{R}} = S^-_{\mathbf{R}}$, $a^\dagger_{\mathbf{R}} a_{\mathbf{R}} = S^z_{\mathbf{R}} + m + 1/2$. The Hamiltonian in this regime can be written as [10], $\mathcal{K} = -h\sum_{\mathbf{R}} S^z_{\mathbf{R}} - \sum_{\langle \mathbf{R},\mathbf{R}'\rangle}[J_\perp \mathbf{S}^\perp_{\mathbf{R}} \cdot \mathbf{S}^\perp_{\mathbf{R}'} + J_z S^z_{\mathbf{R}} S^z_{\mathbf{R}'}]$, where $\mathbf{S}^\perp_{\mathbf{R}} = (S^x_{\mathbf{R}}, S^y_{\mathbf{R}})$, $h = \mu - mU + O(t^2/U)$, $J_\perp = (m+1)t$, $J_z = O(t^2/U)$. Superfluid order corresponds to $\langle \mathbf{S}^\perp_{\mathbf{R}} \rangle \neq 0$. The Mott phase corresponds to $\langle S^z_{\mathbf{R}} \rangle = \pm 1/2$.

At $h = 0$, $J_\perp \neq 0$, the system at $T = 0$ is a ferromagnet in the xy-plane (superfluid). The transition temperature is $T_c \sim J_\perp$. As $|h|$ increases, the ordering spin will tilt away from the xy-plane and develop an S_z component. At the same time, the magnitude of $\langle S^\perp_{\mathbf{R}} \rangle$ is reduced, and so as T_c. Using Primakoff-Holstein transformation, it is straightforward to work out the spin wave spectrum and hence the entropy density at temperatures $T < t$ near $\mu \sim mU$, which is $s_m(T, \mu) = Cd^{-3}(\frac{T}{(m+1)t})^3(1 - \frac{|\mu - mU|}{6t(m+1)})^{-3/2}$, and where $C = \sqrt{3}\pi^2/1620$. The fact that s is a local minimum at $\mu = Um$ (or $h = 0$) reflects the weakening of superfluid order when $h \neq 0$.

For $|h| > J_\perp$, (or $|\mu - mU| > (m+1)t$), the system enters the Mott phase. The entropy density will reduce to the Mott value (which is essentially zero) over a chemical potential range $\Delta[\mu - V(r)] \sim (m+1)t$, or spatial distance $\Delta R_m \sim (m+1)t/(M\omega^2 R_m)$. Together with the local minimum structure derived in previous paragraph, the entropy density must therefore have a double peak feature as shown in the inset of Fig. 2.

The maximum of the entropy density appears at $|h| \sim J$. It is difficult to obtain analytic results in this regime, for one has to deal with all the complexity of quantum critical phenomena at temperature T in this regime. Accurate answers will require quantum Monte Carlo treatments. However, with the features of entropy density mentioned above, one can estimate the total entropy to be $S_{\mathrm{cake}} \sim 4\pi\sum_m R_m^2(\Delta R_m)s_m$, or $S_{\mathrm{cake}} \sim \frac{4\sqrt{3}\pi^3}{135}\frac{T^3}{M\omega^2 d^3 t^2}\sum_m \frac{R_m}{(m+1)^2}$. This faster drop of S_{cake} with temperature will reduce the cooling power of adiabatic expansion. However, this will take place at temperature scales so low that it is not visible on the scale of Fig. 3.

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[8] The number of layers in a wedding cake structure may decrease during adiabatic expansion. This will involve mass transport caused by the motion of the conducting shell. The rate for this process is $t/\hbar$ times the Gibbs factor $e^{-E_{\mathrm{ex}}/T}$, where E_{ex} is the excitation energy for removing atoms from one Mott layer to the nearby one (such as $\mathcal{E}_{m-1} - \mathcal{E}_m$). Since this excitation energy vanishes at the center of the conducting shell, this rate is given simply by $t/\hbar$. Hence, as long as this rate is faster than that of change of lattice height, the expansion process will remain adiabatic.

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