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Variational Study on Loop Currents in Bose Hubbard model with Staggered Flux

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Abstract

In view of strongly interacting bosons in an optical lattice with a large gauge field, we study phase transitions in a two-dimensional Bose-Hubbard model with a staggered flux, on the basis of variational Monte Carlo calculations. In the trial states, besides typical onsite and intersite correlation factors, we introduce a configuration-dependent phase factor, which was recently found essential for treating current-carrying states. It is found that this phase factor is qualitatively vital for describing a Mott insulating (MI) state in the present model. Thereby, the Peierls phases attached in relevant hopping processes are cancelled out. As a result, local currents completely suppressed in MI states, namely, a chiral Mott state does not appear for the square lattice, in contrast to the corresponding two-leg ladder model. In addition, we discuss other features of the first-order superfluid-MI transition in this model.

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*Keywords:*optical lattice; cold atom; Bose-Hubbard model; staggered flux; artificial magnetic filed; loop current; Mott transition, variational Monte Carlo method

1. Introduction

Ultracold atoms in optical lattices provide an opportunity for studying condensed matter physics in extremely clean and well-controlled environment. However, the charge neutrality of cold atoms prevents phenomena related to Lorentz force in a magnetic field. Therefore, experimentalists have been attempted a variety of ways to realize an artificial magnetic field (Lorentz force) [1]. In a very recent experiment, uniform artificial magnetic fields were created by laser-assisted tunneling on bosonic ladders, and a phase transition was observed from a Meissner (global current) phase to a vortex (local current) phase. Furthermore, an experiment to realize a staggered artificial magnetic field was carried out [3]; thereby, properties in artificial magnetic fields have been brought to attention for strongly correlated lattice bosons.

These studies for the systems with uniform and staggered fluxes provided a subject to tackle with theoretical analyses [4-6]. Among them, a density-matrix-renormalization-group study for two-leg ladder systems is noticeable [5], in which it was demonstrated that there appear Mott-insulator (MI) phases with and without a staggered flux, and a phase transition is found between an ordinary MI phase and a chiral MI phase, in which local currents flow and a charge gap opens [5]. On the other hand, for two-dimensional systems, mean-field-type approaches were mainly used [4], which are not reliable for studying strongly correlated regimes.

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In this paper, we discuss ground-state properties of a two-dimensional Bose-Hubbard model (BHM) with a staggered flux on the basis of variational Monte Carlo (VMC) calculations. In a recent study for a fermionic Hubbard model [7], it was shown that, for reducing the energy of correlated current-carrying states, a configuration-dependent phase factor, $\hat{\mathcal{P}}_\phi$, has to be incorporated into a conventional doublon-holon (D-H)-binding-type wave function. Here, introducing a factor similar to $\hat{\mathcal{P}}_\phi$ into the trial state, we study features of superfluid (SF)-MI transition and show that a chiral MI state does not appear in the model on the square lattice.

2. Model and Method

As a system of bosons in optical lattice with a staggered flux, we adopt a Bose-Hubbard model (BHM) including Peierls phase θ on the square lattice:

$$\mathcal{H} = \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - t\sum_{i\in A}\left[\mathrm{e}^{\mathrm{i}\theta}\left(\hat{a}_i^\dagger \hat{b}_{i+x} + \hat{a}_i^\dagger \hat{b}_{i-x}\right) + \mathrm{e}^{-\mathrm{i}\theta}\left(\hat{a}_i^\dagger \hat{b}_{i+y} + \hat{a}_i^\dagger \hat{b}_{i-y}\right) + \mathrm{H.c.}\right], \tag{1}$$

where $a_i^\dagger, b_i^\dagger$ (a_i, b_i) creates (annihilates) a boson at i-th site on the A and B sublattices (see Fig. 1), $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i = \hat{b}_i^\dagger \hat{b}_i$, x and y indicate the lattice vectors in x and y directions, respectively; t is the tunneling rate, θ is the Peierls phase corresponding to a local magnetic flux, and U is the on-site Hubbard repulsion. The second (hopping) term in Eq. (1) is readily diagonalized by a Bogoliubov transformation to yield a single-particle band dispersion in the staggered fields: $\epsilon_{\boldsymbol{k}}^{\mathrm{ST}} = \pm 2t\sqrt{\cos^2 k_x + \cos^2 k_y + 2\cos 2\theta \cos k_x \cos k_y}$. Energy minima appear at $\boldsymbol{k}_0 = (0,0)$ and (π,π) for $0 \le \theta \le \pi/4$, and at $\boldsymbol{k}_\pi = (0, \pm\pi)$ and $(\pm\pi, 0)$ for $\pi/4 \le \theta \le \pi/2$. Therefore, two different types of Bose-Einstein condensation occur depending on the value of θ.

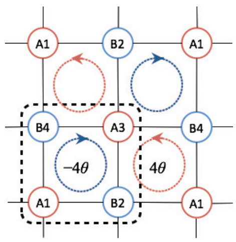

Fig.1. Schematic figure of staggered flux ($\pm 4\theta$) in square plaquettes (square of dashed line) in the BHM. A(1, 3) and B(2, 4) indicate the sublattices.

In VMC calculations for Eq. (1), we employ a Jastrow-type variational wave function: $|\Psi_\phi\rangle = \hat{\mathcal{P}}|\Phi_{\mathrm{ST}}\rangle$, where $|\Phi_{\mathrm{ST}}\rangle$ is the ground state of non-interacting bosons with the staggered flux. As a one-body condensate state $|\Phi_{\mathrm{ST}}\rangle$, we employ a form used in the previous study of a mean-field approach [4], where bosons are created at $\boldsymbol{k}_0$ and $\boldsymbol{k}_\pi$ as quasi-particles described by $\hat{\gamma}_0^\dagger$ and $\hat{\gamma}_\pi^\dagger$. Actually, $|\Phi_{\mathrm{ST}}\rangle$ is written as,

$$|\Phi_{\mathrm{ST}}\rangle = \frac{1}{\sqrt{N!}}\left[\mathrm{e}^{-\frac{\mathrm{i}\xi}{2}}\cos(\sigma)\,\hat{\gamma}_0^\dagger + \mathrm{e}^{\frac{\mathrm{i}\xi}{2}}\sin(\sigma)\,\hat{\gamma}_\pi^\dagger\right]^N |0\rangle, \tag{2}$$

$$\hat{\gamma}_0^\dagger = \frac{1}{\sqrt{N_s}}\sum_{j\in\square}\left[\mathrm{sgn}\left(\cos\tilde{\theta}\right)\left(\hat{a}_{j,1}^\dagger + \hat{a}_{j,3}^\dagger\right) + \left(\hat{b}_{j,2}^\dagger + \hat{b}_{j,4}^\dagger\right)\right], \qquad \hat{\gamma}_\pi^\dagger = \frac{1}{\sqrt{N_s}}\sum_{j\in\square}\left[\mathrm{i}\,\mathrm{sgn}\left(\sin\tilde{\theta}\right)\left(\hat{a}_{j,1}^\dagger - \hat{a}_{j,3}^\dagger\right) + \left(\hat{b}_{j,2}^\dagger - \hat{b}_{j,4}^\dagger\right)\right],$$

where N (N_s) is the total number of bosons (sites), $\sum_{j\in\square}$ denotes the summation over the plaquettes, and $\sigma, \xi, \tilde{\theta}$ are variational parameters. In this study, we consider the case of unit filling $(N/N_s = 1)$.

Taking account of many-body effects in the present case, we use a correlation factor of a form:

$$\hat{\mathcal{P}} = \hat{\mathcal{P}}_\phi(\phi)\hat{\mathcal{P}}_{\mathrm{DH}}(\eta_{\mathrm{D}}, \eta_{\mathrm{H}})\hat{\mathcal{P}}_{\mathrm{J}}(v_r)\hat{\mathcal{P}}_{\mathrm{G}}(g_n), \tag{3}$$

where $\hat{\mathcal{P}}_{\mathrm{G}}(g_n) = \Pi_{\mathrm{i}} g(n_i)|n\rangle_{i\,i}\langle n|$ $(g_{n>6} = 0)$ and $\hat{\mathcal{P}}_{\mathrm{J}}(v_r) = \exp\left[-(1/2)\sum_{i\neq j} v(|\boldsymbol{r}_i - \boldsymbol{r}_j|)\,(\hat{n}_i - 1)\left(\hat{n}_j - 1\right)\right]$ are the onsite (Gutzwiller) and intersite (Jastrow) correlation projections, and $\hat{\mathcal{P}}_{\mathrm{DH}}(\eta_{\mathrm{D}}, \eta_{\mathrm{H}})$ is a nearest-neighbor D-H (H-D) binding projection [8], which is essential for treating Mott physics. These correlation factors were typically used in analyzing the non-flux $(\theta = 0)$ BHM [9-11]. For a current-carrying state in a Mott regime, it is crucial to introduce an additional configuration-dependent phase factor $\hat{\mathcal{P}}_\phi(\phi)$ [7, 8]. Here, $\hat{\mathcal{P}}_\phi(\phi)$ is given by,

$$\hat{\mathcal{P}}_\phi(\phi) = \exp\left[\mathrm{i}\phi \sum_{p=1(A),2(B)} (-1)^{p+1} \sum_{i\in p} \hat{d}_i\left(\hat{h}_{i+x} + \hat{h}_{i-x} - \hat{h}_{i+y} - \hat{h}_{i-y}\right)\right], \tag{4}$$

where $\hat{d}_i = 1$ $(\hat{h}_i = 1)$ and $\hat{d}_i = 0$ $(\hat{h}_i = 0)$, if i-th site is doubly occupied (empty) and otherwise (otherwise), respectively, $p = 1$ (2) specifies the sublattice A (B), i runs over all lattice sites in the sublattice p. The role of this factor is to cancel out the Peierls phase attached in hopping processes in strongly correlated regime, where hopping is almost restricted in the direction of creation or annihilation processes of a D-H pair. For details, see Refs. [7] and [8]. In this article, we compare the results obtained from three types of wave functions: $|\Psi_{\mathrm{G}}\rangle = \hat{\mathcal{P}}_{\mathrm{G}}|\Phi_{\mathrm{ST}}\rangle$, $|\Psi_{\mathrm{DH}}\rangle = \hat{\mathcal{P}}_{\mathrm{DH}}\hat{\mathcal{P}}_{\mathrm{J}}|\Psi_{\mathrm{G}}\rangle$, and $|\Psi_\phi\rangle = \hat{\mathcal{P}}_\phi|\Psi_{\mathrm{DH}}\rangle$.

Optimization of the variational parameters $(\sigma, \xi, \tilde{\theta}, g_n, v_r, \eta_{\mathrm{D}}, \eta_{\mathrm{H}}, \phi)$ is numerically implemented using a quasi-Newton method for each set of model parameters (U, θ), and then calculate physical quantities with 4-5$\times 10^5$ samples for $L \times L$-site lattices (mainly $L = 10$) under the periodic boundary conditions. We confirmed that the L dependence is not essential for the physics below.