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 all 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 is intrinsic and is caused by the adiabatic compression during the raising of red detuned lattices. However, the origin of this heating, which is entirely different from that in the bulk, also shows that one can reverse the temperature rise to reach quantum degeneracy by adiabatic expansion, which can be achieved by a variety of methods.

At present, there are worldwide interests to emulate 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 allow one to vary density, interaction, and dimensionality with great ease. Typically, experiments are performed in the regime where the quantum gas is in a tight binding band. A necessary condition for reaching the strongly correlated regime is that the lattice gas must achieve quantum degeneracy in this narrow band. This can be very challenging, as the temperature for quantum degeneracy can be several orders of magnitude lower than that in the bulk.

In current experiments on bosons, one typically starts with a magnetic trap and then turns on a lattice adiabatically to bring the system into the Mott regime. How temperature changes in this process is a question of key interest. While there are theoretical studies, there are not yet analytic understanding of the cooling power of this process. For a non-interacting gas in a tight binding band, the only energy scale is the hopping integral $t$, which decreases exponentially with lattice height $V_o$. By dimensional analysis, the entropy density of a quantum gas in an infinite lattice must be a function of $T/t$, where $T$ is the temperature. At first sight, this seems to furnish a powerful cooling scheme, for $t$ will drop exponentially with increasing $V_o$, which will force $T$ to do the same to maintain adiabaticity. This, however, does not work in practice. 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 interaction effect is not only important in the Mott regime, but also in the superfluid phases close to the quantum critical point where condensate depletion becomes severe. Thus, even on the superfluid side, the ratio $T/t$ can not be constant for sufficiently large $V_o$.

As a matter of fact, in 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 $V_o$. 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. We shall call this “temperature runaway”.

The presence of an harmonic trap, however, has 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. Between neighboring Mott regions is a shell of mobile atoms (referred to as a “conducting” shell). Since 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 produces an adiabatic compression on these conducting shells which again cause a temperature runaway. However, by understanding how entropy distributes in the system, it is possible to reverse this “runaway” by a simple process, i.e. adiabatic expansion. In this way, one can reach down to the degenerate temperature of the order of $t$ even for deep lattices.

(A). The relevant energy scales: The potential of an infinite optical lattice is $V(x) = V_o \sum_{i=1,2,3} \sin^2(\pi x_i/d)$, 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. In grand canonical form, it is $H = H_t + H_U - \mu \hat{N}$ where $H_t = -t \sum_{(\mathbf{R}, \mathbf{R}')} a_{\mathbf{R}}^\dagger a_{\mathbf{R}'}, \quad H_U = \sum_{\mathbf{R}} U n_{\mathbf{R}} (n_{\mathbf{R}} - 1)/2, \quad \hat{N} = \sum_{\mathbf{R}} \hat{n}_{\mathbf{R}}$, $\hat{n}_{\mathbf{R}} = a_{\mathbf{R}}^\dagger a_{\mathbf{R}}$, and $\mu$ is the chemical potential. Both the hopping integral $t$ and on-site energy $U$ can be calculated from lattice height $V_o$ and recoil energy $E_R \equiv (\pi \hbar^2)/(2 M d^2)$. To give an idea of the energy scales in the Mott regime, we show the values $E_G$, $U$, $t$ and $t^2/U$ in Table 1 for $^{87}$Rb (with scattering length $a_s = 5.45 \text{nm}$) in a lattice with $d = 425 \text{nm}$ for various lattice height, 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 from the Table 1 that for $V_o/E_R \geq 10$, we have $U >> t >> t^2/U$. Since the superfluid-insulator transi-
tion is estimated to be $V_o/E_R = 12 \sim 13$ for $^87\text{Rb}$, the condition $U >> t >> t^2/U$ is well satisfied in the region of transition, and is strongly enforced at higher lattice height. Table 1 shows the great challenge of reaching quantum degeneracy (i.e. the scale $t$[1]) even for $V_o$ as low as $15E_R$, and the even greater challenge of reaching temperatures $\sim t^2/U$.

| $V_o/E_R$ | 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 | 0.00019 | 0.00005 |

### (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 density is high. The lattice is switched on adiabatically in a magnetic trap $V_m(r) = M\omega_o^2 r^2/2$, with frequency $\omega_o$. 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 $\omega$ of the total harmonic trap $V(r) = M\omega^2 r^2/2$ is:

$$\omega^2 = \omega_o^2 + 8V_o/(M\omega^2), \quad (1)$$

where $w$ is the waist of the laser beam. Thus, as the lattice is switched on, it also provides an adiabatic compression. In fact, for strong lattices, the laser contribution can dominate over that of the magnetic trap. For example, for $V_o = 12E_R$, $E_R = h \times 3.2kH\times w = 130\mu m$, and $\omega_o = 2\pi \times 15Hz$, the second term in eq. (1) is already 10 times larger than the first. As we shall see, this adiabatic compression is the source of temperature runaway in a trap.

### (C). Density profile and entropy distribution: We shall focus on the case $U >> t$, and temperatures $U >> T > 0$. Let us distinguish the cases $T > t$, $t > T$, and $T = 0$. ($T$ has the dimension of energy).

- **(C1) $T = 0$:** If $t$ were zero, all sites are decoupled. The eigenstates on each site are number states. The ground state then has $\langle n_o \rangle = m$, ($m = 0, 1, 2..$), when $\mu$ lies in the interval $(m-1)U < \mu < mU$. In a trap, the density profile can be obtained using local density approximation (LDA) by replacing $\mu$ with $\mu(r) = \mu - V(r)$. This leads to a “wedding cake” structure, (see figure 1), with sharp steps located at

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

and $\mu$ determined by the number constraint,

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

The $m$-sum are restricted to $0 \leq m \leq \mu/U$.

Since the energy exciting from $m$ to $(m+1)$ boson state is $E_{m+1} - E_m = mU - \mu$, 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 is rounded off over a shell of width $(\Delta R_m)^{(o)} \sim (m + 1)/(M\omega^2 R_m)$. (See (C6) for more discussions).

It is also important to note that in addition to the adiabatic compression, the increase in $V_o$ will make the Bose gas more repulsive, since $U \sim (V/E_R)^{0.88} \sim V_o[6]$. As a result, $\mu$ also increases almost linearly as $V_o$ (see eq. (3)) and the radii $R_m$ only has a weak $V_o$ dependence. In other words, the trap tightening effect and increase of repulsion, both caused by the rising $V_o$, almost cancel each other. This effect can be verified numerically, and is important for our later discussions.

- **(C2) $U >> T >> t$:** In this case, the thermodynamics is again dominated by on-site interaction $K_o$ with $H_t$ as a perturbation. It is straightforward to show that for $\mu \sim mU$, the number density $n(T, \mu) = (a^\dagger a)/d^3$ is,

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

where $f(x)$ stands for $f(mU - \mu)$, $f(x) = (e^{x/T} + 1)^{-1}$, and $\langle .. \rangle$ 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

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

Eq.(4) shows that the location of the conducting shell (at $f = 1/2$) is still given by (eq.2). Applying the Sommerfeld expansion on eq.(5) shows that the relation between $\mu$ and $N$ is still given by eq.(4) with corrections $O(T/U)^2$. The width of the conducting layer $\Delta R_m$ is now given by $\Delta \mu(r) \sim T$, or

$$\Delta R_m \sim T/(M\omega^2 R_m). \quad (6)$$
In figure 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 (\( \sim O(e^{-UT/T}) \)) in the Mott region. The maximum value of entropy per site \( s(r)d^3 \) 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 \( S_{\text{cake}} = 4\pi \int dr^2 s(T,\mu(r)) \) is then \( \sim 4\pi \sum_m R_m^2 \Delta R_m \ln 2/d^3 \), or \( S_{\text{cake}} \sim \sum_m T R_m/(m\omega^2 d^3) \). Using Sommerfeld expansion, and with the \( (t/T)^2 \) correction, we have \[ S_{\text{cake}}(T) = \frac{4\pi^3}{3} \frac{T}{M\omega^2 d^3} \sum_m R_m \left( 1 + O((t/T)^2, (T/U)^2) \right). \] \((C3)\) Temperature runaway: Eq.(7) is the origin of temperature runaway. Since \( \omega^2 \) increases with lattice height (see eq.(1)), \( T \) 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 \( \omega \); and eq.(3) becomes \( S_{\text{cake}}(T) = \left( \frac{4\pi^3}{3} \right) \frac{T}{M\omega^2 d^3} \left( \frac{4N}{3}\right)^{1/3} \). In the limit of large \( V_o \), eq.(1) implies \( S_{\text{cake}} \propto T/V_o \). 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 \( V_o \). So we again have \( S_{\text{cake}} \propto T/V_o \), hence the same temperature runaway.

\((C4)\) Reversing the temperature runaway: Since the temperature increase is caused by adiabatic compression, the simplest way to reverse it is to reduce \( \omega^2 \), i.e. an adiabatic expansion. Some possible ways are: (a) adding a blue detuned laser to generate a repulsive trap (with negative curvature \( -\omega^2 \)) of variable strength so that eq.(1) becomes \( \omega^2 = \omega_0^2 - 8V_o/mw^2 \). (b) Start with a very tight harmonic trap and use a blue (instead of red) detuned laser so that \( \omega^2 = \omega_0^2 - 8V_o/mw^2 \). Expansion can then be achieved by increase \( V_o \). (c) Turn on a (magnetic) anti-trap which make the sign of \( \omega^2 \) 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. (d) Use a laser beam with large width \( w \) and reduce \( \omega_o \). The reduction of \( \omega^2 \) 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 \((C6)\)).

\((C5)\) Condition for cooling: Before discussing the case \( T < t \), let us illustrate 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 the a Bose gas in harmonic trap (no lattice) has been studied by Giogini, Pitaevskii, and Stringari\[9\] using Popov approximation. For initial temperature \( T_i < \mu_o \), where \( \mu_o \) is the chemical potential in the center of the trap, their results imply the entropy is

\[ S_i(T, N) = \frac{7A(3)}{5\sqrt{2}} \left( \frac{15\sigma N}{\sigma} \right)^{1/5} \left( \frac{T}{\hbar \omega_o} \right)^{5/2}, \]  

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

The temperatures \( T_i \) and \( T_f \) are related as \( S_i(T_i, N) = S_{\text{cake}}(T_f, N; V_o) \), where \( S_{\text{cake}}(T, N; V_o) \) is obtained by inverting the number relation \( N = \int n(T, \mu(r)) = N(T, \mu) \) for \( \mu \) and substituting it into the relation \( S_{\text{cake}} = \int s(T, \mu(r)) \). In figure 3, we have represented \( S_i \) by a black solid line for a system of \( 3.5 \times 10^5 \) \(^{87}\)Rb bosons, \( \omega_o = 2\pi(15Hz) \), \( \sigma_s = 5.45nm \). \( T_i \) is chosen to be 13K. The entropies \( S_{\text{cake}} \) of the final states obtained by raising a red laser lattice to \( V_o/E_R = 15 \) 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 \( S_{\text{cake}} \) deviates from the linear dependence on \( T \) when \( T \) increases is because of the corrections to Sommerfeld expansion in eq.(3) and (4). The dashed line with large slope is the entropy of a final state with low (total) trap frequency \( (\omega = 2\pi(15Hz)) \), produced by the expansion schemes mentioned in Section \((C3)\). 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 \( S_{\text{cake}} \) lies on the right (left) hand side of \( T_i \). Temperature runaway is reflected in the fact that the slope of \( S_{\text{cake}}(T, N; V_o) \) decreases with increasing \( V_o \), and will eventually lie on the right hand side of any \( T_f \). For given \( T_i \), the critical \( V_o \) above which intrinsic heating occurs is given by \( S_i(T_i, N) = S_{\text{cake}}(T_i, N; V_o^*) \). For our example, this critical \( V_o^* \) is about \( 25E_R \). From fig.3, it
is clear that if the initial temperature is above 20nK, raising a red laser lattice will lead to a significant increase in temperature. (See also footnote \[3\]). In contrast, if we use a blue laser for the lattice, one can gain an order of magnitude or more reduction in temperature.

**C6** \( T < t \): In this case, hopping is not a perturbation. We shall focus on the regime \( \mu \sim mU \) where entropy density is highest. This regime is intricate for the following reasons. At \( \mu = mU \), the ground state of the Bose Hubbard model is a superfluid, with transition temperature \( T_c \) of the order \( (m+1)t \). As the difference \( |\mu - mU| \) increases, number fluctuations are suppressed and \( T_c \) drops. At some point, the falling \( T_c \) will reach \( T \) and drop below it. To calculate the entropy as a function of \( T \) and \( \mu \), one must face the complexity of critical phenomenon at some point. While it is possible to calculate the entropy function using quantum Monte Carlo methods, it is desirable to have analytic understanding so as to perform quick estimates, which we do below.

Near \( \mu \sim mU \), dominant number fluctuations are between the number states \( m + 1 \) and \( m \) on each site. Denoting these two states as a “pseudo-spin” \( |1/2 \rangle \) and \( |-1/2 \rangle \), we have \( a_R^\dagger a_R = S_{xR}^z + m + 1/2 \); and the Hamiltonian \( K \) written as \[ \text{(H)}, K = -\hbar \sum_{\langle R,R' \rangle} (J_1 S_{xR}^+ S_{xR'}^- + J_2 S_{yR}^z S_{yR'}^z) \] where \( S_{xR}^\pm = (S_{xR}^0)^\pm \), \( h = \mu - mU + O(t^2/U) \), \( J_1 = (m+1)t \), \( J_2 = O(t^2/U) \). Superfluid order corresponds to \( (S_{xR}^z)^2 \neq 0 \). The Mott phase corresponds to \( (S_{xR}^z)^2 \leq 1/2 \).

At \( h = 0 \), \( J_1 \neq 0 \), the system at \( T = 0 \) is a ferromagnet in the \( xy \)-plane (superfluid). The transition temperature is \( T_c \sim J_1 \). 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 \( (S_{xR}^z)^2 \) 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 \( s_m(T,\mu) = C d^{-3} \left( \frac{T}{m+1} \right)^3 \left( 1 - \frac{|\mu - mU|}{m+1} \right)^{3/2} \), and where \( C = \sqrt{3\pi^2}/1620 \). The fact that \( s \) increases as \( h \) moves away from 0 reflects the weakening of superfluid order when \( h \neq 0 \).

For \( |h| > J_1 \), (or \( |\mu - mU| \gg (m+1)t \)), the system enters the Mott phase. Since \( T < t \sim J_1 \), 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 \( \Delta R \sim (m+1)t/(M \omega^2 R_m) \). (See the inset of fig.2). The case \( |h| \sim J \) is difficult one. 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 \( S_{\text{cake}} \sim \frac{4\sqrt{\pi}^3}{135} \frac{T^3}{M\omega^2 d^4} \sum_m m R_m \), or \( S_{\text{cake}} \sim \frac{4\sqrt{\pi}^3}{135} \frac{T^3}{M\omega^2 d^4} \). This faster drop of \( S_{\text{cake}} \) with temperature will reduce the cooling power of adiabatic expansion. However, this will take place at temperature scale so low that it is not visible on the scale of fig.3.

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\[ \text{[1]} \text{R. Diener, et al. \[cond-mat/0609685\]} \]
\[ \text{[2]} \text{B. DeMarco, C. Lannert, S. Vishveshwara, and T.-C. Wei, Phys. Rev. A 71, 063601 (2005), which calculates density profile in the Mott limit numerically but not the entropy. A. M. Rey, G. Pupillo, and J. V. Porto Phys. Rev. A 73, 023608 (2006); which based on “fermionization” in 1D which is not applicable to 3D} \]
\[ \text{[3]} \text{B.Capogrosso-Sansone, N.V.Prokof'ev, B.V.Svistunov, \[cond-mat/0701178\]} \]

\[ \text{[4]} \text{This result is correct only for temperature sufficiently smaller than the lattice height, which is a regime well satisfied by current experiments. See fig.2 and eq.(8) of P.B. Blakie and T. V. Porto, \[cond-mat/0507655\]} \]
\[ \text{[5]} \text{F. Gerbier, et al. Phys. Rev. A 72, 053606 (2005).} \]
\[ \text{[6]} \text{t/E_R = 1.43 (V_0/E_R)^{0.98} e^{-2.07\sqrt{V_0/E_R}}, U/E_R = (5.97\alpha/\lambda) (V_0/E_R)^{0.88}, where} \ \alpha = 2d \text{ is the wave length of the laser, F. Gerbier, et al. ibid.} \]
\[ \text{[7]} \text{M. Greiner, et al. Nature 415, 39 (2002).} \]
\[ \text{[8]} \text{All the figures we show here are exact numerical evaluations of the number constraint} \ N = \int f(T,\mu(r)), \text{and total entropy} \ S_{\text{cake}} = \int s(T,\mu(r)), \text{as well as other quantities. The validity of the leading and sub-leading contri-} \]
butions of the Sommerfeld expansion have all been verified in the temperature range of interest.

[9] S. Giogini, L. P. Pitaevskii, and S. Stringari, J. Low Temp. Phys. 109, 309 (1997). Eq. (8) is obtained by using eq. (77) therein, and the relation 

\[ T \frac{\partial S}{\partial T} = \frac{\partial E}{\partial T}. \]

Most current experiments have initial states at temperatures \( T_i > \mu_o \). We have consider the case \( T_i < \mu_o \) is to demonstrate the intrinsic heating even under optimal initial conditions. Heating will be very severe for initial state with \( T_i > \mu_o \) at \( V_o \) around \( 10E_R \).

[10] R. Barankov, et.al. cond-mat/0611126