Superfluid-Insuator transitions of Bosons on a Kagome lattice at non-integer fillings

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Refs.

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Outline

1. Mott transition for bosons: an introduction.

2. Dual picture of the transition: a dual vortex theory.

3. Superfluid-Mott transition on Kagome (also XXZ spin model on Kagome)

4. Results from dual vortex theory: comparison with QMC.

5. RG and possible application of NPRG

Bose-Hubbard Model

$$H_B = -t \sum_{\langle ij \rangle} \left(b_i^\dagger b_j + \text{h.c} \right) + \frac{U}{2} \sum_i \widehat{n}_i \left(\widehat{n}_i - 1 \right) - \mu \sum_i \widehat{n}_i$$

Question: What are the T=0 phases of the model?
Answer: For what filling factor?

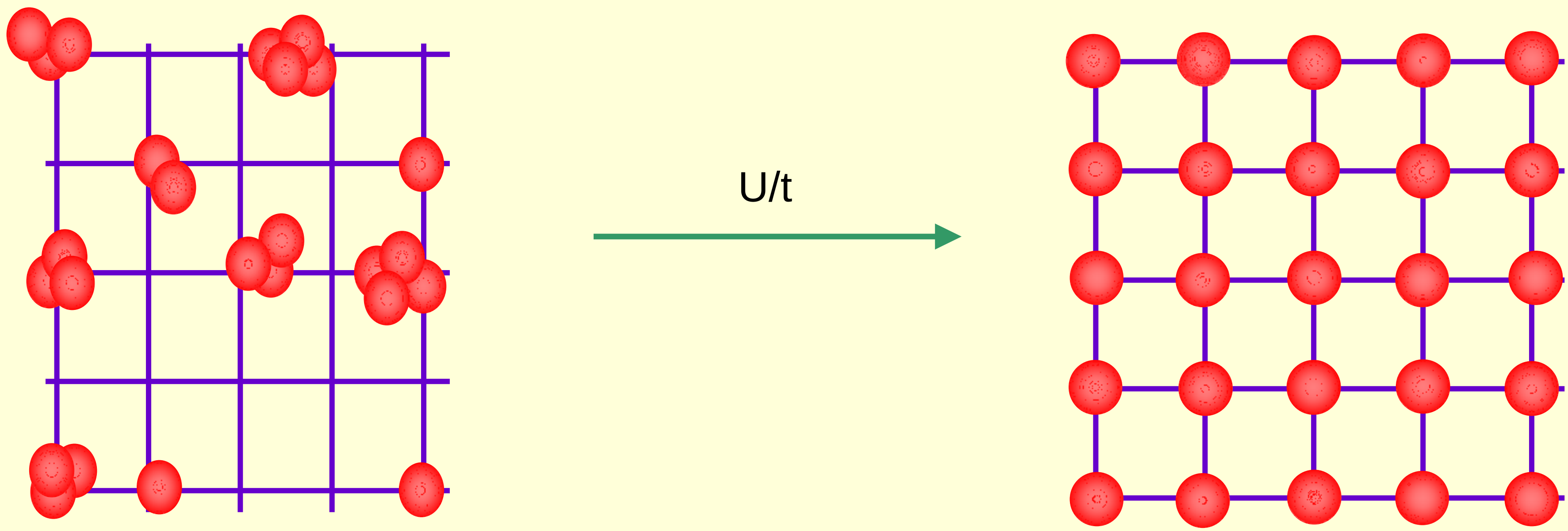
Integer filling

Interesting:
1) Mott phase for t<<U and Superfluid for t>>U
2) Quantum phase transition at a critical t_c
3) Critical theory may have z=1 or z=2.

Fractional filling

Boring: always a featureless superfluid

Cartoon of the states on a simple 2D square lattice



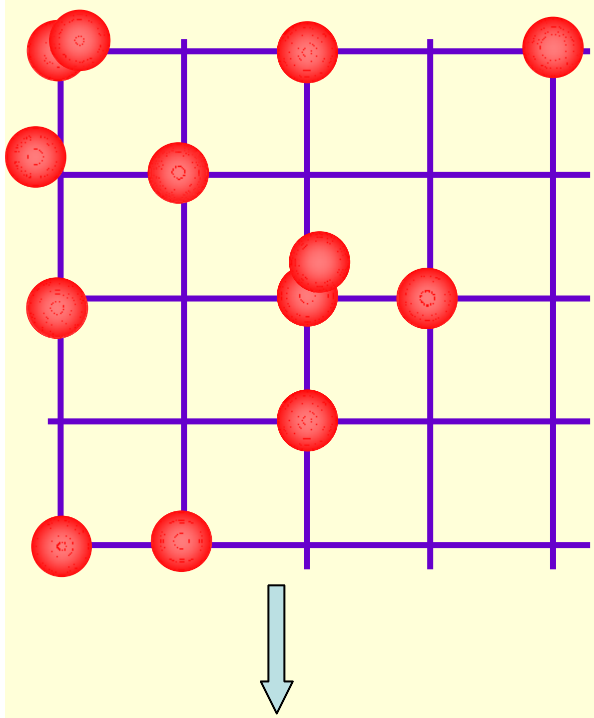
Question: Experimental verification of this picture?
Answer: Yes, using ultracold atoms in optical lattices.

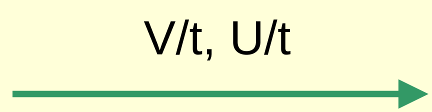
Greiner et al. Nature 2002.

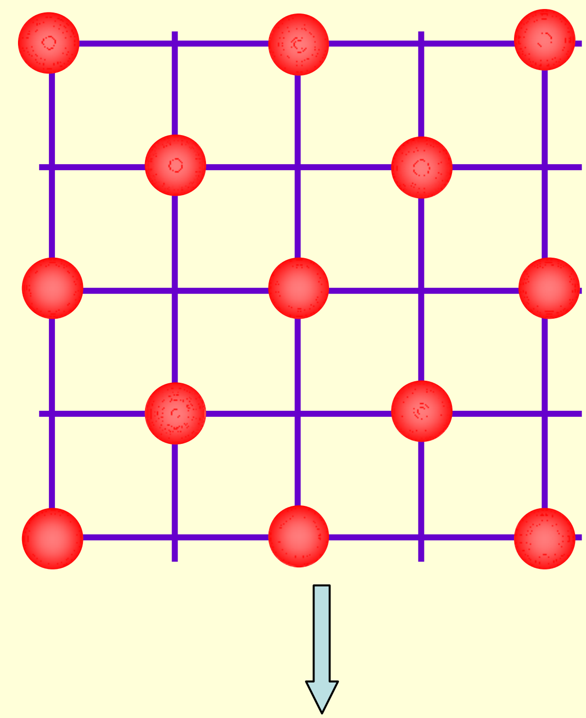
Fractional filling and extended Bose-Hubbard Model

$$H_{\text{Bose}} = -t\sum_{\langle ij\rangle}\left(b_i^\dagger b_j + \text{h.c}\right) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + V\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j - \mu\sum_i \hat{n}_i$$

Simplest case: Boson at filling f=1/2 on a square lattice







Broken U(1) symmetry

Question: Nature of quantum phase transition?

Broken translation symmetry

Superfluid-Insulator transition at generic filling f

The transition is characterized by multiple distinct order parameters (boson condensate and density-wave order).

Traditional (Landau-Ginzburg-Wilson) view:

Such a transition is either first order or has a coexisting supersolid phase, and there can be no second order transition between the superfluid and the Mott states.
As a result, there are no precursor fluctuations of the order of the insulator in the superfluid.

Theory of transition described in terms of order parameters of either sides.

Recent theories:

Quantum interference effects can render such transitions second order, and the superfluid does contain precursor CDW fluctuations [additional possibility]

Transition described in terms of vortices which are not the order parameter in either side of the transitions: non-LGW paradigm.

T. Senthil, A. Vishwanath, L. Balents, S. Sachdev and M.P.A. Fisher, *Science* **303**, 1490 (2004)
L. Balents, L. Bartosch, A. Burkov, S. Sachdev and K. Sengupta, PRB **71**, 144509 (2005).

Basic points of non-LGW paradigm applied to bosons

1. The quantum phase transition from Mott to superfluid phase is described by vortices which are non-local topological excitations of the superfluid phase.

2. These vortices are not the usual order parameter in either side of the transitions; hence the name non-LGW paradigm.

3. The superfluid phase has $\langle \phi \rangle = 0$ while the Mott phase has $\langle \phi \rangle \neq 0$

4. The vortex fields form multiplets which transform according to the symmetry group of the underlying lattice: natural incorporation of the geometry of the lattice and hence natural way to address issues related to frustration.

5. A duality analysis of the Hubbard-Boson model leads to an effective action of the vortices:

$$S_{\rm dual} = \frac{1}{2e^2}\sum_p \left(\epsilon_{\mu\nu\lambda}\Delta_\nu A_{b\lambda} - f\delta_{\mu\tau}\right)^2 - y_v \sum_{b,\mu}\left(\psi^\dagger_{b+\mu} e^{2\pi i A_{b\mu}}\psi_b + \text{h.c.}\right) + \sum_b r|\psi_b|^2 + u|\psi_b|^4 + \ldots$$

ψ_b: vortex fields living on dual lattice., f: average boson filling, $A_{b\mu}$: gauge fields which the vortices see., y_v: vortex fugacity

Operational Procedure: What to do with the vortex action

1. Treat the action at a saddle point level: the vortices see a dual magnetic field proportional to the boson filling factor f.

2. Solve the corresponding Hofstadter problem and find out the minima of the vortex kinetic energy spectrum.

3. When one approaches the transition from the superfluid side, the fluctuations about these minima will be most important for destabilizing the superfluid phase.

4. Expand the vortex field about these minima and construct the most general effective Landau-Ginzburg action which respects all the symmetries of the underlying lattice.

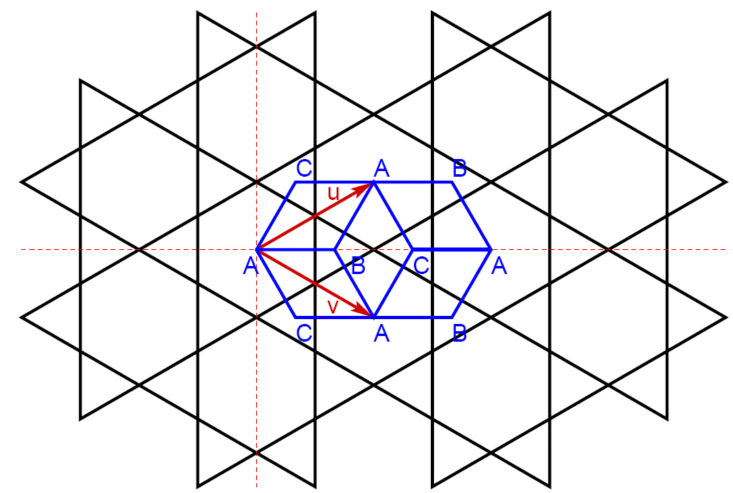
5. Construct the possible density-wave orderings based on symmetry from the effective action. These are the competing orders for the Mott states.

6. In this picture, the superfluid-Mott transition naturally leads to competing orders for the Mott state.

Extended Bose-Hubbard models on Kagome lattice

$$H_{\text{Bose}} = -t\sum_{\langle ij\rangle}\left(b_i^\dagger b_j + \text{h.c}\right) + \frac{U}{2}\sum_i \hat{n}_i\left(\hat{n}_i - 1\right) + V\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j - \mu\sum_i \hat{n}_i$$

Kagome and its
dual dice lattice



Holstein-Primakoff transformation

$$H_{\text{XXZ}} = \sum_{\langle ij\rangle}\left[-J_x\left(S_i^x S_j^x + S_i^y S_j^y\right) + J_z S_i^z S_j^z\right] - B_l\sum_i S_i^z$$

Duality Mapping

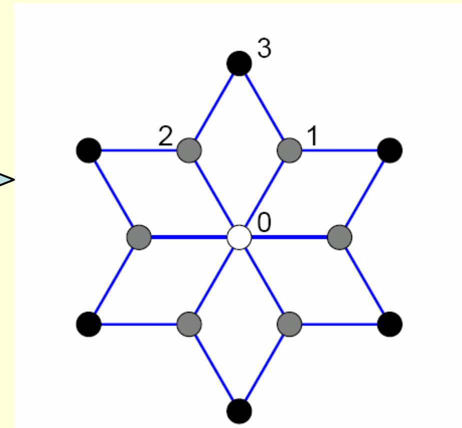
$$S_{\text{dual}} = \frac{1}{2e^2}\sum_p\left(\epsilon_{\mu\nu\lambda}\Delta_\nu A_{b\lambda} - f\delta_{\mu\tau}\right)^2 - y_v\sum_{b,\mu}\left(\psi_{b+\mu}^\dagger e^{2\pi i A_{b\mu}}\psi_b + \text{h.c.}\right) + \sum_b r|\psi_b|^2 + u|\psi_b|^4 + \ldots$$

1) Nature of the superfluid-Mott insulator transition?

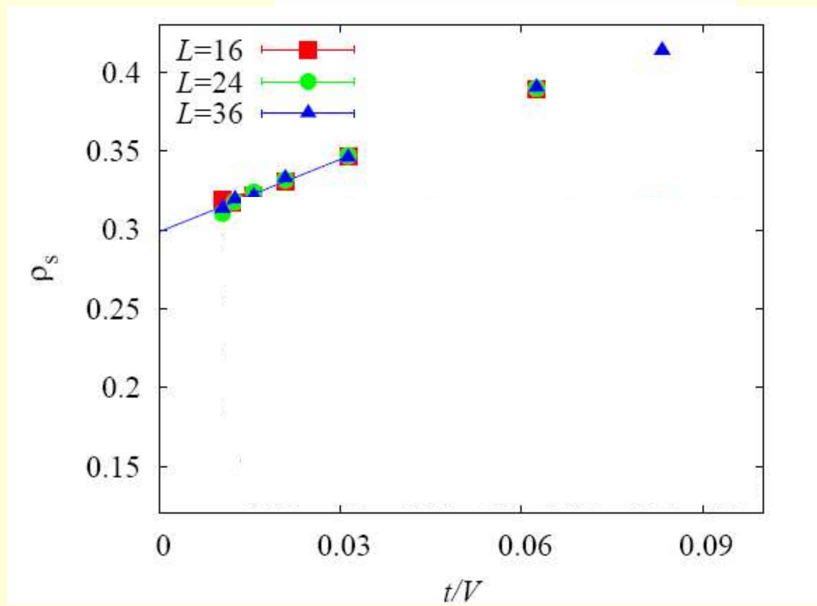
f=1/2

Solution of the Hofstadter problem shows that the entire vortex spectrum collapses into three infinitely degenerate bands. There are no well defined minima in the vortex spectrum.

The vortex wavepacket starting at 0 can not move beyond the cage (sites shown as black dots): such dynamic localization of the vortices is termed as Aharanov-Bohm caging. (Vidal,2004)



In the presence of such localization, it becomes energetically unfavorable to condense the vortices and hence the superfluid phase persists for arbitrarily strong U and V.



Persistence of superfluidity confirmed by QMC for Kagome Lattice.

Explains the absence of S_z ordering for XXZ model on Kagome lattice at B=0 for J_x/J_z <<1.

f=2/3 or 1/3

Two well defined minima within the magnetic Brillouin zone.

$$(k_x a, \sqrt{3}/2 k_y a) = (0, \pi/3) = (2\pi/3, 2\pi/3)$$

The vortex wavefunctions at these minima are given by

$$\psi \equiv (\psi_a, \psi_b, \psi_c),\ (x,y) \equiv (3ma/2, \sqrt{3}na/2)$$

$$\psi_1 = \frac{1}{\sqrt{2}} \exp(2\pi i n/3 + i\pi m)(1,0,-1)$$

$$\psi_2 = \frac{1}{\sqrt{2}} \exp(i\pi n/3)(1,-1,0)$$

The low energy properties of the system can be described by fluctuations about these minima.

$$\Psi = \psi_1 \varphi_1 + \psi_2 \varphi_2$$

One needs to construct an effective Landau-Ginzburg theory in terms of the vortex fields, consistent with the symmetries of the underlying dice lattice.

$$T_u : \varphi_1 \to \varphi_1 \exp(-i\pi/3) \quad \varphi_2 \to \varphi_2 \exp(i\pi/3)$$

$$T_v : \varphi_1 \to \varphi_1 \exp(i\pi/3) \quad \varphi_2 \to \varphi_2 \exp(-i\pi/3)$$

$$I_x : \varphi_{1(2)} \to \varphi^*_{1(2)}$$

$$I_y : \varphi_{1(2)} \to \varphi^*_{2(1)}$$

$$R_{2\pi/3} : \varphi_{1(2)} \to \varphi_{1(2)}$$

$$R_{\pi/3} : \varphi_{1(2)} \to \varphi_{2(1)}$$

Landau-Ginzburg action

$$L = \sum_{\alpha=1,2}\left[\left|(\partial_\mu - iA_\mu)\varphi_\alpha\right|^2 + r\left|\varphi_\alpha\right|^2\right] + u\left(|\varphi_1|^4 + |\varphi_2|^4\right) + v|\varphi_1|^2|\varphi_2|^2 + w\left[(\varphi_2^*\varphi_1)^3 + \text{h.c.}\right]$$

The U(1) symmetry associated with the relative phase θ of the vortex fields is broken by the 6th order term.

The 6th order term is marginal at the tree level. Its relevance/irrelevance is not easy to determine analytically.

Possibilities for the second order phase transition

$v > 0$: $\varphi_1 = 0, \varphi_2 \neq 0$ or vice versa

Only one of the two vortex fields condense and the relative phase θ do not play a role.

$v < 0$: $\varphi_1 \neq 0, \varphi_2 \neq 0$

- $w > 0$ $\theta = \pi/3$
- $w < 0$ $\theta = 2\pi/3$

If w turns out to be irrelevant, θ becomes gapless at the critical point. Emergence of a gapless mode at the critical point.

Quantum Monte Carlo study

Measurement of superfluid density ρ_s, density structure factor S(q), static susceptibility χ(q), and bond structure factor S_b(q).

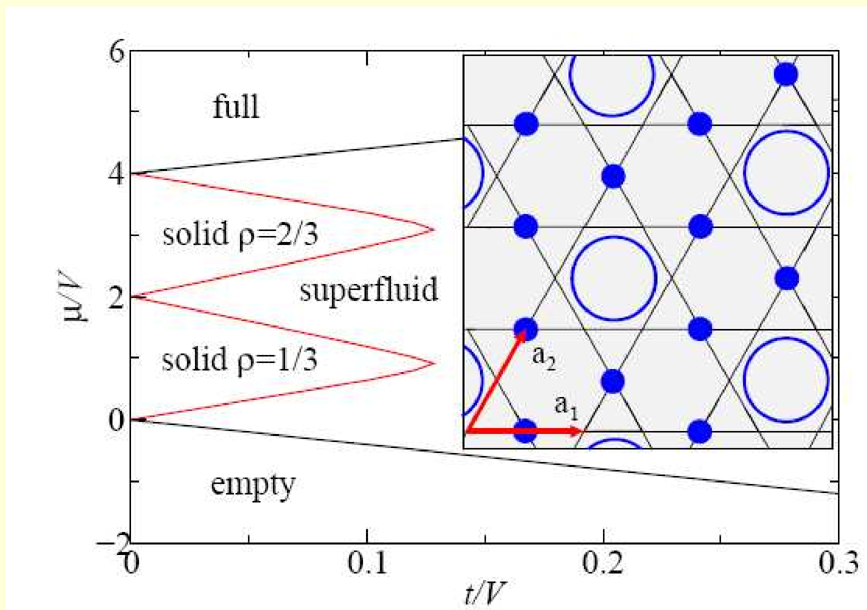
$$\rho_{q\tau} = \frac{1}{N}\sum_i \rho_{i\tau}\,\mathrm{exp}(i\mathbf{q}\cdot\mathbf{r_i})$$

$$S(\mathbf{q}) = N\langle \rho_{q\tau}\rho_{q\tau}\rangle$$

$$\chi(\mathbf{q}) = N\left\langle \int d\tau\, \rho_{q\tau}\rho_{q0}\right\rangle$$

$$S_b(\mathbf{q}) = N\left\langle B_{q\tau}B^\dagger_{q\tau}\right\rangle \quad B_{(i,j),\tau} = t(b_i^\dagger b_j + \mathrm{h.c})$$

Ground state Phase diagram



f=1/3 or 2/3

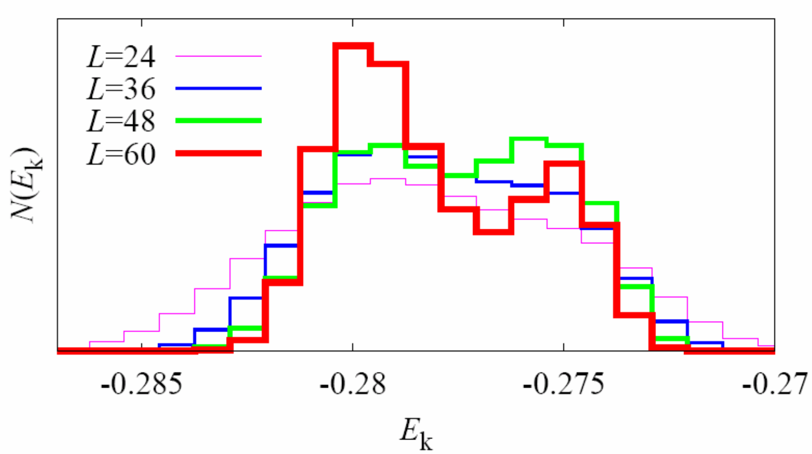
The ground state, for low t/V, is found to be comprised of resonating bosons in one third of the hexagons and localized ones in the rest. Such an R-3-3 state is also suggested as one of the competing states by duality analysis and also supported by ED studies [Kabra et al]

Peak structure of S(q) and χ(q) measured in QMC is consistent with this state.

Measurement of P_n or probability of having hexagons with n bosons is consistent with this state.

$P_{0,1,2} < 0.001$, $P_3 = 0.338$,
$P_4 = 0.38$, $P_5 = 0.225$, $P_6 = 0.052$

Sharp peak in S_b(q) confirms presence of resonating bonds.



Emergence of double-peaked structure at the critical point implies a very weak first-order transition. The transition may be second order if one sits exactly at the tip of the Mott lobe where the boson density is conserved at the transition.

RG results on relevance and irrelevance of w

$$L = \sum_{\alpha=1,2} \left[\left| (\partial_\mu - i\mathcal{A}_\mu)\varphi_\alpha \right|^2 + r\left|\varphi_\alpha\right|^2 \right] + u\left(|\varphi_1|^4 + |\varphi_2|^4\right) + v\,|\varphi_1|^2|\varphi_2|^2 + w\left[(\varphi_2^*\varphi_1)^3 + \text{h.c.} \right]$$

The critical theory consists of 2 boson fields coupled to an U(1) gauge field in 2+1 D.

→ *No reliable conventional analysis for 2+1 D and N=2.*

Halperin, Lubensky and Ma PRL 1974.
E. Brezin and J. Zinn-Justin PRL 1976
Chen, Lubensky, Nelson PRB 1978.
Balents et al. PRB 2004

↓ *So far, the only reliable means of addressing the nature of these phase transitions have been QMC: however here restricting oneself exactly at the tip of the Mott lobe is a numerically difficult task*

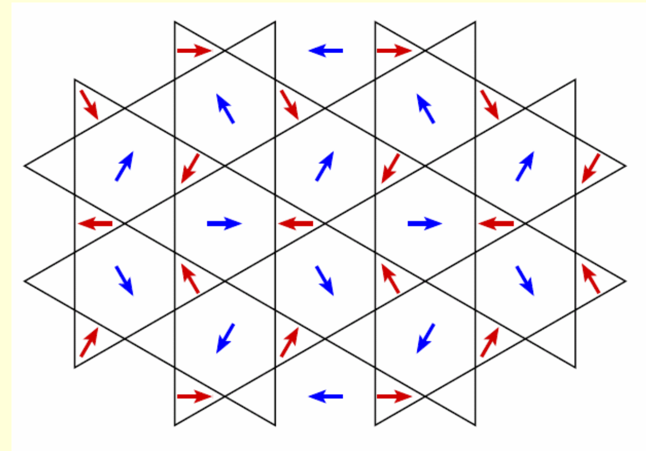
Two key issues: 1) Can there be a second order quantum phase transition at the tip of the Mott lobe for these models as predicted by recent non-LGW theories?

2) Relevance or irrelevance and sign of w [marginal at tree level] which dictates the Mott phase and presence/absence of an additional gapless mode at the QCP.

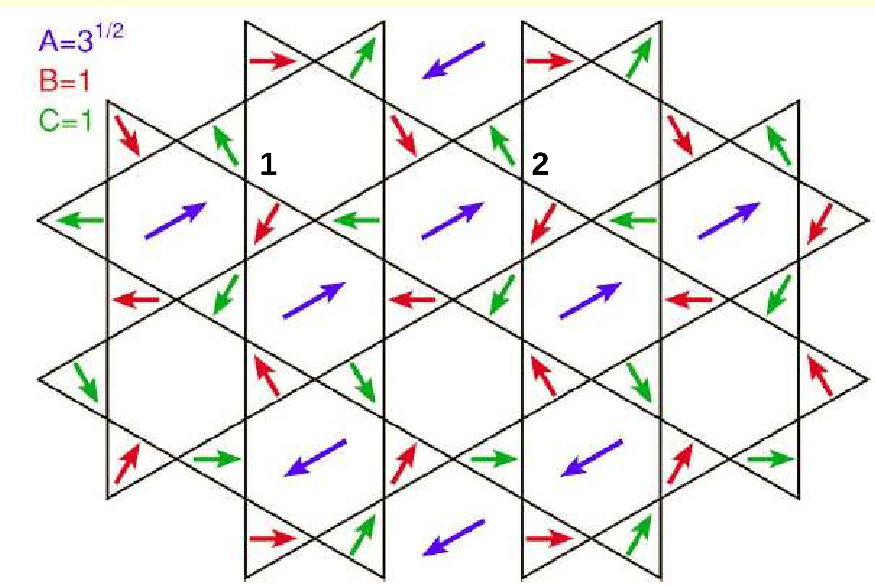
It would be interesting to see if ERG/NPRG can tackle this problem

Plot of vortex wavefunction for v>0

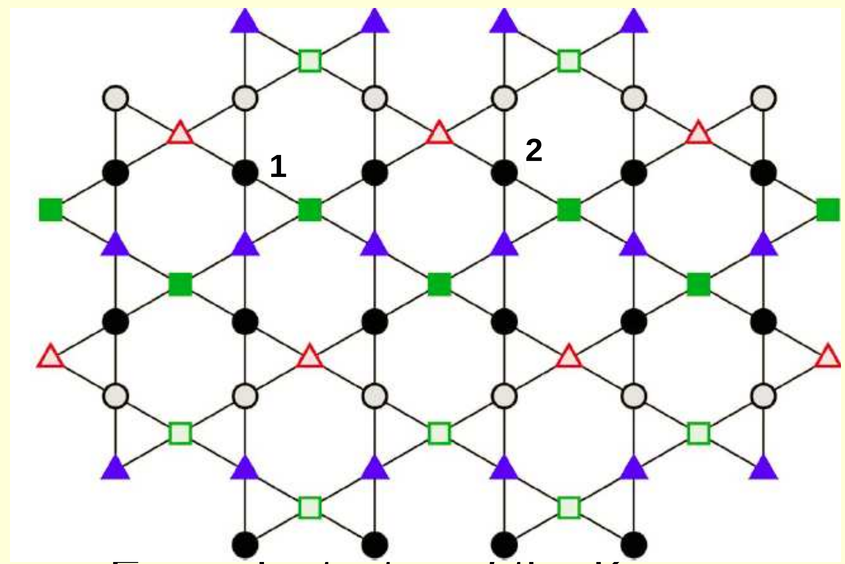
All sites on the lattice are equivalent
The Mott phase corresponds to state with equal amplitude of bosons around the up and down triangles. There is no density wave of bosons



Plot of vortex wavefunction for v<0

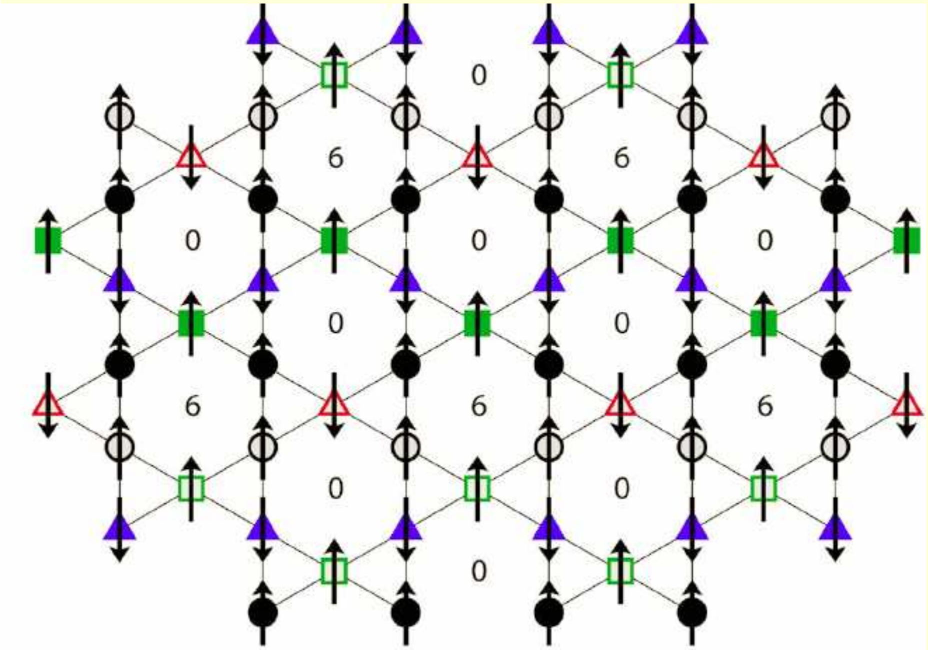


Vortex wavefunction for w>0.

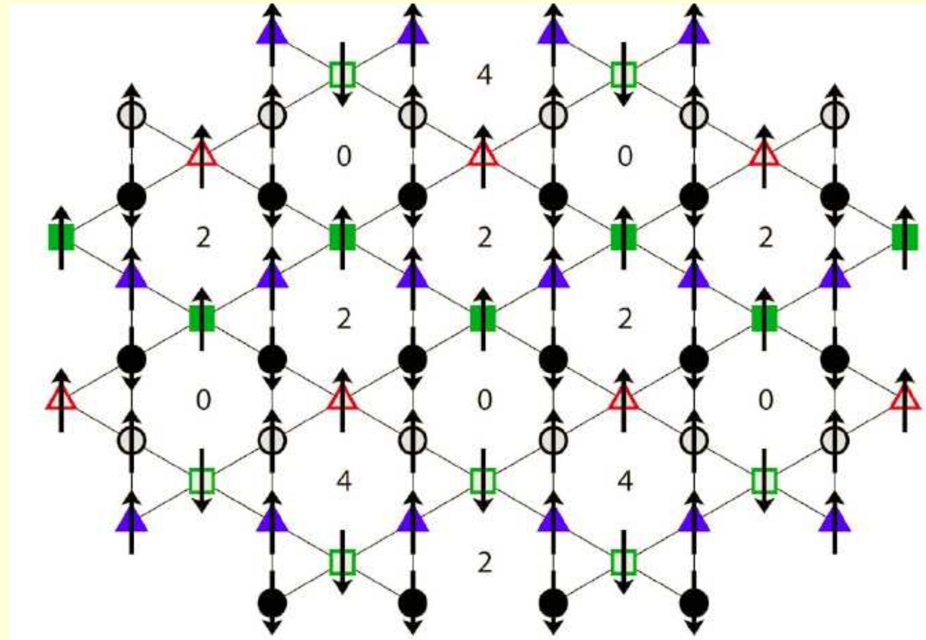


Equivalent sites of the Kagome lattice for v<0, w>0. There are six inequivalent sites.

Density wave states for v<0 at f=2/3



A possible 3 by 3 order predicted by the vortex theory at f=2/3.



More complicated 9 by 9 order (full ordering pattern not shown)

Note that the spins on black and green sites can be flipped. This does not change the filling, but switches 2->4 and makes the hexagon marked 0 a resonating one.

Expect quantum fluctuations to cause partially resonating state with a R-3-3 pattern.

Appendix A: Hopfstadter Equations on dice lattice

$$\epsilon\psi_A(x,\kappa) = \psi_B(x+a) + \psi_C(x-a) + 2\cos\left[\frac{\gamma}{a}(x-a/4)+\kappa\right]\psi_B(x-a/2) + 2\cos\left[\frac{\gamma}{a}(x+a/4)+\kappa\right]\psi_C(x+a/2),$$

$$\gamma = 2\pi f = 2\pi\phi/\phi_0$$

$$\kappa = \sqrt{3}k_y a/2$$

$$\epsilon\psi_B(x,\kappa) = \psi_A(x-a) + 2\cos\left[\frac{\gamma}{a}(x+a/4)+\kappa\right]\psi_A(x+a/2),$$

$$\epsilon\psi_C(x,\kappa) = \psi_A(x-a) + 2\cos\left[\frac{\gamma}{a}(x-a/4)+\kappa\right]\psi_A(x-a/2),$$

Closed equation for non-zero energies involving a single sublattice

$$\psi_A(x=3ma/2,\kappa) \equiv \psi_A(m,\kappa)$$

$$\left(\frac{\epsilon^2-6}{2\cos(\gamma/2)}\right)\psi_A(m,\kappa) = 2\cos(3\gamma m+2\kappa)\psi_A(m,\kappa) + 2\cos\left[\frac{3\gamma}{2}\left(m-\tfrac{1}{2}\right)+\kappa\right]\psi_A(m-1,\kappa) + 2\cos\left[\frac{3\gamma}{2}\left(m+\tfrac{1}{2}\right)+\kappa\right]\psi_A(m+1,\kappa),$$

App. B: Symmetry transformation of wavefunctions on a dice lattice

$$T_{\alpha=u,v}\colon\ \psi(x,y) \rightarrow \psi(x-\alpha_x, y-\alpha_y)\,\omega^{\alpha_x y 2/\sqrt{3}}$$

$$I_x\colon\ \psi(x,y) \rightarrow \psi^*(x,-y),$$

$$R_{\pi/3}\colon\ \psi_A(x,y) \rightarrow \psi_A([x+\sqrt{3}y]/2,[y-\sqrt{3}x]/2) \times \omega^{[(y^2-x^2)/4+\sqrt{3}xy/2]},$$

$$\psi_B(x,y) \rightarrow \psi_C([x+\sqrt{3}y]/2,[y-\sqrt{3}x]/2)\,\omega^{[(y^2-x^2)/4+\sqrt{3}xy/2]},$$

$$\psi_C(x,y) \rightarrow \psi_B([x+\sqrt{3}y]/2,[y-\sqrt{3}x]/2)\,\omega^{[(y^2-x^2)/4+\sqrt{3}xy/2]},$$

$\mathbf{u}=(3a/2,\sqrt{3}a/2)$ and $\mathbf{v}=(3a/2,-\sqrt{3}a/2)$