Vortex Quantum Dynamics of Two Dimensional Lattice Bosons

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We study hard-core lattice bosons in a magnetic field near half filling. The bare vortex hopping rate is extracted from exact diagonalizations of square clusters. We deduce a quantum melting of the vortex lattice above vortex density of 6.5×10^{-3} per lattice site. The Hall conductivity reverses sign abruptly as the density crosses half filling, where its characteristic temperature scale vanishes. We prove that at precisely half filling, each vortex carries a spin-1/2 quantum number ("v spin"). Experimental implications of these results are discussed.

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Properties of two dimensional lattice bosons are relevant to diverse systems of current interest, e.g., cold atoms on optical lattices, arrays of Josephson junctions, and underdoped cuprate superconductors. Particularly interesting are vortices in such systems, which can be introduced by a rotation, or a magnetic field (if the bosons carry charge). The periodic potential scatters the vortices by units of reciprocal lattice momenta, enhancing their mobility and modifying their effective Magnus field.

When many vortices are introduced into the system, they tend to localize in a lattice configuration which coexists with superfluidity [1–3]. In two dimensions a vortex lattice can melt by quantum fluctuations resulting in a nonsuperfluid quantum vortex liquid (QVL). Present microscopic understanding of vortex dynamics of lattice bosons is insufficient to predict the actual melting density. A missing energy scale, which is difficult to obtain perturbatively or semiclassically, is the "bare" vortex hopping rate t_v on the dual lattice. Another puzzle is the temperature-dependent Hall conductivity $\sigma_H(T)$, which reflects the effective vortex Magnus dynamics in the QVL phase.

In this Letter we compute t_v and $\sigma_H(T)$ by exact diagonalization of finite clusters near half filling. We find t_v to be similar to the boson hopping rate. Mapping our effective vortex Hamiltonian to the boson Coulomb liquid simulated in Ref. [4], we expect a QVL above a melting density of 6.5×10^{-3} vortices per lattice site. The Hall conductivity near half filling reverses sign in a sharp transition. The energy scale governing the transition at finite temperatures vanishes at the transition point. Furthermore, we show that at this point vortices carry spin-1/2 degrees of freedom ("v spins"), as a consequence of local noncommuting SU(2) symmetries.

Model.—We consider N_b hard-core bosons (HCB) hopping on a square lattice of unit lattice constant and size $N = L^x L^y$. The filling fraction is $n_b = N_b/N$. An external vector potential **A** modulates the hopping amplitude (Josephson energy) *t*. The system is placed on a torus with periodic boundary conditions, as shown in Fig. 1. **A**

describes a uniform magnetic field of total N_{ϕ} flux quanta, which penetrates the torus surface. In addition, **A** describes two Aharonov-Bohm (AB) fluxes which thread the two holes of the torus. We define Θ^x and Θ^y as the fluxes through contours which encircle the torus at x = 0 and y = 0, respectively.

In the spin-1/2 representation of HCB, the angular momentum raising and lowering operators $S_{\mathbf{r}}^{\pm}$ create and annihilate bosons; the occupation number is $n_{\mathbf{r}} = S_{\mathbf{r}}^z + \frac{1}{2}$. The Hamiltonian we study is a gauged *XXZ* model,

$$\mathcal{H} = -\frac{t}{4} \sum_{\mathbf{r},\boldsymbol{\eta}} (e^{iA_{\mathbf{r},\boldsymbol{\eta}}} S_{\mathbf{r}}^+ S_{\mathbf{r}+\boldsymbol{\eta}}^- + \text{H.c.}) + \frac{V}{2} \sum_{\mathbf{r},\boldsymbol{\eta}} S_{\mathbf{r}}^z S_{\mathbf{r}+\boldsymbol{\eta}}^z. \quad (1)$$

Here $\eta = \pm \hat{\mathbf{x}}, \pm \hat{\mathbf{y}}$ is the link direction on which the lattice gauge field $A_{\mathbf{r},\eta}$ is defined. Here we only consider the superfluid regime of weak nearest neighbor repulsion $0 < V \ll t$.

In the absence of external magnetic field, the classical ground state of \mathcal{H} is a ferromagnet in the XY plane. The



FIG. 1 (color online). The gauged torus. Geometry of HCB Hamiltonian Eq. (1) which serves to extract its vortex mass and Hall conductivity. The torus surface is penetrated by a uniform magnetic field, and threaded by two Aharonov-Bohm fluxes $\boldsymbol{\Theta} = (\boldsymbol{\Theta}^{x}, \boldsymbol{\Theta}^{y})$. For one flux quantum there is no translational symmetry on the torus. Red circles denote cycles of zero flux, and the vortex center $\mathbf{R}_{v}(\boldsymbol{\Theta})$ is localized on the antipodal point to their intersection, the *null point*.

mean field superfluid stiffness is given by $\rho_s^{\text{mf}} = tn_b(1 - n_b)$. Consequently, the superfluid transition temperature, which is proportional to ρ_s , is maximal at half filling [5].

An important distinction between lattice hard-core bosons and continuum models is the existence of a charge conjugation operator $C \equiv \exp(i\pi\sum_{\mathbf{r}} S_{\mathbf{r}}^x)$ on the lattice. *C* transforms boson "particles" into "holes" $n_i \rightarrow (1 - n_i)$, and the Hamiltonian into

$$C^{\dagger} \mathcal{H}[\mathbf{A}, n_b] C = \mathcal{H}[-\mathbf{A}, 1 - n_b].$$
(2)

A consequence of (2) is that the Hall conductivity is *antisymmetric* in $n_b - 1/2$:

$$\sigma_H(n_b, T) = -\sigma_H(1 - n_b, T).$$
(3)

In terms of vortex motion, this relation implies that below and above half filling vortices drift in opposite directions relative to the particle current. Sign reversal of Hall conductivity is familiar from tight binding electrons at half filling on bipartite lattices. Here, however, the mechanism of sign reversal is different: it arises from the hard-core interactions of bosons and occurs for any lattice structure.

Single vortex Harper Hamiltonian.—Let us consider the case of $N_{\phi} = 1$, which introduces a single vortex on the surface of the torus. The vortex center **R** is treated as a quantum point particle, which hops between dual lattice sites (centers of plaquettes). Its hopping amplitude is modulated by a dual gauge field **a**, whose circulation yields a flux of $\sum_{\mathbf{R},\boldsymbol{\eta}}^{\text{plaq}} a_{\mathbf{R},\boldsymbol{\eta}} = 2\pi n_b$ per dual plaquette. This construction results in a Harper hopping model, which implements the well-known hydrodynamical Magnus action on the vortex motion [6,7].

On the torus, translational symmetry is broken by the magnetic fluxes [8], and the vortex feels an effective confining potential of the form $U_N(\mathbf{R}) = \frac{1}{2}K|\mathbf{R} - \mathbf{R}_v|^2/(L_xL_y)$. The constant *K* is calculated variationally from Eq. (1) using spin coherent states. By minimizing the variational energy with respect to the position of the vortex centered at \mathbf{R} , we calculate the force constant *K*, which for V = 0 fits the value $K \simeq 39.2tn_b(1 - n_b)$.

The minimum of the confining potential $\mathbf{R}_{\nu}(\Theta^{x}, \Theta^{y})$ depends on the values of the AB fluxes as follows [8–10]:

$$R_{v}^{\alpha} = L^{\alpha} \left(\frac{1}{2} + \epsilon^{\alpha \beta} \frac{\Theta^{\beta}}{2\pi} \right) \mod L^{\alpha}, \tag{4}$$

where $\epsilon^{\alpha\beta}$ is the antisymmetric tensor and indices α , $\beta = x$, *y* are not summed.

Thus we arrive at the low energy Harper Hamiltonian of the single vortex, which is given by

$$H^{\nu}_{\mathbf{R},\mathbf{R}'} = -\frac{t_{\nu}}{2} \sum_{\boldsymbol{\eta}} e^{ia_{\mathbf{R},\boldsymbol{\eta}}} \delta_{\mathbf{R}',\mathbf{R}+\boldsymbol{\eta}} + U_N(\mathbf{R}) \delta_{\mathbf{R},\mathbf{R}'}.$$
 (5)

Here we ignore coupling of the vortex to the superfluid phonons [11–13], which are gapped on the finite lattice by the energy scale $2\pi t/L$.

For a quantitative quantum theory of vortices we need to evaluate the effective hopping t_v . Since vortex tunneling between lattice sites depends on short-range many-body correlations, we extract t_v from exact numerical diagonalizations of \mathcal{H} on 16–20 sites clusters, in the presence of a single flux quantum. By tuning t_v , we fit the lowest three eigenenergies E_n of \mathcal{H} to those of the effective Harper Hamiltonian (5).

Our results for $t_v(n_b, V/t)$, for N = 20, fit the analytical approximations,

$$t_{\nu}(n_b, 0) = t - 12.6 \left(n_b - \frac{1}{2} \right)^2 + 1264 \left(n_b - \frac{1}{2} \right)^4,$$

$$t_{\nu} \left(\frac{1}{2}, V \right) = t + 1.5V + 2.7 \frac{V^2}{t}.$$
 (6)

The system parameters were varied in the range $|n_b - \frac{1}{2}| \le 0.2$, and V/t < 0.5. We find that at half filling, t_v varies very little between the N = 16 and N = 20 lattices.

We have argued that the low energy eigenstates $|\Psi_n\rangle$ of \mathcal{H} describe fluctuations of the vortex positions. We expect the low energy vortex wave functions to be localized by the confining potential near \mathbf{R}_v . To test these expectations, we compare the vorticity density $\langle \nabla \times \mathbf{j} \rangle$ of the states $|\Psi_n\rangle$ to the probability density of the eigenstates of H^v . As shown in Fig. 2, using the fitted value of t_v we obtain similar distributions for both sets of wave functions.

Vortex tunneling.—In (6) we find that near half filling, vortices are as light as bosons, $t_v \approx t$. This implies that the vortex tunneling rate between two localized pinning potentials of strength V, which are separated by distance d, decays exponentially as $\Gamma \sim V e^{-d/\lambda}$. The localization length $\lambda \propto \sqrt{t/V}$ diverges at weak pinning. This result is to be contrasted with weakly interacting continuum Bose gas. There, the vortex tunneling rate between pinning sites



FIG. 2 (color online). (a) The vorticity $\langle \nabla \times \mathbf{j} \rangle$ for the first three doublets of the HCB model, Eq. (1), with $N_{\phi} = 1$ and $\mathbf{\Theta} = 0$ on a 4 × 4 lattice. The uniform background vorticity has been subtracted. (b) Single particle probability density of the lowest three excitations of H^{ν} , Eq. (5) with $t_{\nu} = t$.

is much smaller, and decays as a Gaussian $\Gamma \sim e^{-(\pi/2)n_b d^2}$ [14,15]. From this comparison, we conclude that at half filling $n_b = 1/2$ the lattice and the interactions enhance vortex mobility considerably.

Quantum melting transition.—Having calculated t_v , we can write down the effective multivortex Hamiltonian in the thermodynamic limit. We drop U_N at large N. By (5), at half filling there is dual magnetic flux π per plaquette. In the magnetic Brillouin zone, there is a twofold degenerate dispersion $E_{\mathbf{k},s}$, $s =\uparrow, \downarrow$. We later return to explain the origin of this v-spin degeneracy. The vortex effective mass is $M_v^{-1} = \partial^2 E_{\mathbf{k}} / \partial \mathbf{k}^2 = t_v a^2 / \hbar^2$. Integrating out the phonon fluctuations produces an instantaneous logarithmic (2D Coulomb) interaction between vortices, plus retarded (frequency-dependent) interactions [12,13]. Since we are interested in the short wavelength fluctuations which are responsible for quantum melting of the vortex lattice, we ignore these retardation effects.

Thus, for half filled bosons and a vortex density n_v we arrive at the multivortex Hamiltonian

$$\mathcal{H}^{\mathrm{mv}} = \sum_{i,s=\uparrow\downarrow} \frac{\mathbf{p}_i^2}{2M_v} + \frac{\pi t}{4} \sum_{i\neq j} \log(|\mathbf{r}_i - \mathbf{r}_j|) - \frac{n_v \pi^2 t}{4} \sum_i |\mathbf{r}_i|^2.$$
(7)

The single spin version of \mathcal{H}^{mv} is the boson Coulomb liquid studied by Magro and Ceperley (MC) [4] by diffusion Monte Carlo simulation. Their dimensionless parameter which governs the phase diagram is $r_s^{-2} = \pi n_v a_0^2$. We set their $a_0 = (\frac{\hbar^2}{\pi t M_v})^{1/2}$ as the microscopic length which matches between their model and \mathcal{H}^{mv} . MC found that below $r_s \approx 12$ the boson lattice undergoes quantum melting. Using our values of t_v in Eq. (6), the critical $r_s = 12$ translates into a vortex melting density of

$$n_v^{\rm cr} \le \left(6.5 - 7.9 \frac{V}{t}\right) \times 10^{-3} \text{ vortices per site.}$$
(8)

This is a surprisingly low vortex density, which implies that a QVL can be created at manageable rotation frequencies for cold atoms, and moderate magnetic fields for Josephson junction arrays and cuprate superconductors.

Hall conductance.—The temperature-dependent Hall conductance of the finite cluster is given by the thermally averaged Chern numbers [16]:

$$\sigma_{H}(n_{b},T) = \frac{1}{\pi} \sum_{n=0}^{\infty} \int_{0}^{2\pi} \int_{0}^{2\pi} d^{2} \Theta \frac{e^{-E_{n}/T}}{Z} \operatorname{Im} \left\langle \frac{\partial \Psi_{n}}{\partial \Theta_{x}} \middle| \frac{\partial \Psi_{n}}{\partial \Theta_{y}} \right\rangle.$$
(9)

 $E_n(\Theta)$ and $|\Psi_n(\Theta)\rangle$ are the exact spectrum and eigenstates of (1). The results are matched at high temperatures with the ones obtained by the Kubo formula [8]. A typical Hall conductance as a function of filling for $N_{\phi} = 1$ is plotted in Fig. 3. At zero temperature, $\sigma_H = N_b$ below half filling, reminiscent of the behavior in the continuum $\sigma_H \propto N_b/N_v$ which holds irrespective of temperatures. However, for HCB, $\sigma_H(T, n_b)$ decreases with temperature. Moreover, σ_H reverses sign at half filling, as expected by (3).

Our results show a striking general feature. We find that σ_H undergoes a sharp transition between $\sigma_H > 0$ ($\sigma_H < 0$) just below (above) half filling. As the temperature is lowered, the sign reversal of the Hall conductance happens across a narrower region around half filling. This suggests a singularity in the thermodynamic system with a vanishing energy scale. We define $T_H(n_b)$ by $\sigma_H(T_H) = \frac{1}{2}\sigma_H(0)$. In the inset of Fig. 3, we show that T_H seems to vanish with $|n_b - \frac{1}{2}|$, although we cannot yet investigate this behavior further in larger systems.

Spin-1/2 vortices.—Half filling is a special density for \mathcal{H} . First, the Hall coefficient vanishes by (3), which implies that the vortices see no static Magnus field. Second, the external magnetic field creates a multitude of doublet degeneracies. To be precise, for any odd number N_{ϕ} of flux quanta, there are N (the system size) distinct values of AB fluxes Θ_i where all eigenstates are twofold degenerate. We have found that these degeneracies are associated with noncommuting local symmetry operators

$$\Pi^{\alpha} = \frac{1}{2} U^{\alpha} C P^{\alpha}[\mathbf{R}_{v}], \qquad \alpha = x, y.$$
(10)

C is the charge conjugation [see Eq. (3)], and U^{α} is a pure gauge transformation. $P^{x(y)}$ is a lattice reflection about the x(y) axis passing through the vorticity center \mathbf{R}_{v} . For *N* discrete AB fluxes, \mathbf{R}_{v} can be placed on each one of the lattice positions, where $[\mathcal{H}, \Pi^{\alpha}] = 0$. These symmetries follow from the fact that CP^{α} preserves the magnetic field and the AB fluxes. If Θ_{i} are tuned by (4) to position \mathbf{R}_{v} on



FIG. 3 (color online). Hall conductance as a function of boson number N_b for hard-core bosons, Eq. (1) on the torus. Temperatures, in units of t, vary in intervals of $\Delta T = 0.05t$. The jump of the zero temperature conductance at half filling is smoothened at finite temperatures. Inset: Hall temperature scale as a function of density deviation from half filling. T_H is defined by $\sigma_H(T_H) = \frac{1}{2}\sigma_H(0)$.

a lattice site, CP^{α} sends \mathcal{H} to itself up to a pure gauge transformation $(U^{\alpha})^{\dagger}$.

A straightforward, though cumbersome, calculation [8] yields the commutation rule

$$\Pi^{y}\Pi^{x} = (-1)^{N_{\phi}}\Pi^{x}\Pi^{y}.$$
(11)

We define the vector $\mathbf{\Pi} = (\Pi^x, \Pi^y, \Pi^z)$, where $\Pi^z = 2i\Pi^x\Pi^y$. For any odd number N_{ϕ} of vortices it is easy to show using (11) that each of the energy eigenstates is at least twofold degenerate.

Since $\Pi^2 = 3/4$, they obey the algebra of spin-1/2 operators. Thus the doublets reflect the Kramers degeneracy expected for an odd number of interacting spin-1/2 degrees of freedom which we label v spins. As shown by the form of Π^{α} , the v spins are attached to the vortex positions. The z-direction polarization corresponds to a boson charge density wave (CDW) modulation. Variational calculation shows the CDW to be exponentially localized in the vortex core [17]. Thus v-spin interactions between different vortices decay exponentially, and are very weak in the vortex lattice regime.

Nature of the QVL.—Theoretical treatments of lattice bosons have found a myriad of vortex-antivortex condensate (VC) phases at all rational boson filling fractions, $n_b = p/q$, due to q-fold degeneracies of the Harper Hamiltonian on an infinite lattice [18–21]. VCs are, in effect, insulating phases where the dual Anderson-Higgs mechanism produces a Mott gap [11]. However, the QVL we study, which contains a net density of vortices, differs from the proposed VC phases in two important respects.

(i) MC [4] have found that the liquid phase of \mathcal{H}^{mv} (7) has vanishing condensate fraction. Although in a strictly Galilean invariant model one expects a dual superfluid density $\rho_s^v \propto n_v$ [22], superfluidity does not necessarily persist in the presence of weak impurity potentials. Furthermore, retardation effects act to suppress superfluidity [23]. The QVL can therefore differ from the charge-gapped insulator. Whether it is a metal is an open possibility. Away from half filling, our results for σ_H show that the vortices are subject to a strong magnetic field, which further suppresses their condensation. At low boson fillings and large vortex density, $n_b/n_{\phi} < 1$, there is evidence for fractional quantum Hall phases [24,25].

(ii) Away from the commensurate filling VC phases at $n_b = p/q$, the Hall conductivity is expected to cross zero and be proportional to the excess density from p/q. We found that the Hall conductance has a very different be-

havior: it has only one abrupt jump between a positive value below, and is negative above half filling.

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