Simulation of gauge transformations on systems of ultracold atoms

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Abstract. In this paper, we propose a method for simulating gauge transformations on ultracold atoms trapped in an optical lattice coupled to an artificial magnetic field. We discuss an observable that is invariant under these gauge transformations and compute it using a tensor network ansatz that escapes the phase problem. We find that the Mott-insulator-to-superfluid critical point is monotonically shifted as the induced magnetic flux increases. This result is stable against the inclusion of entanglement in the variational ansatz.

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1. Introduction

Ultracold gases are a powerful instrument for creating quantum devices that can simulate, in a controlled manner, a variety of condensed matter and particle physics models. The emerging possibility of acting on the system with carefully tuned electromagnetic fields invites the design of a new generation of experiments [1, 2]. It is possible to implement synthetic Abelian [3]–[6] and non-Abelian [7, 8] gauge fields coupled to neutral ultracold atoms. The non-Abelian fields may be designed to simulate Dirac [9, 10] or Wilson [11, 12] fermions on an optical lattice. Recently, synthetic Abelian fields for neutral atoms were successfully created [13]–[15]. For a recent review on this topic see [16].

There are several approaches to quantum simulation: analogue simulators—where the dynamics of a real physical system are approximated by another one in a laboratory—have been proposed; quantum circuits whose outputs are strongly correlated ground states of relevant physical systems have been put forward [17]; also, devices that reproduce exactly the dynamics of a real-world system have been presented [18]. In this paper, for the first time we propose the simulation of a gauge symmetry or, to be more precise, of a gauge transformation. The main aim of this paper is to show that one of the setups proposed to simulate a magnetic field for ultracold atoms on an optical lattice accommodates the possibility of performing gauge transformations on the vector potential. More precisely, we will show that different geometrical configurations of the experiment amount to different vector potentials and that some of these configurations are related by a gauge transformation. Then, by performing gauge-invariant measurements on the system in different gauges, it will be possible to test the quantum simulator. That is to say, as the Hamiltonian that is conjectured to describe the system is gauge invariant [19], the extent to which the actual cloud of atoms in the laboratory is gauge invariant is a proxy for the quality of the simulator.

The second aim of this paper is to compute the gauge-invariant observable that we propose for testing the simulator, which is the phase diagram of the Bose–Hubbard (BH) Hamiltonian with complex, position-dependent hopping amplitudes. We will do this in mean-field theory. In order to determine the validity of the mean-field approximation, we will benchmark the results against those of a tensor network ansatz and against exact diagonalization. The model we study, despite being bosonic, is considered to be difficult for Monte Carlo simulations due to the phase problem, a generalization of the fermionic sign problem, and is of great relevance for ultracold atomic systems on optical lattices. Although there is an extensive body of literature devoted to the study of this model with mean-field techniques (see [20] and references therein), it has not been approached using methods that go beyond mean field for system sizes that are beyond the reach of exact diagonalization. Using a projected entangled-pair state (PEPS) ansatz with bond dimension \(\chi = 1, 2\), we compute the ground state and determine the quantum critical point of the Mott-insulator-to-superfluid phase transition [21] as a function of the magnetic flux going through the system. We find that the result for \(\chi = 2\), which allows for some degree of entanglement in the ground state, is not qualitatively different from that found with \(\chi = 1\), i.e. with a mean-field ansatz.

This paper is organized as follows. Section 2 is devoted to a review of the proposal by Jaksch and Zoller [3] to create an artificial magnetic field and a discussion of the scheme that allows for gauge transformations. In this section, we also introduce the phase diagram as a gauge-invariant observable. Section 3 is devoted to determining the phase diagram of the system under study in mean-field theory and determining the accuracy of the results by comparing them to PEPS and exact diagonalizations.

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2. Simulation of gauge transformations on ultracold atoms

2.1. A synthetic magnetic field on an optical lattice

Our starting point will be the BH Hamiltonian, which describes bosonic atoms loaded on an optical lattice [22, 23]. By increasing the laser intensity in one of the directions of the lattice, it is possible to create an array of uncoupled two-dimensional (2D) lattices, each of which is governed by a 2D BH Hamiltonian,

\[ H = - \sum_{m,n=-\infty}^{\infty} (J_x a_{m+1,n}^\dagger a_{m,n} + J_y a_{m,n+1}^\dagger a_{m,n} + \text{h.c.}) + \frac{U}{2} \sum_{m,n=-\infty}^{\infty} N_{m,n} (N_{m,n} - 1) - \sum_{m,n=-\infty}^{\infty} \mu_{m,n} N_{m,n}, \]

where the bosonic operators \(a_{m,n}^\dagger\) and \(a_{m,n}\) create and destroy, respectively, an atom at the lattice site \(x_{m,n} = a(m, n)\), with \(m\) and \(n\) being integers and \(a\) being the lattice period. The constant \(J_x\) (\(J_y\)) is the site-to-site tunneling energy in the \(x\) (\(y\)) direction. The parameter \(U\) is the pair interaction energy at each site, \(\mu_{m,n}\) is the local chemical potential and \(N_{m,n} = a_{m,n}^\dagger a_{m,n}\) is the local occupation.

The next step is to make the lattice state dependent. That is, let us suppose the atoms can be in two hyperfine states \(|g\rangle\) and \(|e\rangle\) and that the lifetime of the excited state is such that spontaneous decays from \(|e\rangle\) to \(|g\rangle\) are negligible. Then, if the two states are trapped in different rows of the lattice and we increase the laser intensity in the direction that is orthogonal to these rows, we will obtain an array of uncoupled 1D lattices that trap atoms of each state in every other row. This is achieved by setting the relative polarizations of the lasers that form the standing wave in one of the directions of the plane to the appropriate value [24].

Now, let us couple the states \(|g\rangle\) and \(|e\rangle\) by shining two Raman lasers on the system with wave vectors \(k_g\) and \(k_e\). It follows that an atom on the lattice will undergo Rabi oscillations between the two levels with a (crucially) position-dependent Rabi frequency

\[ \Omega(x) = \Omega_0 e^{i(k_e - k_g)x}, \]

where \(\Omega_0\) is a constant depending on the Raman laser intensity and the detuning. When an atom undergoes a transition from \(|g\rangle\) to \(|e\rangle\) and vice versa, it finds itself in a maximum of the optical potential and tends to fall towards a neighboring row of the lattice at a rate given by

\[ J_R = \frac{1}{2} \int \omega^*(x - x_{m,n+1}) \Omega(x) \omega(x - x_{m,n}) \]

where \(\omega(x - x_{m,n})\) is a Wannier function centered at the site \((m, n)\). Setting \(q \equiv k_e - k_g\) parallel to the \(m\)-direction we obtain \(J_R = J_0 \exp(2\pi i am)\), as in [3], with \(\alpha = |q|a/(2\pi)\).

However, allowing for \(q\) to point in any direction of the plane, that is, setting \(q = |q|(\cos \theta, \sin \theta)\), the induced tunneling rate in the \(n\) direction becomes

\[ J_R = \frac{\Omega_0}{2} e^{iA_y(m,n)} \int dx |\omega_x(x)|^2 \cos(2\alpha \cos \theta x) \int dy \omega_y(y) e^{2\pi i a \sin \theta} \omega_y(y \leftarrow \frac{\pi}{2}), \]

where \(A_y\) is the \(y\)th component of the vector potential,

\[ A_y(m, n) = 2\pi \alpha \left( \cos \theta m + \sin \theta n/2 \right), \]

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Figure 1. Circulation around a plaquette and phases picked up at each transition between lattice sites. The plaquettes in rows adjacent to the one in the diagram get opposite phases as in those cases the transitions between the two levels of the atoms take place in the other direction (first from $|e\rangle$ to $|g\rangle$ as opposed to $|g\rangle$ to $|e\rangle$). This configuration gives rise to a staggered magnetic field. Filled circles trap atoms in state $|g\rangle$ and empty circles trap those in state $|e\rangle$.

plus an irrelevant constant. As we show in the appendix, the integrals in $x$ and $y$ depend very weakly on $\theta$ and can thus be set as a constant. The final result is

$$J_R = J_0 e^{2\pi i\alpha (\cos \theta m + \sin \theta n/2)}.$$  \hspace{1cm} (6)

Note that for $\sin \theta = 0$ the model reduces to the Hofstadter Hamiltonian \footnote{Hofstadter, D. R., Phys. Rev. B 14, 2239 (1976).}. The Hamiltonian for the system, because $\Omega_0$ can be tuned in order to set $J_x = J_0$, now reads

$$H = -J \sum_{m,n=-\infty}^{\infty} \left( a_{m+1,n}^{\dagger} a_{m,n} + e^{iA(m,n)} a_{m,n+1}^{\dagger} a_{m,n} + h.c. \right)$$

$$+ \frac{U}{2} \sum_{m,n=-\infty}^{\infty} N_{m,n}(N_{m,n} - 1) - \sum_{m,n=-\infty}^{\infty} \mu_{m,n} N_{m,n}.$$ \hspace{1cm} (7)

Hence, by coupling the two hyperfine states with Raman lasers and thus inducing transitions between them with a position-dependent Rabi frequency, an atom going around a plaquette of the lattice will acquire a non-vanishing phase in the same way that charged particles acquire an Aharanov–Bohm phase in a magnetic field (see figure 1),

$$|m, n\rangle \rightarrow e^{i(A(m,n)-A(m+1,n))} |m, n\rangle,$$ \hspace{1cm} (8)

where the symbol $\square$ means circulation around a plaquette.

However, if the atom starts the closed path at an adjacent site $(m+1)$ it will acquire the opposite phase because the tunneling amplitude for the $|g\rangle \rightarrow |e\rangle$ transition is the complex
conjugate of that for the $|e\rangle \rightarrow |g\rangle$ transition. In other words, an atom going from an even to an odd row will pick up the opposite phase to atoms going from odd to even rows. This is the most important drawback of the scheme, as it leads to a staggered magnetic field. In order to remedy the problem, the authors of [3] proposed to break the symmetry between both transitions by tilting the lattice, which seems very challenging from an experimental point of view. Recently, a way around this problem was offered in [26]. There, the authors proposed the introduction of an optical superlattice that breaks the degeneracy between transitions in adjacent plaquettes. Because the degeneracy is broken, it is possible to drive, e.g., the transitions $|m, n\rangle \rightarrow |m, n + 1\rangle$ and $|m, n\rangle \rightarrow |m, n - 1\rangle$ with different lasers, thus rectifying the staggered magnetic field.

The scheme we propose for transforming the vector potential to other gauges requires a modification if it is implemented with an optical superlattice. It is necessary that the lasers that drive the different transitions, which were originally degenerate, be rotated by the same angle.

2.2. Simulation of gauge transformations

In this section we discuss how the geometry of the Raman lasers used to induce the artificial vector potential can be changed in order to transform the vector potential into another gauge. The issue of gauge invariance related to artificial magnetism in systems of cold atoms is discussed in [27, 28].

The Hamiltonian (7) is invariant under a global transformation where all the creation and annihilation operators are replaced according to $a_{m,n}^\dagger \rightarrow e^{-i\beta} a_{m,n}^\dagger$ and $a_{m,n} \rightarrow e^{i\beta} a_{m,n}$. This leads to global particle number conservation. However, if the phase $\beta$ is allowed to vary from one lattice site to another, the Hamiltonian is no longer invariant. This is because the vector potential $A_y(m, n)$ does not transform in the experiment, it is not a true gauge field.

Nevertheless, it is possible to make this local transformation a symmetry of the system by changing the configuration of the Raman lasers that generate the vector potential. Let $A$ be the vector potential induced by a given configuration in which the Raman-laser wave vectors form a given angle $\theta$ and their difference is given by the vector $q = k_x - k_y$. Then, it is straightforward to see that there always exists another configuration that gives rise to another vector potential $A'$ determined by $\theta'$ and $q' = k'_x - k'_y$ such that $|q| \cos \theta = |q'| \cos \theta'$, i.e. such that the magnetic flux is the same (figure 2). Hence, by changing $q$ and $\theta$ accordingly, it is possible to transform the vector potential into a whole family of gauges that differ by a linear function of $n$, $A = (0, \Phi m + f(n), 0)$, where $\Phi = \alpha \cos \theta$ is the flux and $f$ is a linear function. Let us stress that these gauge transformations are forced upon the system; they do not possess a dynamical origin.

The spectrum of the Hamiltonian in equation (7) is invariant under a broader set of gauge transformations [19]. Indeed, one can see that the Hamiltonian remains unchanged if the hopping phases, i.e. the artificial vector potential, are changed according to

$$
A_x(m, n) \rightarrow A_x(m, n) - (\Lambda(m + 1, n) - \Lambda(m, n)),
$$

$$
A_y(m, n) \rightarrow A_y(m, n) - (\Lambda(m, n + 1) - \Lambda(m, n)),
$$

as long as one redefines the creation and destruction operators following

$$
da_{m,n} \rightarrow e^{i\Lambda(m,n)} a_{m,n}, \quad a_{m,n}^\dagger \rightarrow e^{-i\Lambda(m,n)} a_{m,n}^\dagger,
$$

where $\Lambda(m, n)$ is an arbitrary function.
Figure 2. Two different Raman laser configurations that give rise to the same magnetic flux as long as $|q'\cos\theta'| = |q|\cos\theta$. Each laser configuration leads to different vector potentials; hence changing the experimental setup determined by $k_1, k_2$ to $k'_1, k'_2$ amounts to performing a gauge transformation.

The simplest configuration of the magnetic field is $\Phi = 0$ everywhere. In the Landau gauge, the vector potential is also zero everywhere, $A_y = 0$. However, there are infinitely many other vector potentials that give rise to $\Phi = 0$. They are called pure-gauge configurations. The pure-gauge configuration that is within reach of the method that we propose is $A'_y = \alpha n/2$ and is obtained by setting $\theta = \pi/2$. Hence, the simplest test of the gauge invariance of the system, and therefore of the quality of the quantum simulator, would be to verify that gauge-invariant measurements give the same result for $A'_y = \alpha n/2$ as for $A_y = 0$.

A fundamental difference between systems coupled to real gauge fields and systems coupled to synthetic gauge fields is that in the first system only gauge-invariant quantities are physical, whereas in the second system this is not necessarily the case. Indeed, in [13] the authors reported of having experimentally distinguished between two pure-gauge configurations. By definition, this is only possible if the measurements carried out were not gauge invariant. While a gauge-dependent quantity in the ultracold gas system may be physically meaningful and accessible, it cannot have a counterpart in a system with charged particles coupled to a real gauge field, as in this case they are neither meaningful nor accessible.

2.3. The phase diagram as a gauge-invariant observable

In this section we will discuss the phase diagram of the BH model, which is gauge invariant. This will allow us to propose an experimental protocol to test the gauge invariance of the actual system in the laboratory.

It is well known that the BH Hamiltonian exhibits a phase transition in its ground state that depends on the ratio $J/U$. For $J/U \to 0$ and commensurate filling the ground state is a product
state with a definite occupation at each site,

$$|MI\rangle = \bigotimes_{m,n=1}^L |N_{m,n} = \bar{n}\rangle,$$

(11)

where $\bar{n} = N/L^2$ is the ratio between the total number of atoms, $N$, and the total number of lattice sites, $L^2$. In the other limit, $J/U \to \infty$ the ground state is a product of $N$ single-particle Bloch with momentum at the minimum of the first energy band. In the limit where the system is very large both in the number of atoms and lattice sites, keeping $\bar{n}$ fixed, the ground state can be shown to be a product over coherent single-site occupation states,

$$|SF\rangle = \bigotimes_{m,n=1}^L \exp(\sqrt{\bar{n}}a^\dagger_{m,n})|0\rangle,$$

(12)

where $N$ is the number of atoms and $|0\rangle$ is the vacuum state. It is possible to distinguish between these two ground states by the presence or not of long-range order or, equivalently, by the condensate fraction

$$\rho_0 \equiv \langle a_{k_0}^\dagger a_{k_0} \rangle = \frac{1}{L^4} \sum_{m,m',n,n'} \langle a_{m,n}^\dagger a_{m',n'} \rangle,$$

(13)

which counts the number of atoms with momentum located at the minimum of the first energy band, $k_0$. As $J/U$ decreases the condensate is depleted until the Mott-insulator state is reached. Hence the phase transition between the two states is continuous. A large condensate fraction is a signature of the superfluid phase, as it possesses long-range order. Indeed, in the thermodynamic limit the only way $\rho_0$ can be large is by manifesting long-range non-vanishing correlations. Conversely, the Mott-insulator state does not present long-range order. Off-diagonal correlations decay exponentially fast, and $\rho_0$ is vanishingly small in the limit of an infinite lattice.

The location of the critical point between the two phases cannot be changed by a gauge transformation. If the order parameter is zero in a certain gauge, i.e. the system is an insulator, it is zero independently of the choice of gauge. Indeed, the two-point correlators in any two gauges will at most differ phase $\exp(i(\Lambda(R) - \Lambda(R')))$.

3. Phase diagram

3.1. The mean-field approach

We now turn to the study of the superfluid–insulator phase diagram of the BH model in a magnetic field. This problem has been approached using strong-coupling perturbation theory in [29], although we proceed with variational techniques.

An arbitrary state of the Hilbert space is given by

$$|\Psi\rangle = \sum_{N_{1,1}, N_{1,2}, \ldots, N_{L,L}} C^{N_{1,1}, N_{1,2}, \ldots, N_{L,L}} |N_{1,1}, N_{1,2}, \ldots, N_{L,L}\rangle.$$

(14)

If we allow at most $d$ atoms to occupy each site, then the dimension of the many-body Hilbert space, which is the tensor product over all single-site Hilbert spaces, will have dimension $d^{L^2}$. The exponential dependence of the many-body Hilbert space dimension makes it impossible to attempt an exact diagonalization or a variational approach on the complete
Hilbert space already for a $4 \times 4$ lattice with $d = 3$. Consequently, an approximate scheme is needed where most of the states of the Hilbert space are ignored.

The fact that in both limits, $J \gg U$ and $J \ll U$, the ground state can be expressed as a product over single-site states allows for the quantum phase transition to be probed by a mean-field ansatz, also known as Gutzwiller’s ansatz, which neglects quantum correlations between neighboring sites,

$$|\Psi_{MF}\rangle = \bigotimes_{m,n} \sum_{N} f_{m,n}^N |N_{m,n}\rangle.$$  \hspace{1cm} (15)

This approximation is completely inadequate in 1D, whereas it is exact in infinite dimensions. It was used in [30] to determine the phase diagram of the BH model in 2 + 1 dimensions without magnetic field.

The mean-field energy $E_{MF}$ is the sum of single-site energies,

$$E_{MF}\left(\{f_{m,n}^N\}\right) = \sum_{m,n} E_{m,n}\left(\{f_{m\pm 1,n}^N, f_{m,n\pm 1}^N\}\right),$$  \hspace{1cm} (16)

where $E_{m,n}$ depends only on the single-site states neighboring site $(m, n)$. The authors of [31] approximate the ground state of the BH model with a magnetic field by sequentially minimizing the local quantities $E_{m,n}$ with respect to the parameters $\{f_{m\pm 1,n}^N, f_{m,n\pm 1}^N\}$ using a self-consistent method. However, instead of using the general mean-field ansatz of equation (15), they impose the $q$-periodicity of the Hamiltonian when the flux per plaquette, in our notation $\alpha \cos \theta = p/q$, is a rational number. Imposing this periodicity and translational invariance in the other direction on the trial state reduces the problem of minimizing $E_{MF}$ on an infinite lattice to that on a $q \times 1$ lattice. The optimization of the ansatz is carried out by defining a local Hamiltonian $H_{m,n}$ that depends only on the local states in the neighboring sites, $\{f_{m\pm 1,n}^N, f_{m,n\pm 1}^N\}$. Then $H_{m,n}$ is diagonalized in the occupation basis and the lowest-lying eigenvector becomes the updated state at the site $(m, n)$.

However, if the above method is applied to an unconstrained mean-field ansatz, where the symmetries are not imposed by hand, it often converges to local minima and there is no guarantee that the energy is being minimized at each step. To bypass this problem we optimize $|\Psi_{MF}\rangle$ by Euclidean evolution. The results are shown in figure 3.

### 3.2. The tensor network approach

The Hamiltonian under study, equation (7), presents the so-called phase problem, which hinders progress through Monte Carlo calculations. Hence, in order to obtain results beyond mean field, we resort to a tensor network approach, which has proven to be very successful in describing 1D systems [32]. A great deal of effort has been put into developing a tensor network ansatz for 2D systems. In this section we employ one of these ansatzes, namely the PEPS ansatz [33]–[35], to determine the phase diagram allowing for some degree of quantum correlation between different sites of the lattice. The ansatz replaces the quantities $f_{m,n}^N$ at each lattice site with tensors $A_{N_{m,n}}^{N_{m,n}}$ where the Greek indices can take up to $\chi$ values. The trial state now reads

$$|\Psi_{PEPS}\rangle = F\left(A_{N_{1,1}}^{N_{1,1}}, \ldots, A_{N_{1,L}}^{N_{1,L}}, \ldots, A_{N_{L,1}}^{N_{L,1}}\right) |N_{1,1} \cdots N_{1,L} \cdots N_{L,L}\rangle,$$  \hspace{1cm} (17)

where the operator $F(\cdot)$ stands for the contraction of the whole tensor network according to the connectivity of the lattice (in our case a square one) and the indices $N_{m,n}$ are summed over.
Figure 3. Critical value of $J/U$ for which the ground state of the BH Hamiltonian, equation (7), undergoes an insulator-to-superfluid transition as a function of the magnetic flux $\Phi = \alpha \cos \theta$. The phase diagram was determined using the mean-field approximation for a $10 \times 10$ square lattice with open boundary conditions for $\mu_{m,n} = 0.5U$ maximum one-site occupation $d = 2$. As the angle of external lasers is changed, a transfer from the transverse component to longitudinal component of the effective gauge field takes place and modifies the location of the critical value of $J/U$. For $\cos \theta \to 0$, the hopping phase is $A_y(m, n) = \alpha n / 2$, and the Mott-insulator-to-superfluid transition point appears at the known value $(J/U)_c = 0.043$. Although site-dependent phases are present, this transition point remains unchanged because $A_y(m, n)$ is completely gauged away, as it only depends on $n$ and hence the derivative in the $m$ direction is zero. Only the interval $\Phi \in [0, 0.5]$ is considered because the Hamiltonian in equation (7) is invariant under the replacement $\Phi \to 1 - \Phi$ and is periodic in $\Phi$ with unit period.

To compute local quantities all the indices of the tensors must be contracted. This can be done, approximately, in an efficient manner. This means that the amount of resources needed to carry out the contraction scales polynomially in $\chi$.

We will follow the algorithm described in [36], which is based on two different ways of finding the ground state of a given Hamiltonian. The first approach consists in iteratively minimizing the expected value of the Hamiltonian (the so-called direct minimization). The second one is called Euclidean evolution and consists in evolving a given PEPS state in imaginary time by minimizing the distance between the evolved state and a new PEPS state. The computational effort is the same in each case and grows as $\chi^{12}$.

The implementation of the algorithm in this work has been done by combining both methods. Direct minimization is used for initializing the state and then the approximate ground state is reached by an evolution in imaginary time. Furthermore, we take the $\chi = 1$
PEPS (mean-field solution) as the initial state for the $\chi = 2$ PEPS in order to accelerate the convergence. Each converged PEPS is obtained with an imaginary time step $dt = 10^{-3}$ and using a second-order Suzuki–Trotter expansion of the evolution operator.

We compute the condensate fraction for different values of $\alpha$ for a $3 \times 3$ lattice of 3-valued sites, i.e. sites whose occupation may be between 0 and 2. We choose two different values of $\alpha \cos \theta$, 0 and 1/2, in order to compare the two curves. The results are shown in figure 4.

For an infinite system the insulator-to-superfluid quantum phase transition is located at the value of $J/U$ for which the condensate fraction computed in the ground state becomes larger than $1/N$. However, for finite systems there is no exact phase transition. In order to estimate the position of the critical value of $J/U$ as accurately as possible for the infinite system from studying a finite system, we compute the derivative of the condensate fraction with $J/U$ and determine the point where it is greatest. As the size of the lattice increases, this criterion yields the correct result for the location of the critical point.

### 3.3. Results

The two phases of the infinite BH model in equation (7) can be distinguished using as order parameter the condensate fraction $\rho_0$. In the superfluid phase corresponding to large $J/U$, the condensate fraction is nonzero because the ground state presents long range order. Conversely, in the Mott-insulator phase there is no such order and $\rho_0 = 0$. In the case of a finite size system, the transition does not appear at the point where $\rho_0$ is no longer vanishing but, rather, as a sharp transition from a small to a large value of $\rho_0$. The point of the phase transition is then determined as the point where the derivative of the order parameter reaches a maximum.

In figure 3, we plot the phase diagram in the $J/U$ versus $\Phi_1 = \alpha \cos \theta$ plane; that is, we analyze the value of the critical coupling $J/U$ as a function of the flux per plaquette. The system we have studied corresponds to a $10 \times 10$ lattice with possible local occupations 0, 1 and 2. The result shown in this plot has been obtained by optimizing a mean-field ansatz, which is a PEPS ansatz with $\chi = 1$. Let us note that, for $\Phi = 0$, we recover the well-known mean-field value for the quantum phase transition $J/U = 0.043$. Then, as the magnetic field increases, the critical value of $J/U$ raises monotonically until roughly $J/U = 0.07$. This result offers a clear experimental prediction. The action of external laser fields as described in previous sections should shift the transition point to larger values than those measured in the absence of effective magnetic fields.

In order to determine whether or not this result is an artifact of the mean-field approximation, we have studied a smaller $3 \times 3$ lattice using $\chi = 1$ (mean field) and $\chi = 2$ tensor networks as well as an exact diagonalization. Again, the possible occupation per site is $d = 0, 1$ and 2 and the chemical potential is set equal to $\mu = 0.5U$, which ensures that the Mott state has $\bar{n} = 1$. The main result we obtain is that a $\chi = 2$ PEPS does not differ significantly from that obtained with a $\chi = 1$ ansatz, and both of them are very close to the exact result. We conclude that the phase diagram of the BH model obtained by variational means with a product state ansatz does not change significantly when a small amount of entanglement is included. The consistency between mean-field and $\chi = 2$ PEPS results holds for all values of the flux, although the departure of the $\chi = 2$ results from the $\chi = 1$ ones is larger when $\Phi = \alpha \cos \theta$ increases.
Figure 4. Condensate fraction $\rho_0$ as a function of $J/U$ for $\mu_{m,n} = 0.5U$ and for two different values of the magnetic flux $\Phi = \alpha \cos \theta = 0$ (top) and $\Phi = 0.5$ (bottom) computed by exact diagonalization and by PEPS ansatzes with bond dimension $\chi = 1, 2$ on a $3 \times 3$ lattice with maximum local occupation $d = 2$. In all cases, $\rho_0$ tends to $1/N$ for small enough values of $J/U$ and approaches a macroscopic value for $J/U \to 1$, which is a sign of long-range order. In order to compute the critical point, we determine the value of $J/U$ where the variation of $\rho_0$ reaches its maximum. As can be seen with the naked eye, the critical point for $\alpha = 0$ is located at a smaller $J/U$ than that for $\alpha = 0.5$. The discontinuities in the exact curves are due to changes in the total particle number of the ground state and are smoothed out in the thermodynamic limit. Insets are blowups of the critical region.
Figure A.1. Running of $J_y(\alpha, \theta)$ for fixed $\theta$ (left) and for fixed $\alpha$. Clearly the variation is markedly larger in the former case than in the latter. It must be stressed that in both cases the effective flux felt by the atoms on the lattice varies from its minimum to its maximum value.

4. Conclusion

We have proposed a method for performing gauge transformations on ultracold atoms coupled to an artificial vector potential. We have also discussed gauge-invariant observables, which can be measured in an experiment, and computed them using a mean-field anzatz and using more powerful tensor network techniques.

Since the Hamiltonian we want to simulate is gauge invariant, a test of the gauge invariance of the system in the laboratory is also a test that reveals how faithfully it is described by this Hamiltonian. It is, therefore, a test of the quality of the quantum simulator. Let us stress that this test is independent of the choice of observable, as long as it is gauge invariant, and of the accuracy of the approximation scheme used to compute it theoretically.

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Appendix

In the calculation of the Raman-assisted tunneling rate $J_R = J e^{i A_y(m,n)}$, we neglected to observe that the constant $J$ depends on $\alpha$ and $\theta$. In order to justify this assumption, we numerically compute

$$J = \frac{\Omega_0}{2} \int dx \left| \omega_x(x) \right|^2 \cos(2\alpha \cos \theta x) \int dy \, \omega_y(y) e^{2\pi i x \sin \theta} \left( y - \frac{\pi}{2} \right). \quad (A.1)$$

As can be seen in figure A.1, the dependence of $J$ on $\alpha$ in units of the recoil energy $E_R$ is somewhat more significant than its dependence on $\theta$. This suggests that, in order to vary the
magnetic flux going through the system, it would be far more efficient to vary $\theta$ instead of $\alpha$. Indeed, to ensure that the system remains isotropic it is necessary to tune the value of $\Omega_0$ such that for every value of $\alpha$ we have $J_x = J$. By changing $\theta$ this compensation is not necessary because the maximum variation of $J$ as a function of $\theta$ is 4%, as opposed to 25% when $\alpha$ is varied.

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