Using Off-diagonal Confinement as a Cooling Method

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In a recent letter [Phys. Rev. Lett. 104, 167201 (2010)] we proposed a new confining method for ultracold atoms on optical lattices, which is based on off-diagonal confinement (ODC). This method was shown to have distinct advantages over the conventional diagonal confinement (DC), that makes use of a trapping potential, such as the existence of pure Mott phases and highly populated condensates. In this manuscript we show that the ODC method can also lead to lower temperatures than the DC method for a wide range of control parameters. Using exact diagonalization we determine this range of parameters for the hard-core case; then we extend our results to the soft-core case by performing quantum Monte Carlo (QMC) simulations for both DC and ODC systems at fixed temperature, and analyzing the corresponding entropies. We also propose a method for measuring the entropy in QMC simulations.

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I. INTRODUCTION

With recent experimental developments on cold atoms in optical lattices, the interest in the bosonic Hubbard model [1, 2] has dramatically increased. This model is characterized by a superfluid-to-Mott quantum phase transition for large onsite repulsion and integer values of the density of particles. In actual experiments the atoms are confined to prevent them from leaking out of the lattice. This is currently achieved by applying a spatially dependent magnetic field. A parabolic potential is added into the Hubbard model [3] to mimic the effect of the magnetic field. Therefore, the resulting model does not exhibit a true superfluid-to-Mott transition, since Mott regions always coexist with superfluid regions. This was predicted theoretically [3], and later confirmed experimentally [3].

Recently, we have proposed a new confining technique [6] where the atoms are confined via a hopping integral that decreases as a function of the distance from the center of the lattice. Since the confinement of the particles is due to the hopping or off-diagonal operators, we called it Off-Diagonal Confinement (ODC), as opposed to the conventional diagonal confinement (DC) which makes use of a parabolic confinement potential that is reflected in the density profile [4]. For large on-site repulsion the ODC model exhibits pure Mott phases at commensurate filling while at other fillings it exhibits more populated condensates than the DC model. Another advantage of ODC is that simple energy measurements can provide insights into the Mott gap, while the presence of the harmonic potential may renormalize the value of the gap with respect to the uniform case [7].

In this paper, we show that the ODC method can also lead to lower temperatures than the DC method for a wide range of parameters. Producing low temperatures in experiments is challenging, especially with fermions for which laser cooling is not as efficient as for bosons. In current experiments, fermions are cooled down by convection in the presence of cold bosons, leading to Bose-Fermi mixtures [8, 11]. Achieving lower temperatures for bosonic condensates will therefore result in colder Bose-Fermi mixtures.

This manuscript is organized as follows. In section II we define our model and describe our methods. The hard-core limit is studied in section III in order to illustrate analytically how ODC produces temperatures that are lower than those obtained with DC. This will also serve to benchmark the quantum Monte Carlo (QMC) simulations we use for analyzing the general soft-core case. In section IV we present the algorithm we use for QMC simulations, and we propose a method for measuring the entropy with this algorithm. Results for the soft-core case are presented in section V. Finally we conclude in section VI.

II. MODEL AND METHOD

We consider bosons confined to a one-dimensional optical lattice with $L$ sites and lattice constant $a = 1$. The Hamiltonian takes the form:

$$
\hat{H} = - \sum_{\langle i,j \rangle} t_{ij} \left( a_i^\dagger a_j^\vphantom{\dagger} + \text{h.c.} \right) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + W \sum_i (i - L/2)^2 \hat{n}_i \quad (1)
$$

The creation and annihilation operators $a_i^\dagger$ and $a_i$ satisfy bosonic commutation rules, $[a_i, a_j^\vphantom{\dagger}] = [a_i^\dagger, a_j^\dagger] = 0$, $[a_i^\dagger, a_j^\vphantom{\dagger}] = \delta_{ij}$, and $\hat{n}_i = a_i^\dagger a_i$ is the number of bosons on site $i$. The sum $\sum_{\langle i,j \rangle}$ runs over all distinct pairs of first neighboring sites $i, j$, and $t_{ij}$ is the hopping integral between $i$ and $j$. The parameter $U$ is the strength of the local on-site interaction, and $W$ describes the curvature of the external trapping potential.

In this work we consider the grand-canonical partition function,

$$
\mathcal{Z} = \text{Tr} \ e^{-\beta (\hat{H} - \mu N_0)} \quad (2)
$$
where $\beta = \frac{1}{k_B T}$, $k_B$ is the Boltzmann constant and $T$ the temperature. The chemical potential $\mu$ controls the average number of particles, $N = \langle \hat{N} \rangle$, with $\hat{N} = \sum_i \hat{n}_i$. The conventional DC model is obtained by setting $t_{ij} = 1$ for all pairs of first neighboring sites $i, j$, and using $W > 0$. For this model the value of $L$ is irrelevant as it is sufficiently large to contain the whole gas. The ODC model is obtained by setting $W = 0$ and using a hopping integral $t_{ij}$ that decreases as a function of the distance from the center of the lattice, and vanishes at the edges. For this model, $L$ fully determines $t_{ij}$ as described below.

Typically the temperature is not a control parameter in cold-atoms experiments, and once laser cooling has been performed, the system has a fixed entropy which can be considered the control parameter. Then the temperature can be estimated numerically knowing the isentropies of the system. Therefore, our strategy for determining which of the two confining methods can achieve the lowest temperature is based on switching adiabatically from DC to ODC, so the entropy is conserved. Then we determine the temperatures $T_{dc}$ and $T_{ode}$ of the DC and ODC systems by equating the entropies.

We will consider an experiment in which a fixed number $N$ of atoms is loaded into an optical lattice with a DC trap, described by Eq. (1) with parameters $t_{ij} = 1$, $W = 0.008$ (as in Ref. [4]). We use $L = 400$ in order to ensure the confinement of the whole gas. Then, we adiabatically switch to the ODC trap by slowly varying $t_{ij}$ and $W$ to $t_{ij} = (i + j + 1)(2L - i - j - 1)/L^2$ with $L = 70$, and $W = 0$ (as in Ref. [5]), keeping $N$ and $U$ the same.

However, in our calculation, it is actually more convenient to control the temperature than the entropy. Thus we consider both DC and ODC systems for a set of temperatures $T$, and measure the corresponding entropies, $S_{dc}(T)$ and $S_{ode}(T)$. Then, knowing the initial temperature $T_{dc}$, the final temperature $T_{ode}$ can be extracted graphically by imposing the equality, $S_{dc}(T_{dc}) = S_{ode}(T_{ode})$, as described in the next section.

### III. THE HARD-CORE CASE: EXACT ANALYTICAL RESULTS

The hard-core limit ($U = +\infty$) of the model can be solved analytically. These exact results provide a solid benchmark for our study of the general soft-core case in the next section. We follow here the method used by Rigol [13]. In the hard-core limit, the $U$ term in (1) can be dropped if the standard bosonic commutation rules are replaced by $[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = [a_i, a_j^\dagger] = 0$ for $i \neq j$, and $a_i a_i^\dagger + a_i^\dagger a_i = 1$, and $a_i^2 = a_i^{12} = 0$. With this algebra, the model (1) reduces to

$$\hat{\mathcal{H}} = -\sum_{\langle i,j \rangle} t_{ij} (a_i^\dagger a_j + \text{h.c.}) + W \sum_i (i - L/2)^2 \hat{n}_i,$$

which describes hard-core bosons. By performing a Jordan-Wigner transformation, the hard-core creation and annihilation operators can be mapped onto fermionic creation and annihilation operators, $f_i^\dagger$ and $f_i$, where

$$a_j^\dagger = \frac{1}{\sqrt{2}} \sum_{q=1}^{j-1} e^{\pm i \pi f_q^\dagger f_q} f_j, \quad a_j = \frac{1}{\sqrt{2}} \sum_{q=1}^{j-1} e^{-i \pi f_q^\dagger f_q} f_j,$$

which satisfy the usual fermionic anticommutation rules, $\{f_i, f_j^\dagger\} = \{f_i^\dagger, f_j\} = 0$, $\{f_i, f_j\} = \delta_{i,j}$. This leads to a model that describes free spinless fermions,

$$\hat{\mathcal{H}} = -\sum_{\langle i,j \rangle} t_{ij} (f_i^\dagger f_j + \text{h.c.}) + W \sum_i (i - L/2)^2 \hat{n}_i,$$

where $\hat{n}_i = f_i^\dagger f_i$ represents the number of fermions on site $i$. Because the model is a quadratic form of $f_i^\dagger$ and $f_i$, it can be solved by a simple numerical diagonalization of the $L \times L$ matrix. Denoting by $\epsilon_k$ with $k \in [1, L]$ the eigenvalues of this matrix, the partition function (2) takes the form

$$Z = \prod_{k=1}^L \left(1 + e^{-\beta(\epsilon_k - \mu)}\right).$$

The entropy is defined as $S = -k_B \text{Tr} \ln \mathcal{D}$ with the density matrix $\mathcal{D} = \frac{1}{Z} e^{-\beta(\hat{\mathcal{H}} - \mu \hat{N})}$. Working in a system of units where the Boltzmann constant $k_B = 1$ and using the properties of the density matrix, it follows that $S = \ln Z + \beta \langle \hat{\mathcal{H}} \rangle - \beta \mu \langle \hat{N} \rangle$. Substituting $\langle \hat{\mathcal{H}} \rangle - \mu \langle \hat{N} \rangle = -\frac{\partial}{\partial \beta} \ln Z$ and using expression (6) for $Z$, the entropy takes the form

$$S(\beta, \mu) = \sum_{k=1}^L \left[ \ln \left(1 + e^{-\beta(\epsilon_k - \mu)}\right) + \frac{\beta(\epsilon_k - \mu)}{e^{\beta(\epsilon_k - \mu)} + 1} \right].$$

The average number of particles $N$ is obtained by summing the Fermi-Dirac distribution,

$$N(\beta, \mu) = \sum_{k=1}^L \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}.$$
the initial guess as a vector, \( \nabla E \) form a correction \( \Delta \vec{r} \). Solving this system of equations determines the others correspond to the conservation of the number of particles. Noting that the two curves cross. If the initial temperature \( T \), we calculate the error \( E \). There exists a critical temperature \( T_c \) where the ODC method produces a temperature \( T_{odc} \) that is lower than the temperature \( T_{dc} \) obtained with the DC method. Above \( T_c \) (yellow region), it is the DC method that gives the lowest temperature. For example, the point \( P \) corresponds to a system with 34 particles, an initial temperature \( T_{dc} = 3 \), and a final temperature \( T_{odc} \approx 1.5 \).

Fig. 2 shows the critical temperature \( T_c \) and the DC isotherms as functions of \( N \). For a given number of particles and an initial temperature \( T = T_c(N) \), the ODC and DC systems have the same temperature \( T_{odc} = T_{dc} \) when the confinement is switch adiabatically. Below (above) \( T_c \), the ODC system has a temperature \( T_{odc} \) that is lower (higher) than the temperature \( T_{dc} \) of the DC system. The point \( P \) illustrates how the figure should be read: For a system with 34 particles and an initial DC temperature \( T_{dc} = 3 \), the final ODC temperature is \( T_{odc} \approx 1.5 \). Note that \( T_c \) vanishes when \( N = L = 70 \). The resulting Mott phase found in the ODC case always has lower entropy than the mixed phases found in the DC case. This will be discussed in greater detail in the next section.

IV. QUANTUM MONTE CARLO ALGORITHM AND THE ENTROPY

For the treatment of soft-core interactions, we perform QMC simulations using the Stochastic Green Function (SGF) algorithm [14] with tunable directionality [15]. Although this algorithm was developed for the canonical ensemble, a trivial extension [16] allows us to simulate the grand-canonical ensemble. Our thermodynamic control parameters are the temperature \( T \), the volume \( V \) (number of sites \( L \)), and the chemical potential \( \mu \). Unlike the analytical hard-core case, a direct measurement of the entropy is not possible with a single QMC simulation because the value of \( Z \) is unknown. However it is still possible to eval-
By substituting \( N dE \) differential into Eq. (12), we get an expression for the thermal susceptibility that can be directly measured in our simulations:

\[
\chi_{th} = \beta^2 \left[ \langle \hat{N}'(\hat{\mathcal{H}} - \mu \hat{N}) \rangle - \langle \hat{N}' \rangle \langle (\hat{\mathcal{H}} - \mu \hat{N}) \rangle \right] \tag{12}
\]

Considering the energy \( E = \langle \hat{\mathcal{H}} \rangle \) and the associated differential \( dE = TdS - PdV + \mu dN \), where the pressure \( P \) is defined as \( P = -\frac{\partial E}{\partial V} \bigg|_{S,N} \), and performing a Legendre transformation over the variables \( S \) and \( N \), we can define the grand-canonical potential \( \Omega \) that depends only on our natural variables, \( \Omega(T, V, \mu) = E - TS - \mu N = -PV \). Its differential takes the form

\[
d\Omega = -SdT - PdV - Nd\mu. \tag{13}
\]

We can then extract a useful Maxwell relation,

\[
\frac{\partial S}{\partial \mu} \bigg|_{V,T} = \frac{\partial N}{\partial T} \bigg|_{V,\mu}, \tag{14}
\]

so the entropy can be easily obtained by integrating the thermal susceptibility over the chemical potential and keeping the temperature and the volume constant,

\[
S(T, V, \mu) = \int_{\mu_0}^{\mu} \chi_{th}(T, V, \mu')d\mu', \tag{15}
\]

where \( \mu_0 \) is the critical value of the chemical potential below which the average number of particles \( N \) and the thermal susceptibility \( \chi_{th} \) are vanishing.

In order to check the reliability of Eq. (15), we show on Fig. 3 a comparison of the entropy of the hard-core case obtained with the SGF algorithm by integrating the thermal susceptibility (12), and the entropy computed with Eq. (7). The agreement is good for both DC and ODC cases at high \( T = 3 \) and low temperatures \( T = 0.25 \).

We now release the hard-core constraint and set the thermal susceptibility over the chemical potential and so the entropy can be easily obtained by integrating the expressions for the thermal susceptibility and entropy.

We can then extract a useful Maxwell relation,

\[
\frac{\partial S}{\partial \mu} \bigg|_{V,T} = \frac{\partial N}{\partial T} \bigg|_{V,\mu}, \tag{14}
\]

so the entropy can be easily obtained by integrating the thermal susceptibility over the chemical potential and keeping the temperature and the volume constant,
V. Conclusion

In this manuscript we propose that the adiabatic switch from the DC to the ODC method can produce lower temperatures for a wide range of initial temperatures and system parameters. In the hard-core limit, we determine the critical temperature $T_c$ for which the two methods have the same entropy. Below (above) $T_c$ and at constant entropy, the ODC method leads to temperatures that are lower (higher) than with the DC method. In order to extend our results to the soft-core case, we propose a simple method for evaluating the entropy with QMC, by measuring the thermal susceptibility $\chi_{th}$ in the grandcanonical ensemble and integrating it over the chemical potential $\mu$. Then we make use of the SGF algorithm with tunable directionality, and show that the soft-core results are qualitatively the same as in the hard-core case.

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