Realization of Fully Frustrated Josephson-Junction Arrays with Cold Atoms

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(Received 17 January 2005; published 27 June 2005)

Fully frustrated Josephson-junction arrays (FF-JJA's) exhibit a subtle compound phase transition in which an Ising transition associated with discrete broken translational symmetry and a Berezinskii-Kosterlitz-Thouless transition associated with quasi-long-range phase coherence occur nearly simultaneously. In this Letter we discuss a cold-atom realization of the FF-JJA system. We demonstrate that both orders can be studied by standard momentum-distribution-function measurements and present numerical results, based on a successful self-consistent spin-wave approximation, that illustrate the expected behavior of observables.

DOI: 10.1103/PhysRevLett.95.010401 PACS numbers: 03.75.Lm

The preparation of cold atomic gases trapped in an optical lattice has opened up attractive new possibilities for the experimental study of strongly correlated many-particle systems [1] and has inspired much theoretical activity (see, e.g., Ref. [2] for a review). In particular, the experimental observation by Greiner *et al.* [1] of a superfluid-Mott insulator (SI) transition in a three-dimensional (3D) optical lattice explicitly demonstrated the possibility of realizing strongly correlated cold bosons. The SI transition in an optical lattice was predicted in Ref. [3] and can be described by the Bose-Hubbard model [4], which has also been employed to model 2D granular superconductors [5] and Josephson-juntion arrays (JJA's) [6]. This success has motivated many new proposals [7] for cold-atom simulations of strongly correlated boson phenomena.

In this Letter we propose that cold atoms be used to study the incompletely understood phase transitions that occur in FF-JJA's [6,8]. The boson Hubbard model for JJA's accounts for Cooper pair hopping between small superconducting particles and for Coulomb interactions which can be dominantly intraparticle. For superconducting particles the model applies when the thermal energy $k_B T$ is much smaller than the bulk energy gap, i.e., when the underlying fermionic character of electrons is suppressed. Cold atoms in optical lattice potentials provide, in some senses at least, a closer realization [1,3] of the boson Hubbard model because other degrees of freedom are more completely suppressed and because the interactions are more dominantly on-site. Frustration [8] can be introduced into JJA's by introducing an external magnetic field to change the energetically preferred phase relationship between boson amplitudes on neighboring sites. Frustration in this case refers to the impossibility of choosing the optimal phase difference for each bond. In a cold-atom optical lattice system, frustration can be introduced by altering the phase factors for atom hopping between optical potential minima more explicitly, for example, by following procedures similar to those proposed recently by Jaksch and Zoller [9], Mueller [10], and Sørensen *et al.* [11]. The laser configurations suggested in these papers also enable spatially periodic modulation of the magnitude of boson hopping amplitudes, a feature that is important to the proposal outlined below.

In a FF square-lattice JJA the sum of the optimal phase differences for individual bonds around every plaquette is π, *fully* incompatible with the integer multiple of 2π phase winding constraint imposed by the single-valued condensate wave function. For square-lattice JJA's full frustration can be introduced by applying an external magnetic field that generates one half of a superconducting flux quantum through each plaquette of the array. In the Landau gauge the frustration is imposed by changing the sign of every second vertical hopping parameter. For a FF-JJA, the Gross-Pitaevskii mean-field equation of the corresponding boson Hubbard model has two distinct degenerate solutions, illustrated schematically in Fig. 1, which break the discrete translational symmetry of the lattice, and for each solution a free overall phase factor in the condensate wave function which breaks gauge symmetry. The surprising property of FF square-lattice JJA's, and by extension of FF square-lattice cold atoms, is that the Ising order and the quasi-long-range phase order appear to vanish nearly simultaneously and continuously at a common critical temperature. When quantum fluctuations are included, similar phase changes are expected to occur at zero temperature as the on-site interaction strength is increased. If these orders do, in fact, disappear simultaneously, the phase transition would have to be in a new universality class and could not have a natural description in terms of the condensate wave function order parameter, a situation reminiscent of the deconfined quantum critical behavior discussed recently by Senthil *et al.* [12].

The compound phase change in a frustrated JJA is closely related to the phase changes that occur in the vortex lattices of the mixed state of superconductors, and in rotating ^{4}He and cold-atom systems [13,14]. The vortex lattice ground state has broken translational symmetry

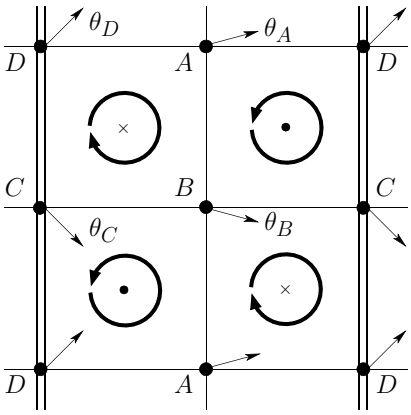

FIG. 1. Ground-state degenerate solutions for a classical FF-JJA. Double vertical lines stand for modulated "antiferromagnetic" bonds ($-\alpha E_J$) while single vertical and horizontal lines stand for unmodulated "ferromagnetic bonds" (E_J). The configuration shown corresponds to $\alpha = 0.5$ for which $\theta_A = -\theta_B = \pi/12$ and $\theta_D = -\theta_C = \pi/4$. The distinct configuration with equal energy is obtained by $(\theta_A, \theta_D) \rightarrow -(\theta_A, \theta_D)$ or equivalently by vertical translation by one lattice constant.

instigated by frustrating order-parameter-phase dependent terms in the Hamiltonian. The key difference between vortex lattices and frustrated JJA's is that the broken translational symmetry is discrete rather than continuous in the latter case. Thermal fluctuations of a vortex lattice imply [15] that quasi-long-range phase order cannot exist at any finite temperature in 2D systems. For superconductors it has been argued [16] that given the absence of phase coherence, broken translational symmetry will not occur either. For the FF-JJA case, the opposite conclusion has been reached in a careful Monte Carlo study by Olsson [17]; he finds that vortex position fluctuations suppress the phase stiffness and instigate a Berezinskii-Kosterlitz-Thouless transition (BKT) as the Ising phase transition temperature is approached from below. If correct, this conclusion would have to be altered when frustration is weakened, as described below, and the Ising transition temperature is driven to zero. In this Letter we point out that these subtle phase changes can be studied by measuring the momentum distribution function (MDF) of a FF cold-atom cloud [18] and report on theoretical estimates for the MDF based on a self-consistent harmonic approximation (SCHA) [19]. Cold atoms can offer a unique opportunity for the experimental study of a system in which there is competition between critical phenomena associated with $\mathbb{Z}_2$ and gauge U(1) broken symmetries.

We assume that atom hopping between sites on the optical lattice is weak enough to justify a single-band Wannier basis [3] with Wannier function $w(\mathbf{x})$. The lattice Hamiltonian we study is

$$\hat{\mathcal{H}}_f = \frac{U}{2}\sum_{\mathbf{x}_i}\hat{n}^2_{\mathbf{x}_i} - \sum_{\mathbf{x}_i,\boldsymbol{\delta}} E^J_{\mathbf{x}_i,\boldsymbol{\delta}} \cos(\hat{\phi}_{\mathbf{x}_i} - \hat{\phi}_{\mathbf{x}_i+\boldsymbol{\delta}}) \qquad (1)$$

where $\mathbf{x}_i = d(n, m)$ with $n, m \in [-\mathcal{N}, \mathcal{N})$ is on a 2D square lattice with lattice constant d, $\boldsymbol{\delta}$ is the vector connecting a lattice site to its neighbors, and the Josephson energy or atom hopping energies $E^J_{\mathbf{x}_i,\boldsymbol{\delta}}$ are identical (equal to E_J) on all bonds except the vertical bonds on every second column. These modulated frustrating bonds have the value $-\alpha E_J$ with $\alpha > 0$ [19]. In Eq. (1) the phase operator $\hat{\phi}_{\mathbf{x}_i}$ has been introduced by approximating the atom annihilation operator on site $\mathbf{x}_i$ by $\hat{b}_{\mathbf{x}_i} \simeq \sqrt{\bar{n}}\exp(i\hat{\phi}_{\mathbf{x}_i})$, allowed when the mean occupation $\bar{n}$ on each lattice site is large. The density $\hat{n}_{\mathbf{x}_i}$ and phase $\hat{\phi}_{\mathbf{x}_i}$ operators are canonically conjugate on each site. The negative hopping parameters introduce frustration, which can be energetically weakened [19] by choosing $\alpha < 1$.

When quantum fluctuations are neglected, the $T = 0$ condensate phase pattern [8] is determined by minimizing the classical energy with respect to the phase difference χ across positive E_J links; the single-valued condition requires that the magnitude of the phase difference across negative E_J links $\chi' = -3\chi$, implying [8] that $\sin(\chi) = \alpha\sin(3\chi)$ and hence that

$$\chi = \pm \arcsin(\sqrt{[(3\alpha - 1)/\alpha]}/2) \qquad (2)$$

for $\alpha > 1/3$, while $\chi = 0$ for $\alpha < 1/3$. For $\alpha < 1/3$, the energy penalty of frustration is paid completely on the negative E_J link and the classical ground-state condensate phase is spatially constant. As α increases beyond this value, the energy penalty of frustration is increasingly shifted to the positive E_J links. The ground-state configuration in this regime is doubly degenerate with currents circulating in opposite directions around alternating plaquettes, as illustrated in Fig. 1. Thermal and quantum fluctuations will degrade both Ising and phase coherence orders. A detailed account of the phase diagram at finite temperature is described in Ref. [19].

Phase coherence of cold atoms in an optical lattice can be directly detected by observing a multiple matter-wave interference pattern after ballistic expansion with all trapping potentials switched off. As time evolves, phase-coherent matter waves that are emitted from each lattice site overlap and interfere with each other. Narrow peaks appear in the MDF due a combination of lattice periodicity and long-range phase coherence [20–22]. The vortex superlattice of the $\alpha > 1/3$ mean-field state results in the appearance of additional peaks in the MDF; $n_f(\mathbf{k}) = \Re e\langle\hat{\Psi}^\dagger(\mathbf{k})\hat{\Psi}(\mathbf{k})\rangle/A$ where A is the system area, and $\hat{\Psi}(\mathbf{k})$ is the 2D Fourier transform of the field operator, $\hat{\Psi}(\mathbf{x}) = \sum_{\mathbf{x}_i} w(\mathbf{x} - \mathbf{x}_i)\hat{b}_{\mathbf{x}_i}$. It follows that

$$n_f(\mathbf{k}) = \frac{\bar{n}|w(\mathbf{k})|^2}{A}\Re e\sum_{\mathbf{x}_i,\mathbf{x}_j} e^{i\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)} C(\mathbf{x}_i, \mathbf{x}_j) \qquad (3)$$

where we have defined a Wannier function form factor $w(\mathbf{k}) = \int d^2\mathbf{x} e^{-i\mathbf{k}\cdot\mathbf{x}} w(\mathbf{x})$ and the phase-phase correlator

$C(\mathbf{x}_i, \mathbf{x}_j) \equiv \langle \exp[i(\hat{\phi}_{\mathbf{x}_i} - \hat{\phi}_{\mathbf{x}_j})] \rangle$. In the broken translation symmetry state $n_f(\mathbf{k})$ is nonzero at superlattice reciprocal lattice vectors $\mathbf{G}_{n,m} = \pi(n, m)/d$; for the classical (i.e., $U = 0$) ground state at zero temperature we find that $n_f(\mathbf{G}) = (N_s^2/A)\bar{n}|w(\mathbf{G})|^2 S_0(\mathbf{G})$ where $N_s = 4\mathcal{N}^2$ is the total number of lattice sites, and the superlattice structure factors are

$$\begin{aligned} S_0(\mathbf{G}_{0,0}) &= [\cos(\chi)\cos(\chi/2)]^2, \\ S_0(\mathbf{G}_{1,0}) &= [\sin(\chi)\sin(\chi/2)]^2, \\ S_0(\mathbf{G}_{0,1}) &= [\sin(\chi)\cos(\chi/2)]^2, \\ S_0(\mathbf{G}_{1,1}) &= [\cos(\chi)\sin(\chi/2)]^2, \end{aligned} \tag{4}$$

with $S_0(\mathbf{G}_{n+2k,m+2k}) = S_0(\mathbf{G}_{n,m})$ for any integers n, m, and k. Phase coherence in a lattice leads to condensation peaks in $n_f(\mathbf{k})$ at all reciprocal lattice vectors $\mathbf{G}_{2n,2m}$. Coherence and Ising broken translational symmetry leads to additional peaks (satellites) with the characteristic pattern of structure factors summarized by Eqs. (4) at the 2×2 superlattice reciprocal lattice vectors. MDF measurements therefore probe both types of order.

These results will be altered by both quantum and thermal fluctuations. At low temperature ($k_B T \ll E_J$) and well inside the superfluid regime ($U \ll E_J$), the phase correlation functions are given reliably by a SCHA [19] in which the density matrix is approximated by that of an effective harmonic model defined by mean condensate phases on each site and harmonic coupling constants K on each nearest neighbor link. Minimizing the variational free energy with respect to mean phases enforces average current conservation at each node of the lattice. Minimization with respect to the harmonic coupling constants sets them equal to the self-consistently determined mean curvature of the Josephson interaction. The phase changes across the vertical and horizontal positive E_J links, θ_h and θ_v, are unequal in this approximation, as are the harmonic coupling constants K_h and K_v and (of course) the coupling constant on frustrated links K_α. For $U \to 0$ and $T \to 0$, the $\theta_h = \theta_v \to \chi$, $K_h = K_v \to E_J \cos\chi$ and $K_\alpha \to -\alpha E_J \cos(3\chi)$.

The SCHA phase correlation function $C(\mathbf{x}_i, \mathbf{x}_j) = C_{\mathrm{NF}}^{\mu,\nu} C_{\mathrm{Q}}^{\mu,\nu}(\mathbf{X}_i, \mathbf{X}_j)$ is the product of a long-range factor $C_{\mathrm{NF}}^{\mu,\nu}$, dependent only on its position within the 2×2 broken-symmetry unit cell, and a Gaussian factor $C_{\mathrm{Q}}^{\mu,\nu}(\mathbf{X}_i, \mathbf{X}_j)$ which captures the power-law decay of phase correlations in 2D superfluids (here $\mathbf{X}_i$ is a lattice vector of the large unit cell so that sites are labeled by μ and i). We find that $C_{\mathrm{NF}}^{\mu,\nu}$ is given by

$$C_{\mathrm{NF}}^{\mu,\nu} = \begin{pmatrix} 1 & e^{i\theta_v} & e^{i(\theta_v+\theta_h)} & e^{-i\theta_h} \\ e^{-i\theta_v} & 1 & e^{i\theta_h} & e^{-i(\theta_h+\theta_v)} \\ e^{-i(\theta_v+\theta_h)} & e^{-i\theta_h} & 1 & e^{-i(\theta_v+2\theta_h)} \\ e^{i\theta_h} & e^{i(\theta_h+\theta_v)} & e^{i(\theta_v+2\theta_h)} & 1 \end{pmatrix}, \tag{5}$$

and that

$$C_{\mathrm{Q}}^{\mu,\nu}(\mathbf{X}_i, \mathbf{X}_j) = \exp\Big\{ -\frac{U}{N_s^2} \sum_{\sigma} \sum_{\mathbf{k} \in \mathrm{BZ}'} \frac{\mathcal{F}_{\mathbf{k},\sigma}^{\mu,\nu}(\mathbf{X}_i - \mathbf{X}_j)}{\xi_{\mathbf{k},\sigma}} \times [1 + 2N_{\mathrm{BE}}(\xi_{\mathbf{k},\sigma}/k_B T)] \Big\}, \tag{6}$$

where [19]

$$\mathcal{F}_{\mathbf{k},\sigma}^{\mu,\nu}(\mathbf{X}_i - \mathbf{X}_j) = |v_\mu^\sigma(\mathbf{k})|^2 + |v_\nu^\sigma(\mathbf{k})|^2 - 2\Re e\{[v_\mu^\sigma(\mathbf{k})]^* v_\nu^\sigma(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{X}_i - \mathbf{X}_j + \mathbf{b}_{\mu\nu})}\}. \tag{7}$$

Here $\mathbf{b}_{\mu\nu}$ is the site separation for $i = j$, $N_{\mathrm{BE}}(x)$ is a Bose-Einstein thermal factor, $\xi_{\mathbf{k},\sigma}^2 = U\lambda_{\mathbf{k},\sigma}$, $\lambda_{\mathbf{k},\sigma}$ and $v_\mu^\sigma(\mathbf{k})$ being the eigenvalues and the μth component of the eigenvectors of the harmonic Josephson interaction.

We have evaluated $S(\mathbf{k}) = n_f(\mathbf{k})A/(\bar{n}N_s^2|w(\mathbf{k})|^2)$ in the presence of both quantum and thermal fluctuations by summing over a finite lattice with $N_s = 1296$ sites in Eq. (3) and applying periodic boundary conditions to make the wave vectors in Eq. (6) discrete. A typical result is reported in Fig. 2. The presence of nonzero Ising satellites at $\mathbf{k} = \mathbf{G}_{1,0}, \mathbf{G}_{0,1}$, and $\mathbf{G}_{1,1}$ is evident. These peaks are a sharp manifestation of the broken discrete translational symmetry and would be absent in an unfrustrated system.

The evolution of $S(\mathbf{k})$ with U at fixed $T = 0.242E_J/k_B$ is illustrated in Fig. 3 where we plot $S(\mathbf{G})$ for $\mathbf{G}_{0,0}$, $\mathbf{G}_{1,0}$, $\mathbf{G}_{0,1}$ and $\mathbf{G}_{1,1}$. All four peaks are slightly suppressed by quantum and thermal fluctuations with respect to the

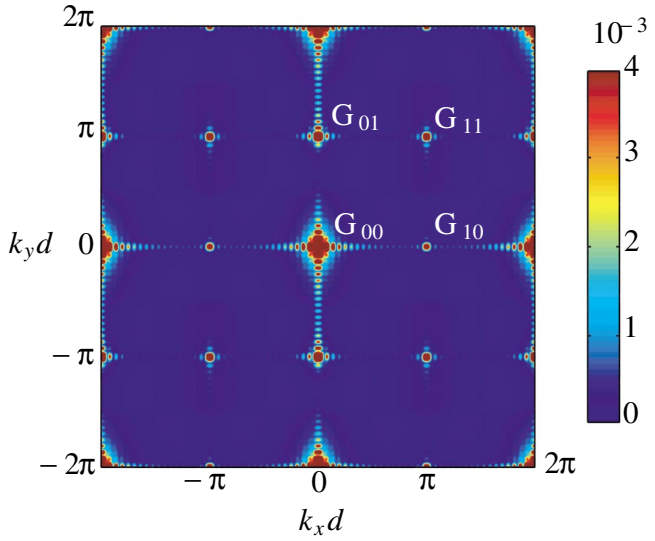

FIG. 2 (color). The structure factor $S(\mathbf{k})$ for FF cold bosons in a 2D array with $\alpha = 0.5$ as a function of the continuous variable $\mathbf{k}d \in [-2\pi, 2\pi] \times [-2\pi, 2\pi]$. Here $T = 0.242E_J/k_B$ [23], and $U = 0.1E_J$. The small undulation in the interference pattern is the result of finite size effects. Clearly finite size effects will be important in any experiment, especially if the confinement potential is quadratic.

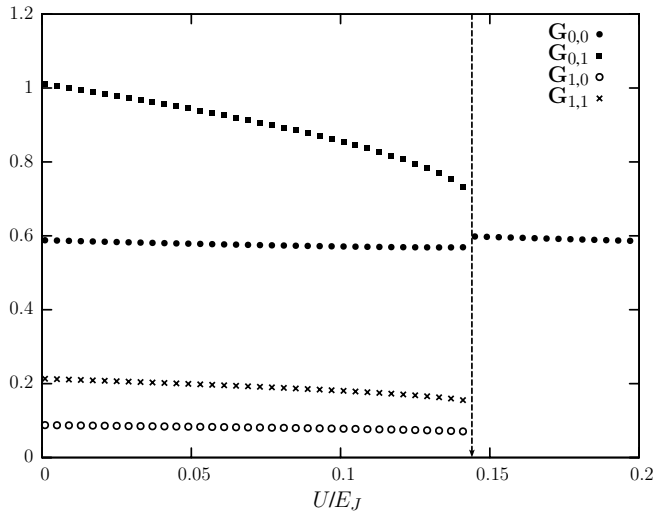

FIG. 3. Condensation and Ising peaks of the structure factor $S(\mathbf{G})$ as a function of U/E_J. The value of $S(\mathbf{G})$ for $\mathbf{G}_{1,0}$, $\mathbf{G}_{0,1}$, and $\mathbf{G}_{1,1}$ has been multiplied by a factor of 10 for clarity. The vertical dashed line indicates the value of U_{IS}^c.

$U = T = 0$ values in Eq. (4). At the critical value $U_{\mathrm{IS}}^c \approx 0.14$ the Ising satellites disappear while the condensation peak survives (the first order character of this transition is an artifact of the SCHA). The superlattice peaks may be regarded as Ising order parameters $\sim S = \sin(\theta_h)$ [see Eq. (4)]. At the Ising point $\theta_h \to 0$, causing $S(\mathbf{G}_{0,0})$ to increase with increasing U, before resuming its decline.

This work was partially supported by EC-RTN "Nanoscale Dynamics" and by an Advanced Research Initiative of S. N. S. A. H. M. acknowledges support from the Welch Foundation and from the National Science Foundation under Grant No. DMR-0115947. We gratefully acknowledge the early contributions to this work by Jairo Sinova. We wish to thank R. Asgari, P. Capuzzi, B. Davoudi, M. Gattobigio, M. Greiner, and K. Madison for useful discussions.

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