Chiral Edge States and Fractional Charge Separation in a System of Interacting Bosons on a Kagome Lattice

Xue-Feng Zhang (张学锋) and Sebastian Eggert

Physics Department and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

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We consider the extended hard-core Bose-Hubbard model on a kagome lattice with boundary conditions on two edges. We find that the sharp edges lift the degeneracy and freeze the system into a striped order at $1/3$ and $2/3$ filling for zero hopping. At small hopping strengths, holes spontaneously appear and separate into fractional charges which move to the edges of the system. This leads to a novel edge liquid phase, which is characterized by fractional charges near the edges and a finite edge compressibility but no superfluid density. The compressibility is due to excitations on the edge which display a chiral symmetry breaking that is reminiscent of the quantum Hall effect and topological insulators. Large scale Monte Carlo simulations confirm the analytical considerations.

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Frustrated systems are a rich playground in the search for new exotic phases and excitations, such as spin liquid phases [1–4], Dirac strings in a spin ice [5,6], and fractional charges in kagome lattice antiferromagnets [7]. Recently, progress of indirect observations of fractional excitations has been made [8], but their detection remains far from trivial since the controlled excitation and separation of fractional charges is difficult. We now show that, by introducing sharp edges on two sides of a kagome lattice with interacting bosons, fractional charges appear spontaneously and are located close to the separate edges depending on their chirality. These chiral edge states are reminiscent of phenomena in quantum Hall physics [9] and topological insulators [10], but on the kagome lattice the topology and chirality are completely controlled by the design of the edges. Moreover, the appearance of the chiral fractional charges with a deconfined interaction gives rise to a new compressible quantum edge phase.

Exotic excitations in frustrated systems such as fractional charges and monopoles can often be understood from rather straightforward geometrical arguments [11]. They appear as local defects in the form of a rearrangement of real charges on the nontrivial background [6,7,12,13]. When two (or more) fractional charges separate they may be connected by a *string* of a slightly disturbed quantum ground state, which normally acts confining. This poses a generic problem for the controlled excitation and observation of the fractional charges: the confining string keeps them close together so that a separate observation becomes impossible, analogously to the difficulty of detecting individual quarks. If the string can be tuned to become deconfining, then the system typically undergoes a quantum phase transition to a complicated sea of closed strings with entirely different properties.

In this Letter we show that a controlled separation of fractional charges is possible using sharp edges in a system of interacting bosons on a kagome lattice. We find that the boundary conditions play an important role due to the huge degeneracy, and deconfining strings appear, which separate the fractional charges. The fractional charges are located near the edges and their internal quantum number (up and down) is locked to the respective topology of the edge.

The model is defined by hard-core bosons on a kagome lattice with nearest neighbor repulsion V and chemical potential μ,

$$H = -t\sum_{\langle ij\rangle}(b_i^\dagger b_j + b_j^\dagger b_i) + V\sum_{\langle ij\rangle} n_i n_j - \mu\sum_i n_i, \qquad (1)$$

where t is the hopping between boson creation and annihilation operators $b_i^\dagger$ and b_j on nearest neighbor sites $\langle i, j\rangle$. The kagome lattice is special since it allows a macroscopic degeneracy even for commensurate fillings of $1/3$ and $2/3$. In particular, without hopping the model in Eq. (1) corresponds to the Ising model with an entropy per site [14] of $S = 0.108$ at filling $1/3$, since all configurations with one particle per triangle are ground states; i.e., there is a ''triangle rule'' analogous to the ''ice rule'' in the spin ice [6]. Finite hopping $t > 0$ lifts this degeneracy which leads to an ordered state with a finite structure factor. At even larger hopping a phase transition to a superfluid phase is observed, which is believed to be weakly first order or possibly second order [15]. At negative hopping $t = -V/2$ the model corresponds to the Heisenberg model which is at half filling one of the most promising candidate for a spin liquid [2].

Fractional charges on the kagome lattice which are connected by strings have been extensively discussed [7] for the fermionic model in Eq. (1) at filling $1/3$. Basically, the fractional charges correspond to one empty triangle, which has two possible chiralities: up or down. Since one up and one down triangle together correspond to a single missing charge [see Fig. 1(b)], it is clear that a single empty triangle has negative fractional bosonic charge $-1/2$.

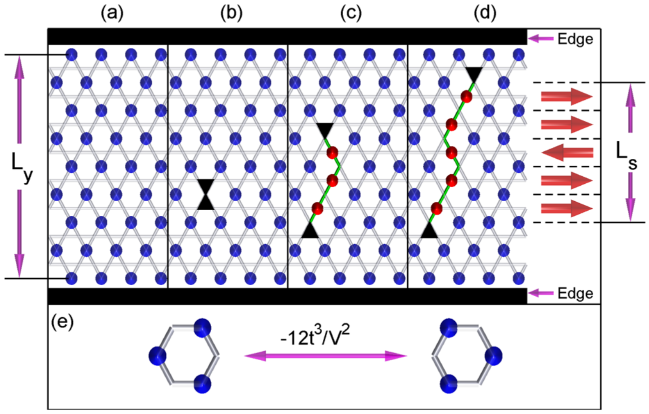

FIG. 1 (color online). (a) Striped order phase induced by edges. (b) One hole corresponds to two fractional charges (black triangles). (c) Hopping of real particles (blue dots) separates the fractional charges and resonant hexagons appear along the connecting string (red dots). (d) The spin (red arrows) representation of the string (green path). (e) Resonant hexagons can be flipped by a third order hopping process.

However, so far there is no proposal on how to directly observe these exotic excitations.

As we will show here, it is possible to make a controlled separation of the fractional charges by introducing sharp edges in the model of Eq. (1) on two sides of the kagome lattice, which also gives rise to a new boundary-induced quantum edge phase. Interestingly, such edges as depicted in Fig. 1 have a macroscopic effect in the kagome lattice, since the edges fix the bosons at the upper corners of the triangles. Therefore, the order becomes frozen for $t = 0$ and there is a unique ground state of bosons in stripes parallel to the edges as shown in Fig. 1(a). In other words, the macroscopic entropy is lost in this "striped order phase," even when the edges are very far apart.

In a system with such edges the role of finite but small hopping t is now dramatically reversed: Instead of lifting the degeneracy, the hopping now facilitates fluctuations, which turn out to be nothing other than strings between fractional charges. As depicted in Fig. 1 the separation of two fractional charges creates a string with configurations of triple occupied hexagons. At finite hopping the triple occupied hexagons are preferred since they lower the energy by $-12t^3/V^2$ via a resonant third order hopping process [15], as shown in Fig. 1(e).

At this point two interesting observations can be made: First, there is a new competition between a frozen ground state due to the edges without any resonant hexagons (striped order phase) on the one hand and possible fluctuating strings on the other hand; second, closed strings cannot appear by a local rearrangement of charges without violating the triangle rule on the frozen configuration shown in Fig. 1(a). Indeed, it is straightforward to convince oneself that fluctuating strings with triple occupied hexagons can only occur if either the triangle rule is violated or holes are introduced into the system. For the case $\mu < V$ we therefore expect that holes may appear spontaneously which separate into two fractional charges since the connecting strings allow additional resonant hexagons and therefore are *deconfining*. However, this phase is not the superfluid phase since the fractional charges are not free. Indeed, we will see that the fractional charges only appear as edge excitations, so we will call this phase the "edge liquid phase."

In order to establish the new edge phase quantitatively, it is important to understand the process of fractional charge separation in detail as illustrated in Fig. 1. In Fig. 1(a) the frozen configuration in the striped order is shown, which is the unique ground state for $t = 0$. If a charge is removed [Fig. 1(b)], two fractional charges can separate for $t \neq 0$, namely, one up and one down triangle [Fig. 1(c)] which are connected by a string (red dots). Because of this string, the down triangle can never move underneath the up triangle. Since there are now resonant configurations (hexagons with three bosons) along the string, it is deconfining and the energy can be lowered by pushing the fractional charges to the upper and lower edges, respectively. When the energy gain from a fluctuating string exceeds the energy cost μ of removing a charge, it can be expected that fractional charges appear spontaneously at the edges, leading to a new quantum edge phase which is compressible.

The energy of a string can in turn be quantitatively estimated by realizing that in fact the resonances on each hexagon correspond to fluctuations of the string as shown in Fig. 1(d). Here the path of the string is mapped to up and down spins depending on whether the string is to the right or left of a resonant hexagon. A flip can occur when the neighboring hexagon has opposite spin, leading to an xy-type model with effective exchange of $-12t^3/V^2$ along the length of the string $L_s \leq L_y$:

$$H_{xy} = -\frac{12t^3}{V^2}\sum_{i=1}^{L_s}(S_i^+ S_{i+1}^- + \text{H.c.}). \quad (2)$$

For a given length L_s the ground state energy of this model is given by

$$E_{xy}(L_s) = \frac{12t^3}{V^2}\left(1 - \cot\frac{\pi}{2(L_s+1)}\right) \approx -\frac{24t^3}{\pi V^2}L_s, \quad (3)$$

which means that there can be a substantial energy gain by maximizing the length L_s. However, this is only part of the story since the ends of the string can move freely up to the total systems size $L_y \geq L_s$, due to the hopping of the fractional charges. This hopping gives an additional kinetic energy of order t and independent of length, but for large systems sizes the leading effect of the xy model in Eq. (2) is to maximize the length of the string L_s, i.e., push the fractional charges apart towards the edges by an effective linear repulsive potential between the fractional charges.

At the top edge the fractional charges appear as down triangles only, and at the bottom edge they appear as up triangles. These edge excitations therefore have a definite chirality, which relates the pseudospin of the fractional charge (up or down) to the direction given by the edge.

We now turn to quantum Monte Carlo simulations of the hard-core boson model in Eq. (1) on the kagome lattice in order to numerically analyze the existence of the edge excitations. We use the stochastic cluster series expansion [16,17] with parallel tempering [18–20] on system sizes up to 1752 sites ($L_y = L_x = 24$) with cylindrical boundary conditions.

In all extrapolations to the thermodynamic limit, we use an isotropic 2D geometry of $L_y = L_x$. Most of the simulations were done for an inverse temperature of $\beta = 200/V$ so that quantum fluctuations of the strings always dominate temperature fluctuations, which we have checked by going to lower temperatures for selected system sizes. In Fig. 2 we show a small section of the phase diagram [15] near the transition to the $1/3$ solid phase for cylindrical boundary conditions. As predicted, the striped order is destroyed by the spontaneous appearance of fractional charges as the hopping is increased. The value of the critical hopping is lower for larger L_y, which is in agreement with the argument that the energy of the string is proportional to L_s. In fact, from the energy of the effective model in Eq. (3) we expect that for a given chemical potential the critical hopping for the appearance of strings will decrease with $t_c \propto 1/L_y^{1/3}$ to leading order, which is confirmed in the inset of Fig. 2. This analytic argument implies that in the thermodynamic limit the edge liquid phase is always the most stable phase, and the striped order phase is just a false vaccum. In all numerical simulations we indeed find that the edge liquid phase becomes more stable with increasing length. In the thermodynamic limit the correlations in the bulk must become independent of the boundary condition, but the presence of boundaries is still manifest by the appearance of fractional charges at the edges and a corresponding "edge compressibility," which are the hallmarks of the edge liquid phase.

In the middle panel of Fig. 3, a typical snapshot of a configuration during a Monte Carlo simulation for $t = 0.102V$ in the edge liquid phase is shown. A string is clearly visible by the shaded resonant hexagons (green) and the shaded up and down triangles (red) which indicate fractional charges near the edges. The distribution of up-triangle fractional charges is shown in the left-hand panel of Fig. 3. In the edge liquid phase ($t = 0.102V$) the interplay of maximizing L_s according to Eq. (3) and the kinetic energy of the fractional charges leads to a characteristic maximum of fractional charges near the edges, which can be predicted from the effective model in Eq. (2) and resembles the solution of a particle in a linear potential (Airy function). In the striped order phase ($t = 0.09V$) no fractional charges are found (except for virtual excitations), and in the superfluid phase ($t = 1.2V$) there are fractional charges in the entire sample, but the maximum near the edge remains. The right-hand panel of Fig. 3 shows the change in resonant hexagon density in the different phases.

The relevant order parameters in the different phases are shown in Fig. 4. The spontaneous appearance of additional

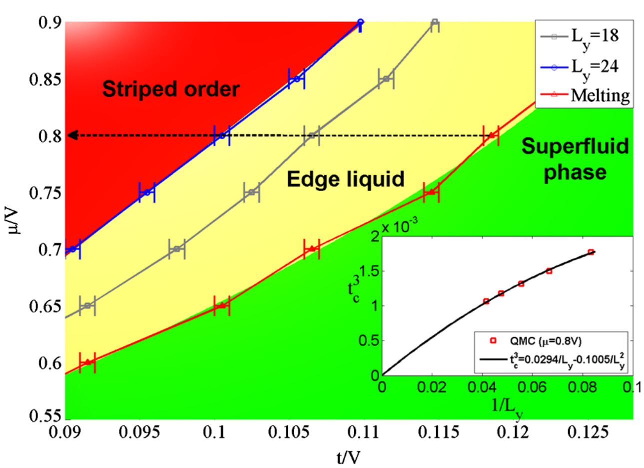

FIG. 2 (color online). The phase diagram of the Bose-Hubbard model with cylindrical boundary conditions for $L_y = 18$ and 24 from quantum Monte Carlo (QMC) simulations at temperature $T = 0.005V$. The melting phase transition line to the superfluid phase was determined on lattices up to $L_y = 24$ with periodic boundary conditions. Inset: The extrapolation of the critical hopping at $\mu = 0.8V$ as a function of length L_y.

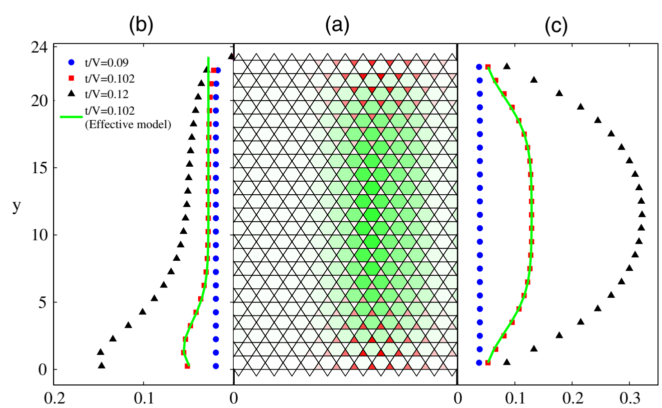

FIG. 3 (color online). A snapshot of a typical configuration during a Monte Carlo run at $\mu/V = 0.8$, $t/V = 0.102$, and $\beta = 200/V$ with $L_x = L_y = 24$ is shown in the middle panel. Red indicates a higher density of empty triangles or fractional charges and green represents a higher density of hexagons in a resonant configuration. The density distribution of up-triangle fractional charges is shown in the left-hand panel for the striped order ($t = 0.09V$), edge liquid ($t = 0.102V$), and superfluid ($t = 0.12V$) phases. The right-hand panel shows the corresponding densities of resonant hexagons.

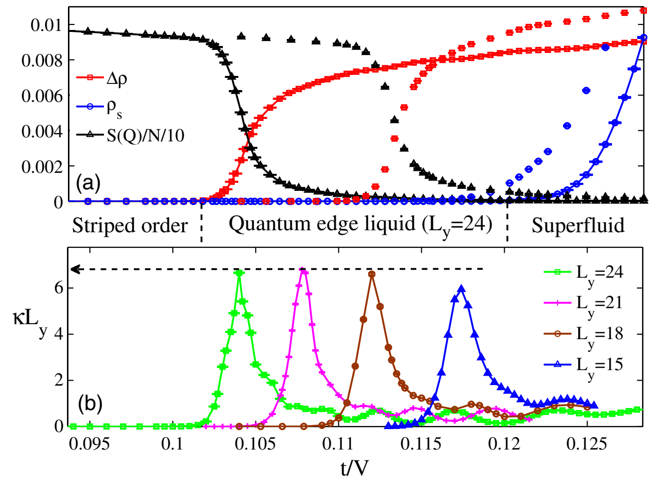

FIG. 4 (color online). (a) The change of hole density $\Delta\rho$ relative to the striped order phase, the structure factor with $Q = (2\pi, 0)$, and the superfluid density ρ_s at $\mu/V = 0.8$ and $\beta = 200/V$ with $L_x = L_y = 24$ (solid line) and 18 (no line) in different phases. (b) The compressibility at $\mu/V = 0.8$ for different sizes.

charges at a critical hopping is clearly seen by the change of total hole density $\Delta\rho = (L_y + 1)/(3L_y + 1) - \sum_i \langle n_i \rangle / N$ (relative to the striped order phase). The structure factor $S(\mathbf{Q})/N = \langle |\sum_{k=1}^{N} n_k e^{\mathbf{i}\mathbf{Q}\cdot\mathbf{r}_k}|^2 \rangle / N^2$ at $\mathbf{Q} = (2\pi, 0)$ is an indication of the striped order, which drops sharply when the fractional charges appear in the edge liquid phase. The length dependence of the critical hopping at which this transition occurs is shown in the inset of Fig. 2. At still larger hopping the system enters the superfluid phase, which has a spontaneously broken U(1) symmetry (off-diagonal order) and a finite superfluid density ($\rho_s = \langle W^2/2\beta t \rangle$ in terms of the winding number W in Monte Carlo simulations [21]). The compressibility per site κ is maybe the most interesting order parameter, since it is zero in the striped order phase and then has a clear maximum close to the phase transition into the edge liquid phase. The bottom panel of Fig. 4 illustrates how this maximum (i.e., the phase transition) moves to lower values of t as the system size increases. At the same time the maximum of the scaled compressibility $L_y \kappa$ approaches a constant; i.e., the compressibility per site *decreases* proportional to $1/L_y$. Indeed, according to the considerations above, the bulk sites do not contribute to the compressibility since there are no fractional charges (see Fig. 3), so we can observe an edge compressibility $\kappa \propto 1/L_y$. The fluctuations of the strings lead to an effective short-range potential between them, so the compressibility is large in the dilute limit close to the phase transition, which is second order. At larger hopping the string density increases and the compressibility is reduced accordingly. The oscillations in the lower panel of Fig. 4 are a finite size effect in L_x: Basically, the compressibility is low when the expectation value of strings is exactly integer valued n. If the hopping is then increased, the number of strings fluctuates between n and $n + 1$, which leads to an increase of the compressibility in regular intervals, analogous to oscillations due to the quantized charging energy of a small capacitor (Coulomb blockade).

In summary, the results show that edges have a dramatic effect for hard-core bosons on a kagome lattice and lead to a new edge liquid phase, which is characterized by a finite edge compressibility but no superfluid density. Quantum Monte Carlo simulations and analytical arguments demonstrate that fractional excitations of up and down triangles can be separated in space and are localized close to the lower and upper edges, respectively. The fractional charges are connected by quantum strings of resonant configurations, which act deconfining. Edge states with a finite compressibility and the locking of an internal quantum number with the direction of the edge (e.g., the chirality of the spin-momentum locking) are also famous characteristics of topological insulators and the quantum Hall effect. However, for the hard-core boson system studied here, the nontrivial topology is not a property of the bulk, but is instead controlled by the design of the sharp edges. In fact, the study of different kinds of edges or defects in the edges are promising future research topics. While fractional excitations at edges have long been known in 1D systems, such as the spin-1/2 degrees of freedom in a spin-1 chain [22], we believe that such an effect has so far been unknown in 2D.

Recently, much experimental progress has been made in the realizations of related models with ultracold bosonic gases. In particular, it is now possible to create an artificial kagome lattice for ultracold bosons [23]. Moreover, a gas of Rydberg atoms was successfully loaded in a two-dimensional optical lattice, and the spatially ordered structures induced by the short-range repulsion interactions have been observed directly [24]. In principle it should be possible to create sharp boundaries on such systems [25]. Together with recent advances in single-site detection [24,26], the effects illustrated above therefore give a promising perspective of actually taking pictures of strings and localized fractional charges analogous to the snapshot in our simulations in Fig. 3.

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