Thermodynamics of quantum degenerate gases in optical lattices

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The entropy-temperature curves are calculated for non-interacting Bose and Fermi gases in a 3D optical lattice. These curves facilitate understanding of how adiabatic changes in the lattice depth affect the temperature, and we demonstrate regimes where the atomic sample can be significantly heated or cooled by the loading process. We assess the effects of interactions on a Bose gas in a deep optical lattice, and show that interactions ultimately limit the extent of cooling that can occur during lattice loading.

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I. INTRODUCTION

Tremendous advances have been made in the preparation and control of bosonic and fermionic atoms in optical lattices (e.g. see [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]). In experiments the gas is typically prepared in the optical lattice by a slow loading procedure that begins with a weakly trapped gas and no lattice. During loading, the lattice is turned on in some prescribed way, and the atoms are localized into the tightly confining potential wells of the optical lattice. This process is accompanied by a massive redistribution of the energy states of the system, and it is poorly understood how the loading process affects the properties of the atoms, such as their temperature. Many of the physical phenomenon that are suitable to experimental investigation in optical lattices are sensitive to temperature and it is therefore of great interest to understand how the temperature of a quantum degenerate gas changes with lattice depth. Experimental results by Kastberg \textit{et al.} [11] in 1995 showed that loading laser cooled atoms into a three-dimensional optical lattice caused the atoms to increase their temperature [12, 13]. Recent studies have shown that there is rich range of behaviour that can be expected to occur during the loading process at temperatures much lower than those explored by Kastberg (e.g. see [12, 13, 14]).

In this work we compare and contrast the behaviour of Bose and Fermi systems in optical lattices as a function of the lattice depth. While some work has been undertaken in the case where an external harmonic potential is also present (but restricted to a non-interacting tight-binding approximation) [8], here we will restrict our attention to the uniform lattice. Schematically, our system is shown in Fig. 1: a system of atoms confined in a 3D cubic lattice. As the lattice depth increases the potential changes from that of a uniform box potential to that of a deep lattice potential. The fundamental question we wish to address is how the properties of the equilibrium state, in particular the temperature, change under this loading procedure. To identify the final thermodynamic state of the system we assume that the loading procedure is isentropic. In practice experiments appear to be approximately reversible when the loading is performed slowly, as has been investigated in Ref. [15].

The paper is organized as follows: In section II we introduce the theoretical approach we use for calculating the single particle spectrum and thermodynamic properties of an ideal quantum gas in an optical lattice. The results of this formalism are presented and discussed in section III. In section IV we address the effects of interactions in application to a bosonic system, before concluding.

II. IDEAL GAS FORMALISM

The single particle spectrum completely determines the thermodynamic properties of an ideal gas. We consider a cubic 3D optical lattice made from 3 independent sets of counter-propagating laser fields of wavelength $\lambda$, giving rise
to a potential of the form

\[ V_{\text{Latt}}(\mathbf{r}) = \frac{V}{2} [\cos(2kx) + \cos(2ky) + \cos(2kz)], \]  
(1)

where \( k = 2\pi/\lambda \) is the single photon wavevector, and \( V \) is the lattice depth. We take the lattice to be of finite extent with a total of \( N_s \) sites, consisting of an equal number of sites along each of the spatial directions with periodic boundary conditions. The single particle energies \( \epsilon_q \) are determined by solving the Schrödinger equation

\[ \epsilon_q \psi_q(\mathbf{r}) = \frac{\mathbf{p}^2}{2m} \psi_q(\mathbf{r}) + V_{\text{Latt}}(\mathbf{r}) \psi_q(\mathbf{r}), \]  
(2)

for the Bloch states, \( \psi_q(\mathbf{r}) \), of the lattice. For notational simplicity we choose to work in the extended zone scheme where \( q \) specifies both the quasimomentum and band index of the state under consideration \[24\]. By using the single photon recoil energy, \( E_R = \hbar^2 k^2 / 2m \), as our unit of energy, the energy states of the system are completely specified by the lattice depth \( V \) and the number of lattice sites \( N_s \) (i.e. in recoil units \( \epsilon_q \) is independent of \( k \)).

For completeness we briefly review some important features of the band structure of Eq. (2) relevant to the thermodynamic properties of the system. The smoothed density of states for the system for various lattice depths is shown in Figs. 2(a)-(d). For sufficiently deep lattices an energy gap, \( \epsilon_{\text{gap}} \), will separate the ground and first excited bands (see Fig. 2(c)). For the cubic lattice we consider here, a finite gap appears at a lattice depth of \( V \approx 2E_R \) \[25\] (marked by the vertical asymptote of the dashed line in Fig. 2(c)). For lattice depths greater than this, the gap increases with lattice depth. In forming the gap, higher energy bands are shifted upwards in energy, and the ground band becomes compressed — a feature characteristic of the reduced tunneling between lattice sites. We refer to the energy range over which the ground band extends as the (ground) band width \( \epsilon_{\text{BW}} \) (see Fig. 2(c)). As is apparent in Fig. 2(e), the ground band width decreases exponentially with \( V \), causing the ground band to have an extremely high density of states for deep lattices.

Our primary interest lies in understanding the process of adiabatically loading a system of \( N_p \) bosons or fermions into a lattice. Under the assumption of adiabaticity the entropy remains constant throughout this process and the most useful information can be obtained from knowing how the entropy depends on the other parameters of the system. In the thermodynamic limit, where \( N_s \to \infty \) and \( N_p \to \infty \) while the filling factor \( n \equiv N_p/N_s \) remains constant, the entropy per particle is completely specified by the intensive parameters \( T, V, \) and \( n \). The calculations we present in this paper are for finite size systems, that are sufficiently large to approximate the thermodynamic limit. We would like to emphasize the remarkable feature of optical lattices that \( V \) is an adjustable parameter, in contrast to solid state systems where the lattice parameters are determined by the constituent atoms and are immutable.

We determine the entropy as follows: We calculate the single particle spectrum \( \{\epsilon_q\} \) for given values of \( N_s \) and \( V \).
will be important in the multiple component case, is beyond the scope of this paper.

III. IDEAL GAS RESULTS

A. Effect of lattice loading on temperature

In Fig. 3 we show entropy-temperature curves for various lattice depths and filling factors \( n \). These curves have been calculated for a lattice with 31 lattice sites along each spatial dimension, i.e. \( N_s \approx 3 \times 10^4 \). A general feature of these curves is the distinct separation of regions where adiabatic loading causes the temperature of the sample to increase or decrease, which we will refer to as the regions of heating and cooling respectively (e.g. see Figs. 3(a)-(c) and (e)). These regions are separated by a value of entropy, \( S_0 \), at which the curves plateau, and we note that this feature is more prominent on the curves for larger lattice depths. This plateau entropy is indicated by a horizontal dashed line and is discussed below. For the case of fermions with unit filling, shown in Fig. 3(f), this plateau occurs at \( S_0 = 0 \), and only a heating region is observed.

We now explicitly demonstrate the temperature changes that occur during adiabatic loading using two possible adiabatic processes labeled \( A \) and \( B \), and marked as dotted lines in Fig. 3(c). Process \( A \) begins with a gas of free particles in a state with an entropy value lying above the plateau entropy. As the gas is loaded into the lattice the process line indicates that the temperature increases rapidly with the lattice depth. Conversely process \( B \) begins with a gas of free particles in a state with entropy below the plateau. For this case adiabatic lattice loading causes a rapid decrease in temperature. This behavior can be qualitatively understood in terms of the modifications the lattice makes to the energy states of the system. As is apparent in Fig. 2(e), the ground band rapidly flattens for increasing lattice depth causing the density of states to be more densely compressed at lower energies. Thus in the lattice all these states can be occupied at a much lower temperature than for the free particle case. As we discuss below, for both Bose and Fermi systems, \( S_0 \) is the maximum entropy available from only accessing states of the lowest band. If \( S < S_0 \), the temperature of the system must decrease with increasing lattice depth to remain at constant entropy. Alternatively, for \( S > S_0 \) the occupation of states in higher bands is important, and as the lattice depth and hence \( \epsilon_{\text{gap}} \) increases, the temperature must increase for these excited states to remain accessible.

1. Bosonic systems

The temperature and entropy at which bosons condense generally changes with lattice depth, and is indicated by circles on the \( S-T \) curves in Figs. 3(a) and (b). We note that for high filling factors the condensation points for different lattice depths occur over a wide entropy range, suggesting that the degree of condensation will be greatly affected by adiabatic lattice loading. For instance, consider the adiabatic process indicated by the dashed line and labeled \( C \) in Fig. 3(b). The system starts as a Bose-condensed gas of free particles. However, as the lattice depth increases the condensate fraction decreases until the system passes through the transition point and becomes unconденded.

2. Fermionic systems

In addition to the effect that lattice loading has on the absolute temperature of a Fermi-gas, it is of considerable interest to understand how the ratio of temperature to the Fermi temperature \( T/T_F \) changes. Indeed, the ratio \( T/T_F \) is the standard figure of merit used to quantify the degeneracy of dilute Fermi gases. In Fig. 3(d) we show how \( T/T_F \) changes with adiabatic lattice loading for the same parameters used in Fig. 3(c). This result indicates the typical behaviour seen: Below the entropy plateau where cooling is observed (e.g. see Figs. 3(c) and (e)), the ratio of \( T/T_F \) remains approximately constant, so that there is little change in the degeneracy of the gas. Above the entropy plateau where heating was observed, the ratio of \( T/T_F \) rapidly increases, so that in this regime the gas will rapidly become non-degenerate as it is loaded into the lattice. For the unit filled Fermi case (Fig. 3(f)), there is no cooling regime, and heating is accompanied by a rapid increase in \( T/T_F \) for all initial conditions of the gas.

We note that for \( n > 1 \) it is possible to observe a reduction in \( T/T_F \) for Fermi systems during the loading process. This occurs because \( T_F \) increases, because the Fermi energy lies in the excited band. We do not consider this case here and refer to the reader to Ref. [13] for details.

B. Entropy plateau

In many \( S-T \) curves a plateau in the entropy is apparent. This occurs when the gap in the energy spectrum between the states of the ground and first excited bands is large compared to the energy width of the ground band, i.e. \( \epsilon_{\text{gap}} > \epsilon_{\text{BW}} \). In this case, there is an intermediate temperature range, sufficiently hot that all the states in the ground band are accessed, yet not hot enough for states in the next band to be accessed. Within the temperature range satisfying these conditions, the entropy remains approximately constant at the value corresponding to the saturated ground band contribution to the entropy – we refer to this value as the plateau entropy. We now provide analytic expressions for this plateau.

The total number of microstates accessible to the ground band, \( \Omega_0 \), for the cases of fermionic and bosonic particles is given by

\[
\Omega_0^F = \frac{N_s!}{N_p!(N_s-N_p)!}, \quad (5)
\]

\[
\Omega_0^B = \frac{(N_s+N_p-1)!}{(N_s-1)!N_p!}, \quad (6)
\]
Figure 3: Entropy versus temperature curves for a $N_s \approx 3 \times 10^4$ site cubic lattice, at various depths $V = 0$ to $20E_R$ (with a spacing of $2E_R$ between each curve). Cases considered are (a) bosons with $n = 1.0$, (b) bosons with $n = 4.0$, (c) fermions with $n = 0.25$, (d) fermions (reduced temperature) with $n = 0.25$ (e) fermions with $n = 0.8$, and (f) fermions with $n = 1.0$. The entropy plateau is shown as a dashed line. The processes indicated by the paths labeled $A$, $B$ and $C$ are discussed in the text. For the bosonic systems the critical point for condensation on each curve is indicated with a hollow circle.
IV. EFFECTS OF INTERACTIONS IN THE BOSONIC SYSTEM

We now briefly comment on the role of interactions on the properties of the Bose gas loaded into an optical lattice. For situations where the number of bosons is commensurate with the number of lattice sites, as the lattice depth increases the system will eventually enter the Mott-insulating state [2,16].

In this state the system exhibits a gapped excitation spectrum which is poorly described by the (gapless) non-interacting system. In a lattice of depth greater than a few recoils, the system is well-described by the Bose-Hubbard model [16]

\[ H_{BH} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i \hat{a}_j \hat{a}_j^\dagger, \]

where \( \hat{a}_j \) is the bosonic annihilation operator of a particle at site \( j = \{ j_x, j_y, j_z \} \), and the sum \( \langle i,j \rangle \) is over nearest neighbouring lattice sites. The interaction parameter \( U \) and the tunneling parameter \( J \) can be determined by band structure calculations [13].

In a deep lattice the tunneling parameter is exponentially suppressed, and can be taken to be approximately zero [23]. In this limit Fock states of the \( \hat{a}_j \) operators diagonalize the Bose-Hubbard Hamiltonian, and in the low temperature limit \( k_B T < U \) and for \( 0 < n \lesssim 1 \) we find that

\[ \mu = \frac{U}{2} \left( \frac{n - 1 + \sqrt{3n(2 - n)} + 1}{2(2 - n)} \right). \]

For the unit filled lattice, \( n = 1 \), the chemical potential is approximately \( \mu = U/2 \) and one can derive an analytic expression for the grand canonical partition function given by (see Ref. [14] for details)

\[ Z = \left[ 1 + e^{\beta \mu} \right]^{N_p}, \]

where \( \beta = 1/k_B T \) and \( \beta \mu \) is the chemical potential. Indeed, as is shown in Ref. [14], for \( k_B T \lesssim 0.05 E_R \), and \( n = 1 \), the final temperature in the deep lattice limit. We also refer the reader to related results in Ref. [17].

In a lattice of depth greater than a few recoils, the system is well-described by the Bose-Hubbard model [16] which we have explicitly written in terms of the filling factor, \( n = N_p/N_s \), with the additional validity conditions \( 1 \ll N_p \ll N_s \) (Fermions) and \( N_s/N_p \gg 1 \) (Bosons). We note an important case for which the above approximation is invalid is for the Fermi system with \( N_p = N_s \), i.e. when we have a filling factor of \( n = 1 \), for which \( S_0 = 0 \). This case corresponds to the unit filling factor result shown in Fig. [30] where, as a result of the entropy plateau occurring at \( S_0 = 0 \), only a heating region is observed.

respectively [28]. The corresponding value of entropy \( S = k_B \log \Omega_0 \), i.e. the plateau entropy, is given by

\[ S_0^p \simeq N_p k_B \left[ -\frac{1}{n} \log (1 - n) + \log \left( \frac{1}{n} - 1 \right) \right], \]

\[ S_0^B \simeq N_s k_B \left[ \log \left( 1 + \frac{1}{n} \right) + \frac{1}{n} \log (1 + n) \right], \]

which we have explicitly written in terms of the filling factor, \( n = N_p/N_s \), with the additional validity conditions \( 1 \ll N_p \ll N_s \) (Fermions) and \( N_s/N_p \gg 1 \) (Bosons). We note an important case for which the above approximation is invalid is for the Fermi system with \( N_p = N_s \), i.e. when we have a filling factor of \( n = 1 \), for which \( S_0 = 0 \). This case corresponds to the unit filling factor result shown in Fig. [30] where, as a result of the entropy plateau occurring at \( S_0 = 0 \), only a heating region is observed.

In this state the system exhibits a gapped excitation spectrum which is poorly described by the (gapless) non-interacting spectrum. Here we develop an analytic description for the unit filled system in the strongly interacting regime to assess the effects that interactions have on adiabatic loading, and the behavior of temperature in the deep lattice limit. We also refer the reader to related results in Ref. [17].

In a lattice of depth greater than a few recoils, the system is well-described by the Bose-Hubbard model [16] and for final lattice depths of (dashed line) \( V = 10E_R \), (dash-dot line) \( V = 20E_R \), and (solid line) \( V = 30E_R \). These results are for the case \( n = 1 \) and for the parameters of $^{87}$Rb.

Figure 4: \( T_f \) versus \( T_i \) for final lattice depths of (dashed line) \( V = 10E_R \), (dash-dot line) \( V = 20E_R \), and (solid line) \( V = 30E_R \). These results are for the case \( n = 1 \) and for the parameters of $^{87}$Rb.
temperature scales linearly with $U$ according to
\begin{equation}
T_f = \frac{U}{3E_R} \left( T_i + 0.177 \frac{E_R}{k_B} \right).
\end{equation}

As $U \sim V^{3/4}$, the temperature must increase with lattice depth, as is observed in Fig. 4. This is in contrast to the non-interacting results that show the temperature of the Bose system (in the low temperature regime where the results of this section hold) scales as $\epsilon_{\text{BW}} \sim J$, and as noted earlier this parameter is exponentially suppressed with increasing lattice depth. Thus we find that the system has two competing behaviours: for low lattice depths, the system will be well-described by the non-interacting result and the temperature will decrease rapidly during loading, as observed in Figs. 4(a) and (b). For deeper lattices, where tunneling between sites is small, the temperature is dominated by the energy gap of the excitation spectrum, i.e. $U$, which increases with increasing $V$. Including tunneling effects (i.e. finite $J$) somewhat suppresses the heating observed in Fig. 4. This can be qualitatively understood in terms of the modifications that hopping makes to the eigenstate energies of the system. A non-zero value of $J$ breaks the degeneracy of the energy gap $U$, leading to a quasi-band whose width is proportional to $J$. As $J$ increases (i.e when the lattice becomes shallower) the energy of the lowest excited states decrease accordingly, while the ground state is only shifted by an amount proportional to $J^2/U$. The lowest energy excitations then lie closer to the ground state and become accessible at lower temperatures. As a consequence, the entropy increases (and thus $T_f$ decreases) with respect to the $J = 0$ case. Of course in the deep lattice case, finite $J$ corrections will become vanishingly small.

V. CONCLUSION

In this paper we have surveyed the physics of loading ultracold bosonic and fermionic atoms into optical lattices. Under the assumption that this loading is approximately adiabatic (isentropic) we have seen that there are regimes where the temperature of the system might be raised or lowered by the loading process. For bosons, the loading process can be used to reversibly condense the sample. For fermions, the Fermi energy sets a new energy scale, and for the case of a filled band no cooling regimes are available. We have examined the effects of interactions on the Bose system, and seen that in the deep lattice limit the temperature of the system is proportional to the on-site interaction strength.

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[23] In fact this study used adiabatic de-loading to reduce the temperature of the constituent atoms.
[24] For a discussion of how the quantum numbers of quasimomentum and band index are introduced we refer the reader to Ref. 20.
[25] The delay in appearance of the excitation spectrum gap until $V \approx 2E_R$ is a property of the 3D band structure. In a 1D lattice a gap is present for all depths $V > 0$.
[26] This also means that a single component Fermi gas is quite well described by a non-interacting theory.
[27] The Fermi temperature is given by $T_F = \epsilon_F/k_B$, where $\epsilon_F$ (the Fermi energy) is the energy of the highest occupied single particle state for the system at $T = 0K$.
[28] In order for the Fermi result to hold we require that $N_b \leq N_a$, so that the excited band isn’t occupied by virtue of the Pauli
exclusion principle.

[29] We note that non-negligible $J$ values in the superfluid regime could be treated using the Hartree-Fock Bogoliubov formalism [21, 22], however we do not consider this regime here.