Kagome lattice structures with charge degrees of freedom

Aroon O'Brien

Max Planck Institute for the Physics of Complex Systems, Dresden

Frank Pollmann, *University of California, Berkeley*

Masaaki Nakamura, *MPI-PKS, Dresden*

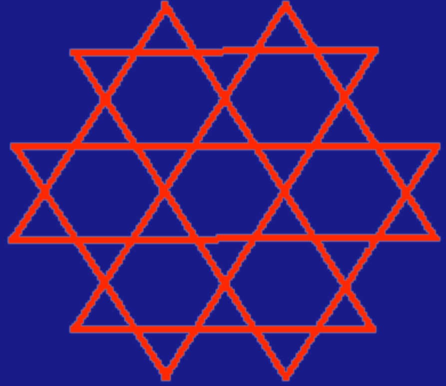
Peter Fulde, *MPI-PKS, Dresden, Asian Pacific Center for the Theoretical Physics, Pohang*

Michael Schreiber, *TU Chemnitz*

NTZ CompPhys08, Nov28 2008

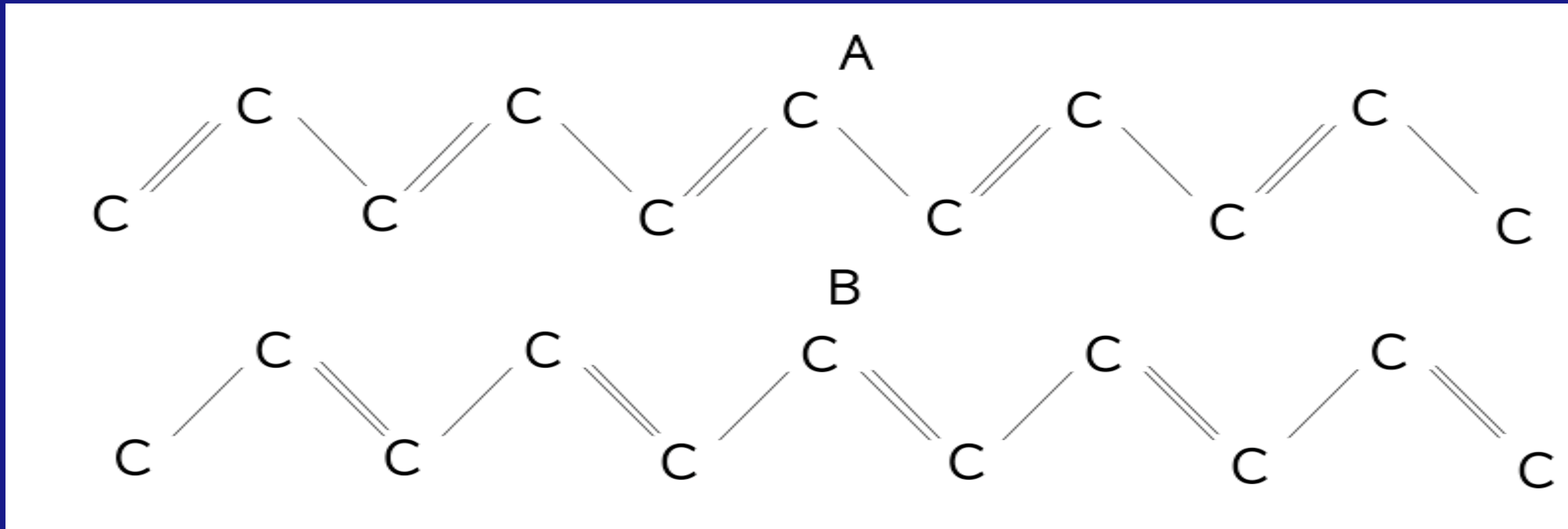
Outline

- Introduction-Frustration and Fractionalization
- A theoretical model of frustration
- Analysing the model
- Current approaches and Outlook



Fractionalization

- First theoretical model supporting fractional excitations-spin-charge separation in polyacetylene molecules [1,2]
- Ground state - idealized chain molecule:



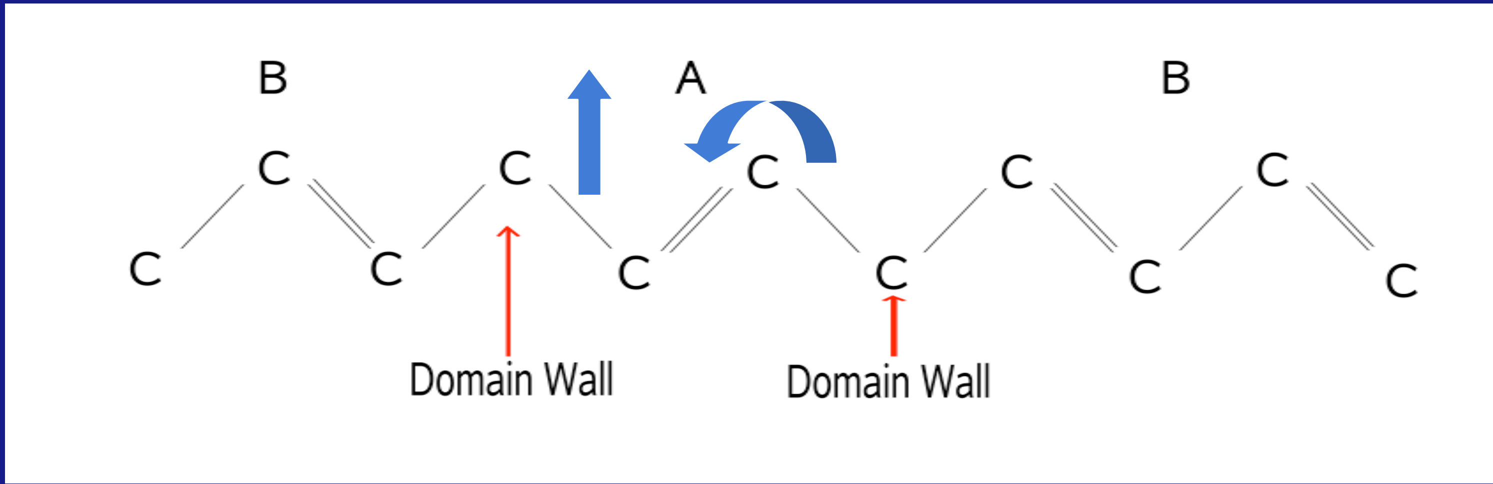
- A bond (= -2e) is removed from either ground state - we obtain two defects both with charge +e and spin 0 (spin charge-separation):

One excitation-decays into two collective excitations

[1]W.P.Su,J.R.Schrieffer, and A.J.Heeger,Phys.Rev.Lett.,v**42**,p1968,1979.
[2]W.P.Su and J.R. Schrieffer, Phys. Rev. Lett.,v**46,**p738,1981.

Fractionalization

- Similarly - removed bond would with charge -e would give rise to fractional charges with charge e/2+!



- Similarly - add/remove one charged particles on a frustrated lattice - gives two fractionally charged excitations

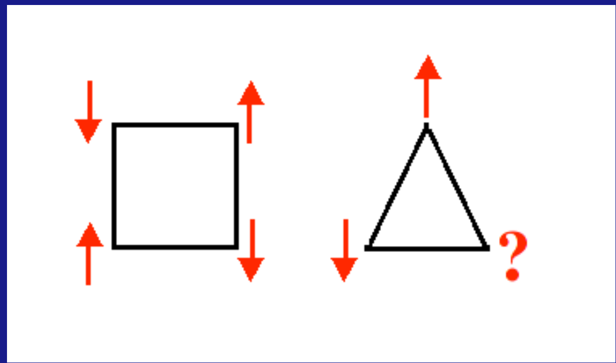
One excitation-decays into two collective excitations

- Fractionalization-observed experimentally in **Fractional Quantum Hall Effect** [3]

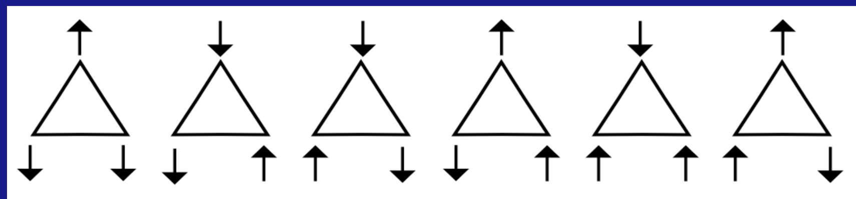
[1]W.P.Su,J.R.Schrieffer, and A.J.Heeger,Phys.Rev.Lett.,v**42**,p1968,1979.
[2]W.P.Su and J.R. Schrieffer, Phys. Rev. Lett.,v**46**,p738,1981.
[3]D.C.Tsui,H.L.Stormer, and A.C.Gossard, Phys.Rev.Lett. 53, 722-723(1984)

Geometric Frustration

- Fractional charges -arise also in theoretical models of **geometrically frustrated systems** [1]
- Occur in lattice structures where it is impossible to minimize the energy of all local interactions:



- Characterised by a **macroscopic ground-state degeneracy**-> high density of low-lying excitations:



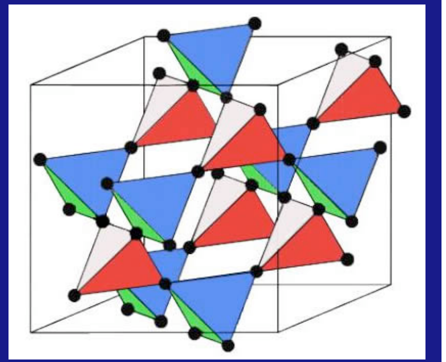
[1] P.Fulde,K.Penc,N.Shannon,Ann.Phys.,v**11,892(2002)**

Geometric Frustration in nature

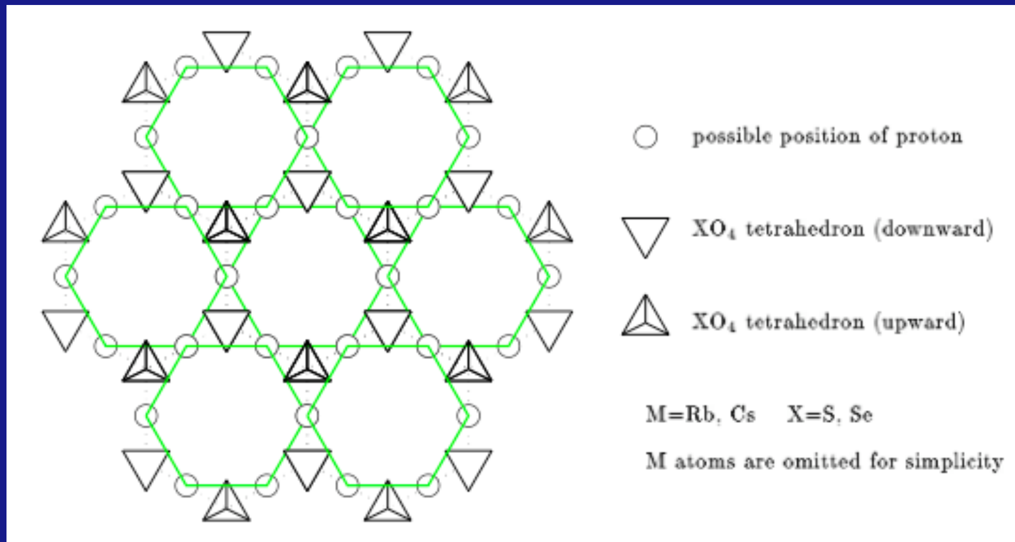
- Spinel minerals form **pyrochlore** structures:

"Samarian Spinel"
(Iranian Crown Jewels)

Spinel structure AB_2X_4
B sites form a pyrochlore lattice



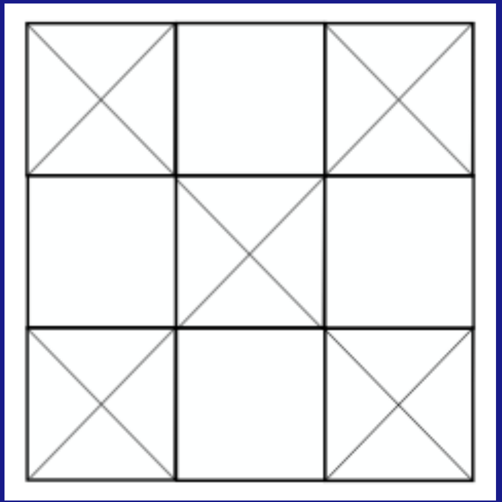
- M_3 $H(XO_4)$ forms a **kagome lattice** structure:



Fractionalised charges due to geometrical frustration

What we know already…

- There are models of 2D lattice structures supporting fractional excitations [5].
- These approaches so far yield fractional excitations that are confined [6].
- 3D lattices have been shown to support deconfined phases[7,8]



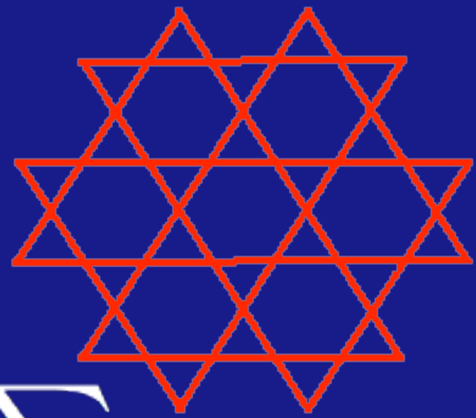
[5]P.Fulde, K.Penc, N. Shannon, Ann. Phys.,v**11**,892 (2002).
[6]F.Pollmann and P.Fulde, Europhys Lett.,v**75**,133 (2006)
[7]Bergmann, G. Fiete, and L.Balents, Phys. Rev. Lett. v**96** (2006)
[8]Olga Sikora et. Al, to be published

Fractionalised charges due to geometrical frustration

What we would like to know…!

- Kagome lattice models-can we investigate the dynamics of systems exhibiting charge fractionalization? Can we determine the **confinement/deconfinement** of the excitations?
- Do these fractionalized excitations exhibit **fractionalised statistics**? What are they?
- Can we use such models to **explain** **experimental observations** in real materials with such structures?

A model of fractionalization



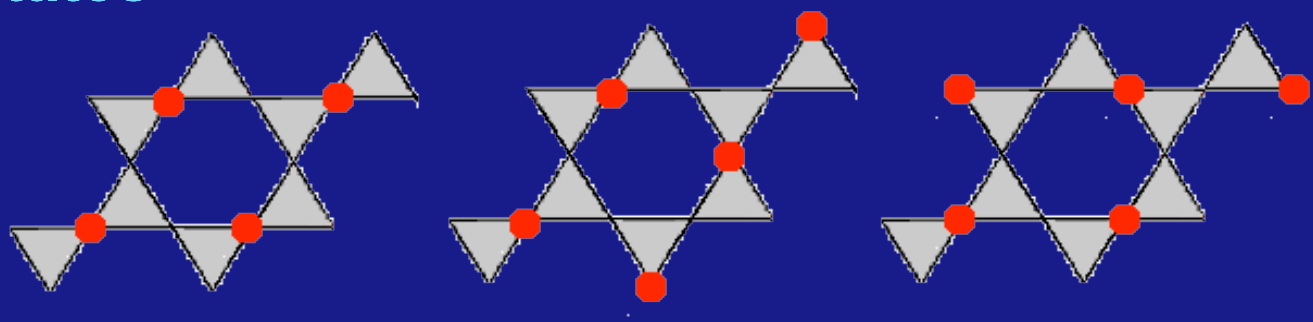
- Consider a model of **spinless fermions** on the kagome lattice

- Extended Hubbard model with **charge degrees of freedom**

$$H = -t \sum_{<i,j>} (c_i^\dagger c_j + H.c.) + V \sum_{<i,j>} n_i n_j$$

- Consider **1/3 filling**

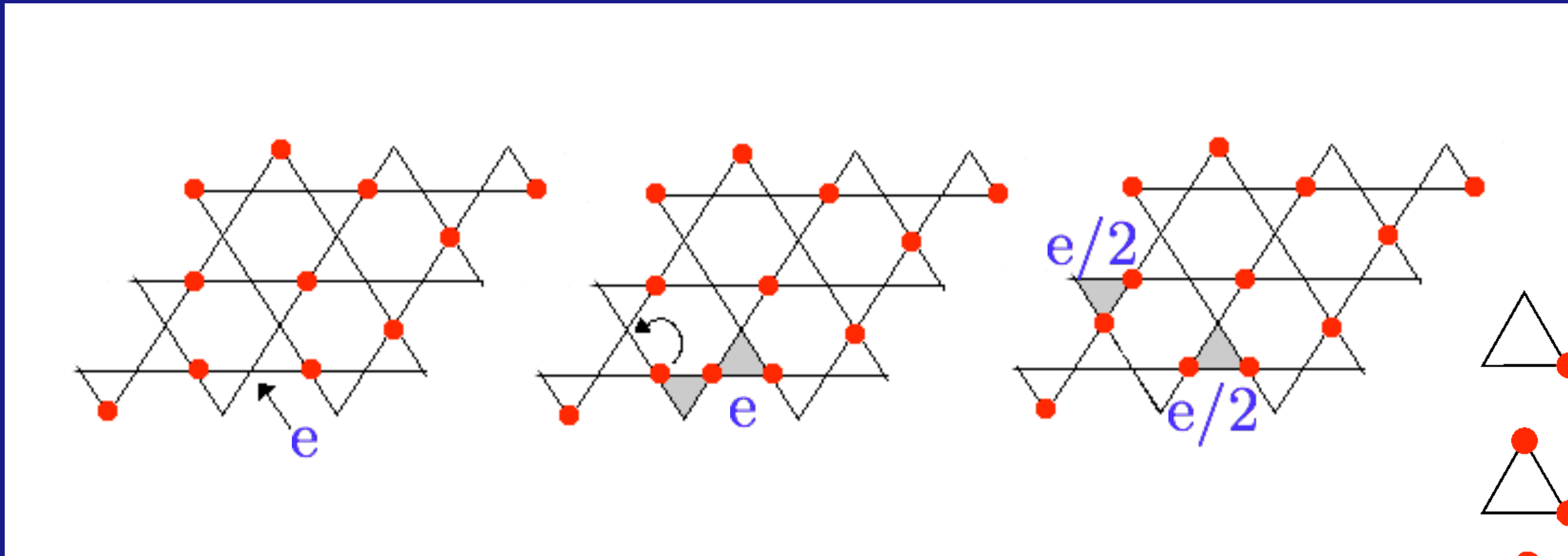
- At t=0, V>0, **macroscopic number of ground states**

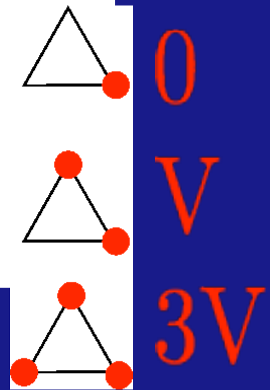


A model of fractionalization

- **Strong correlation limit** (large nearest-neighbour repulsions *V*) -> **local constraint** of 1 particle per triangle on the lattice -> **"triangle rule"**
- Finite hopping of fractional charges in strongly correlated limit where $0 < |t| \ll V$
- Add one particle -> increase system energy by $2V$

A model of fractionalization





- One particle with charge e is added to the system - it can decay into two defects each carrying the charge e/2 -> **2 fractional charges are created**

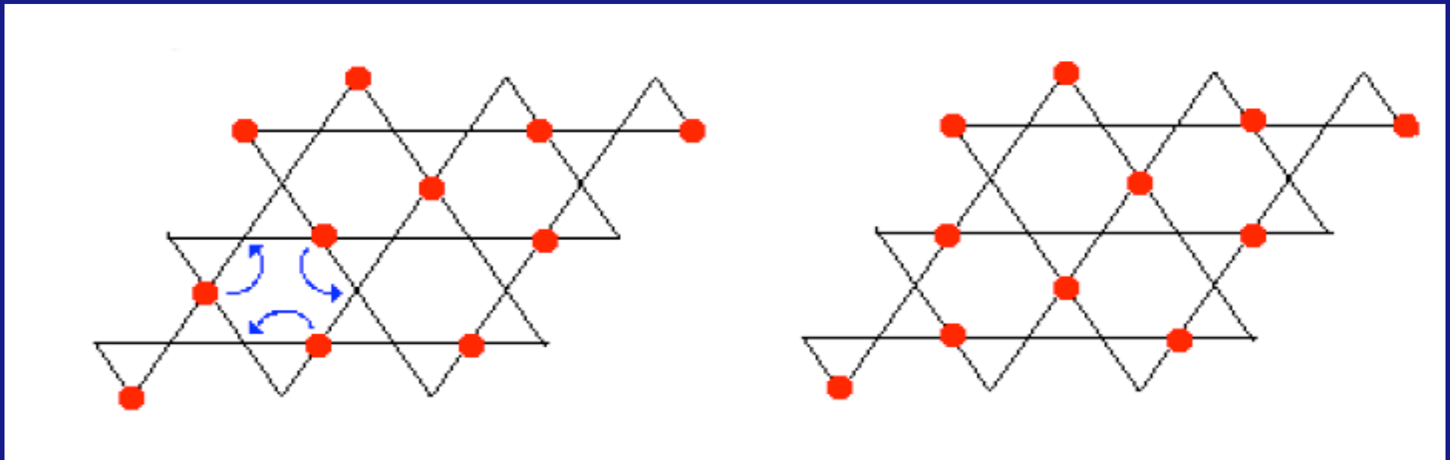
One excitation-decays into two collective excitations

A model of fractionalization

- Large Hilbert space sizes -> limit numerical investigation

Derive an **effective model Hamiltonian** encapsulating behaviour in the strong correlation limit

- Lowest order hopping process lifting degeneracy - **particle hopping around hexagons**:

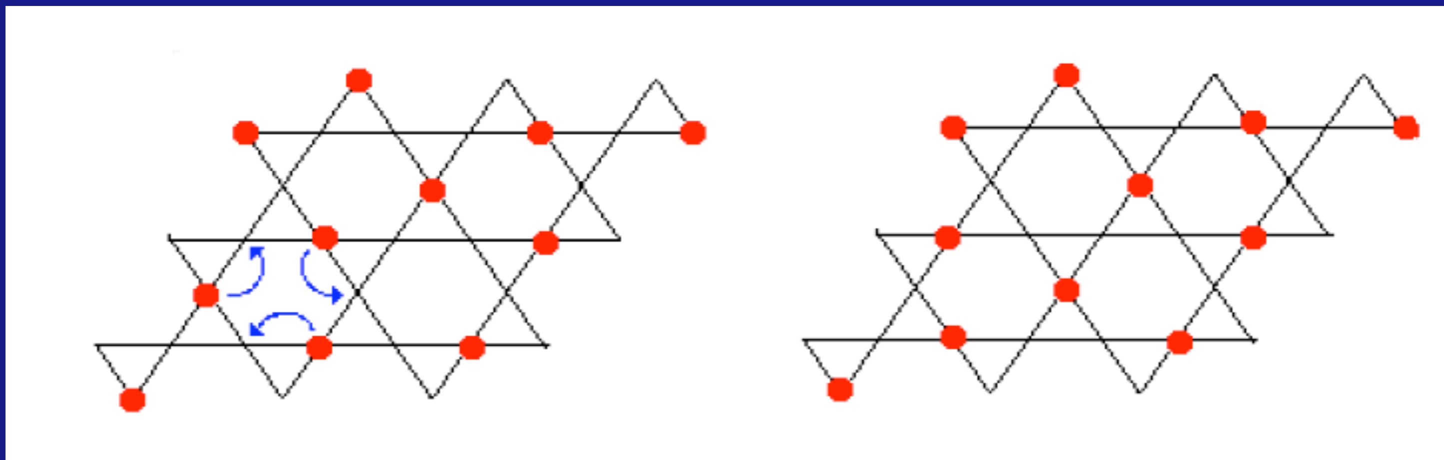


A model of fractionalization

$$H = -t \sum_{<i,j>} (c_i^\dagger c_j + H.c.) + V \sum_{<i,j>} n_i n_j$$

$$H_{eff} = -g \sum_{\langle \hexagon \rangle} \left(| \hexagon \rangle \langle \hexagon | + H.c. \right)$$

Where g = $12t^3/V^2$



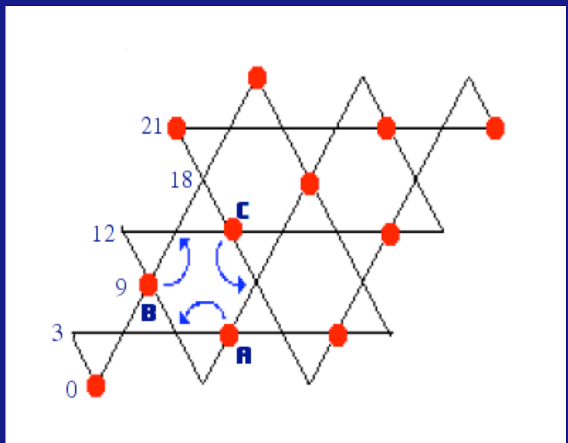
Effective model…

- Exact in the limit of infinitely large V
- Reduces drastically Hilbert space size

Example: No. of configurations for a 147-site cluster at 1/3 filling: $\binom{147}{49} \sim 10^{39}$

No. of configurations for a 147-site cluster at 1/3 filling subject to the triangle rule: $\sim 10^{11}$

- Has no fermionic sign problem!

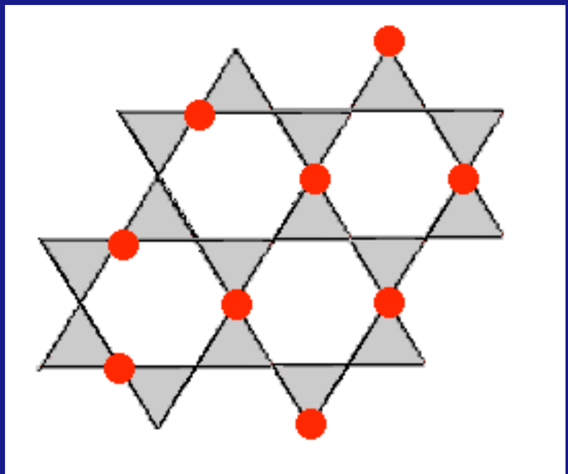


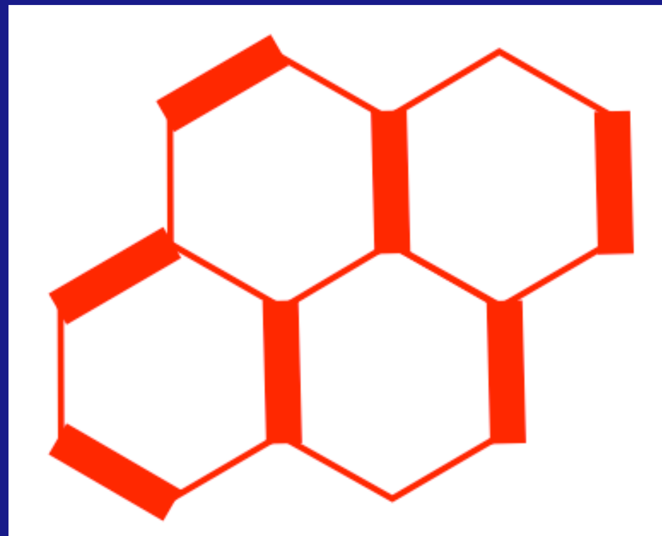
$$\langle final | \text{⬡} \rangle \langle \text{⬡} | initial \rangle \to -1$$

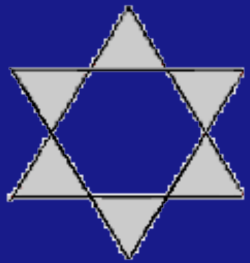
Effective model…

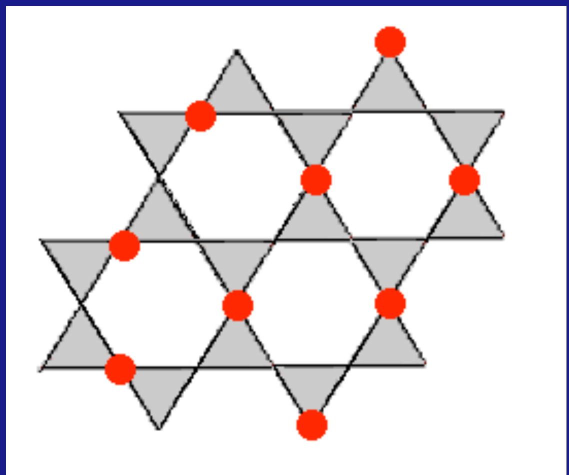
- Is equivalent to a hard-core bosonic model!
- Can be mapped to a Quantum Dimer Model!

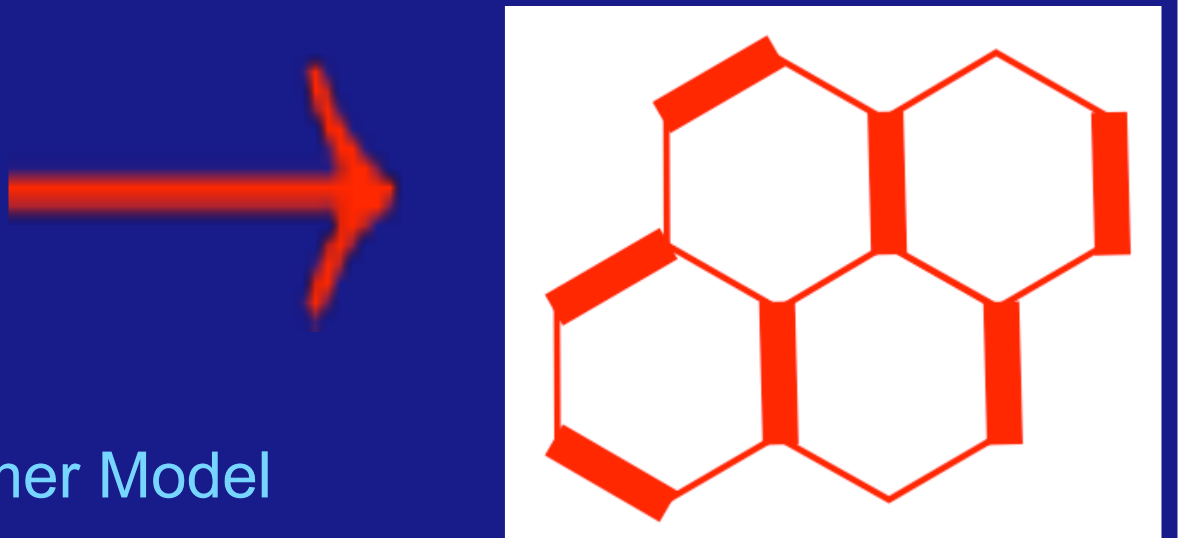
-> kagome lattice model at 1/3 filling maps to honeycomb dimer covering



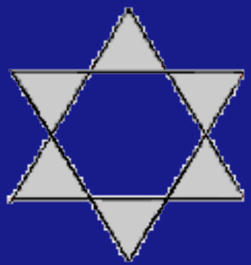


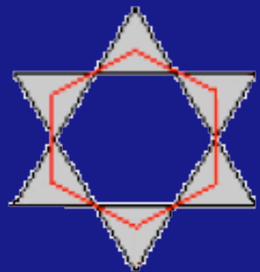


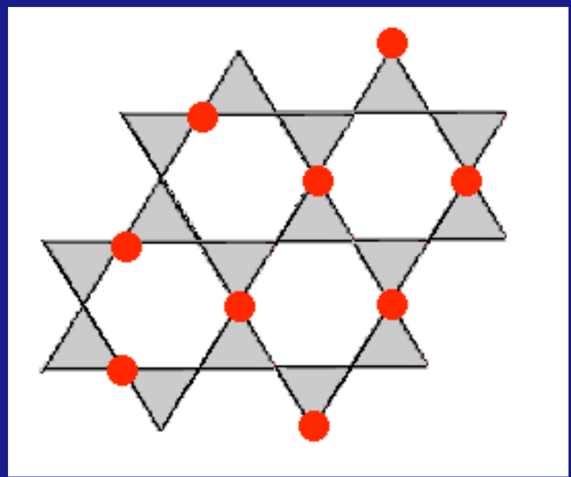




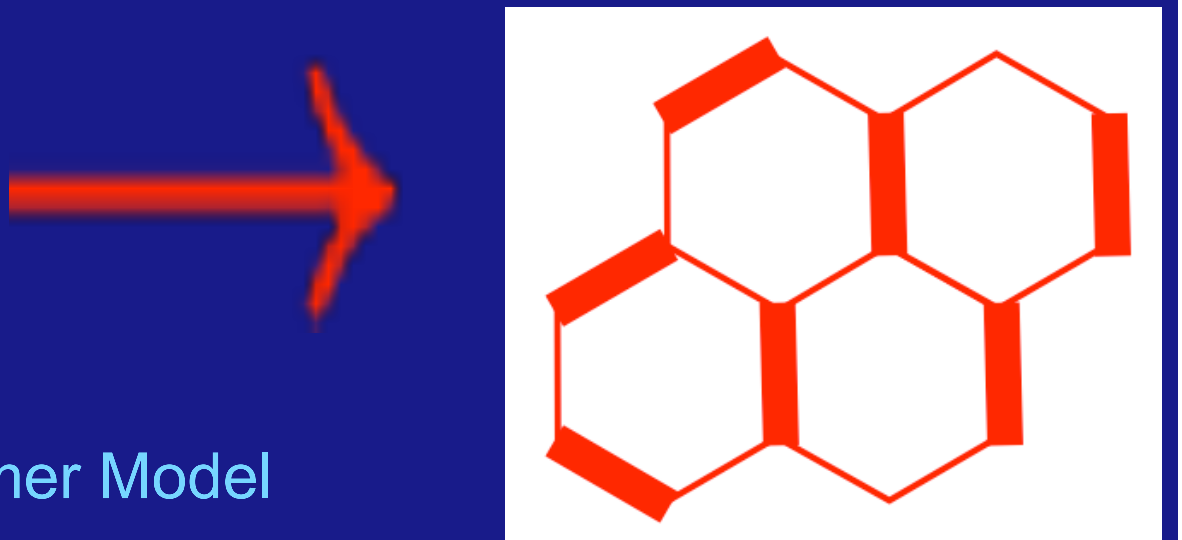
Mapping to Quantum Dimer Model

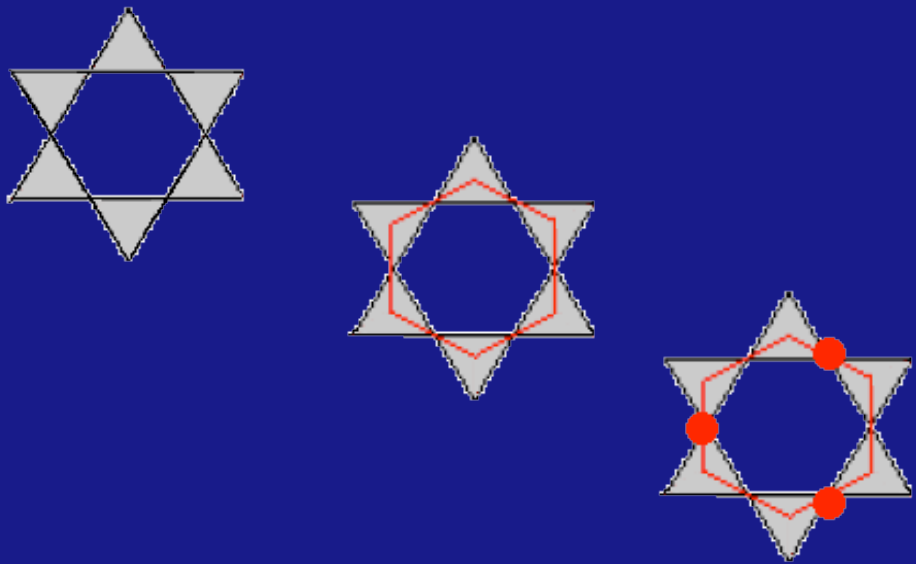


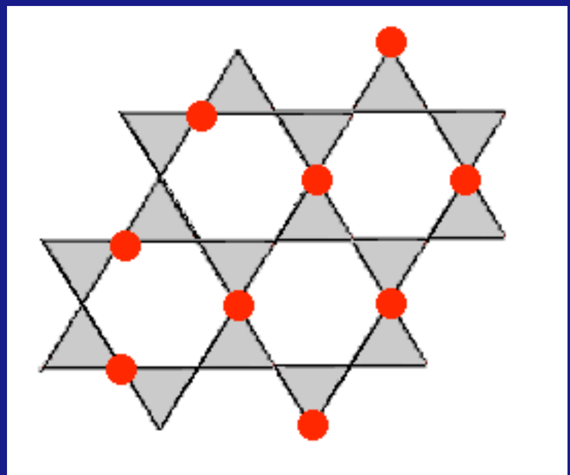


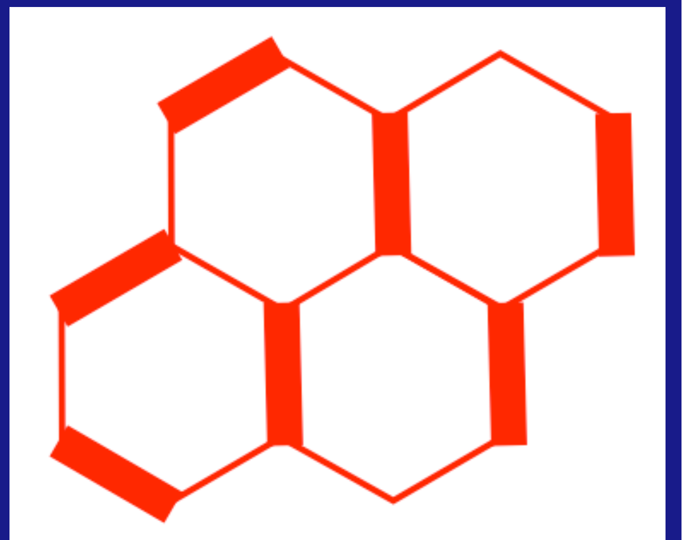


Mapping to Quantum Dimer Model

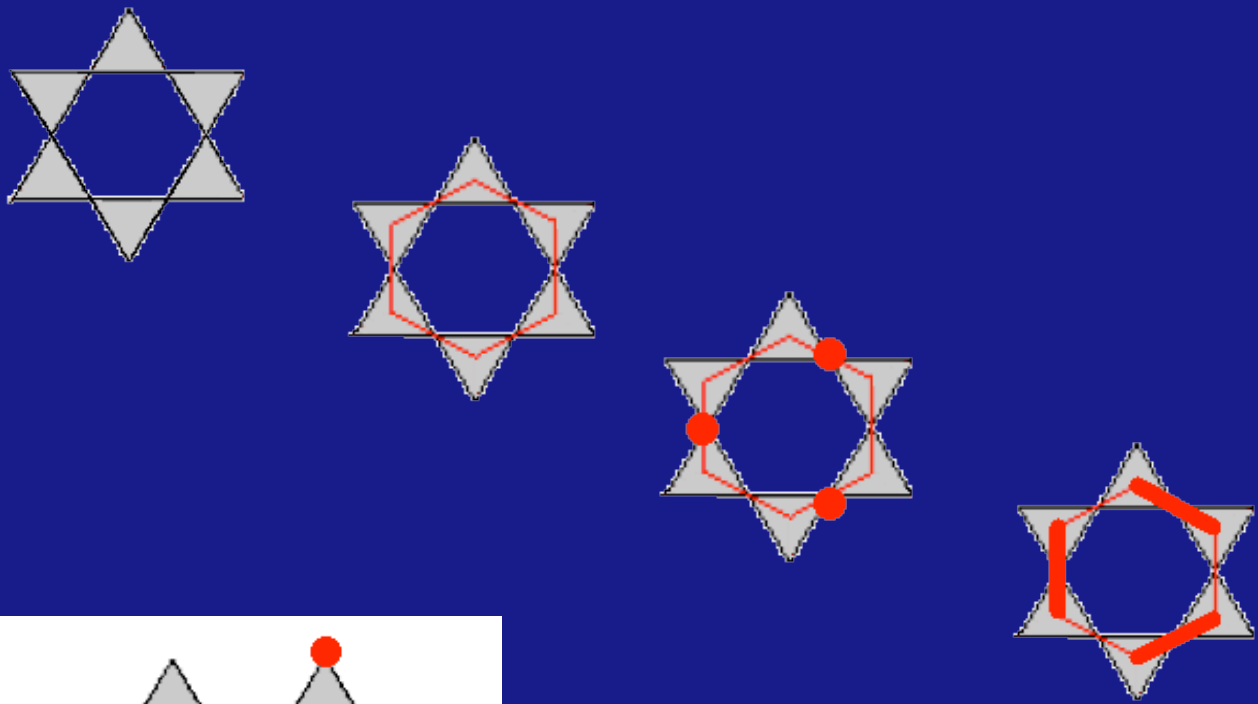


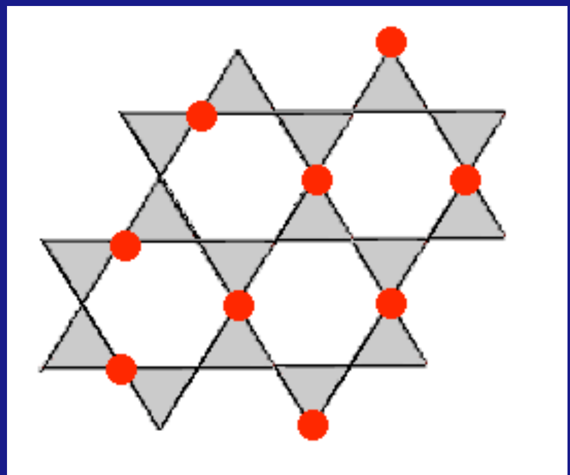


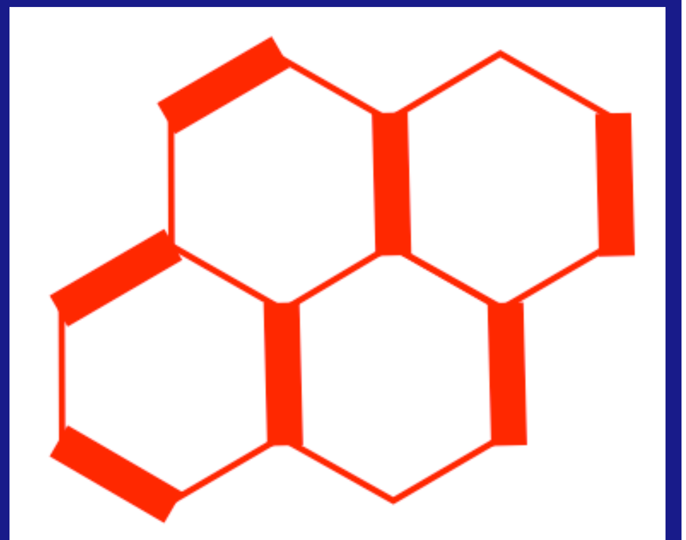




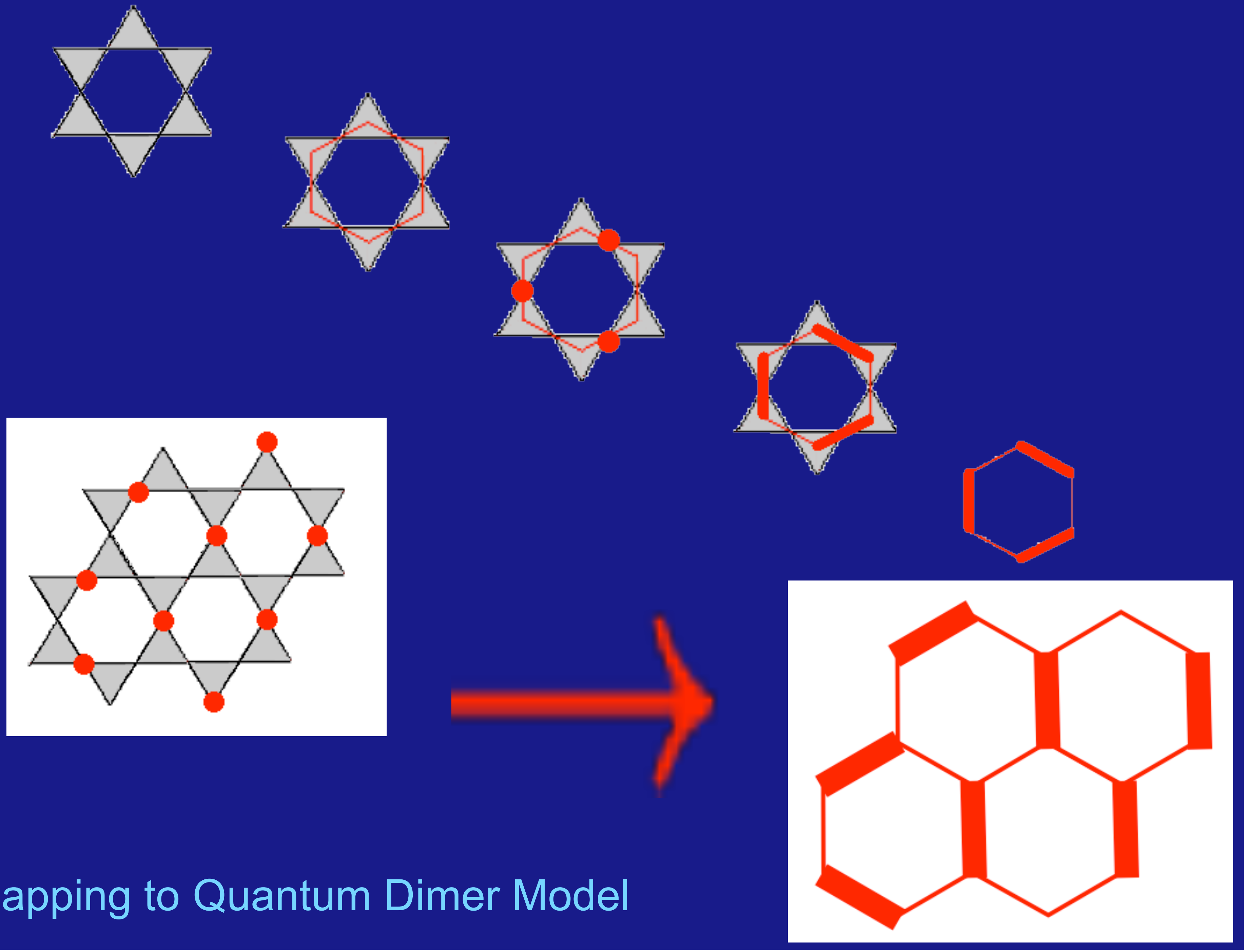
Mapping to Quantum Dimer Model







Mapping to Quantum Dimer Model



Mapping to Quantum Dimer Model

Quantum Dimer Mapping

- Mapping-effective Hamiltonian to 'plaquette phase' (mu=0) of known system [8]:

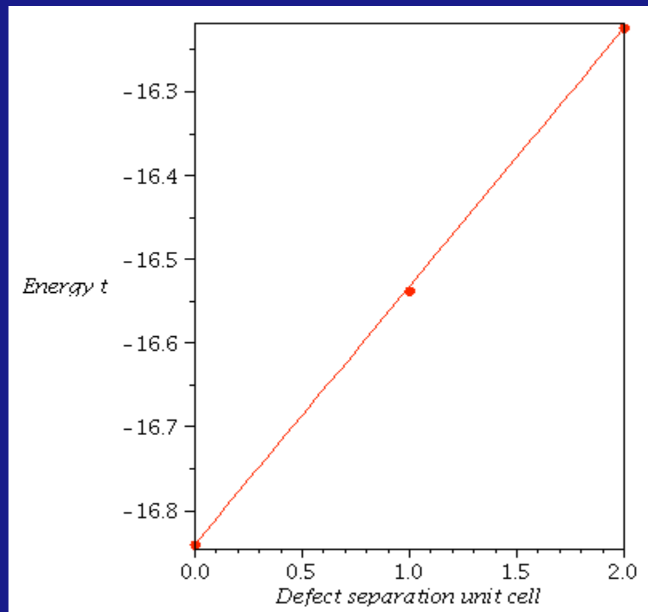
$$H_{QDM} = \sum_{\langle \text{⬡} \rangle} -g(|\text{⬡}\rangle\langle\text{⬡}| + H.c) + \mu(|\text{⬡}\rangle\langle\text{⬡}| + |\text{⬡}\rangle\langle\text{⬡}|)$$

→ Fractional charges confined

→ Numerically confirmed - exact diagonalisation gives ground-states energies

→ Distance between defects 1/# flippable hexagons

Ground-state energies for a 147-site kagome lattice model



[8] R. Moessner, S.L.Sondhi,P.Chandra, Phys.Rev.Lett.53,722-723 (2001)

Investigating dynamical properties…

- With a 'doped system'-consider dynamical properties - add extra term to Hamiltonian

Projected hopping operator

Original effective Hamiltonian

$$H_{doped} = H_{eff} - t\sum_{i,j} P(c_i^\dagger c_j + H.c.)P$$

Describes a system at 1/3 filling +/- one particle

Numerical Methods

- Model Hamiltonian basis transformation -> Lanczos recursion method [9]
- Analyse finite clusters from 25-75 sites
- Direct insight into system dynamics- from spectral function calculations

Spectral function - $A(\mathbf{k},\omega)$ gives probability for adding (+) or removing (-) a particle with momentum k and energy to the system…

$$A(\mathbf{k},\omega) = A^{-}(\mathbf{k},\omega) + A^{+}(\mathbf{k},\omega)$$

Density of states- sum over all k - space contributions:

$$D(\omega) = \frac{1}{N_k}\sum_{\mathbf{k}} A(\mathbf{k},\omega)$$

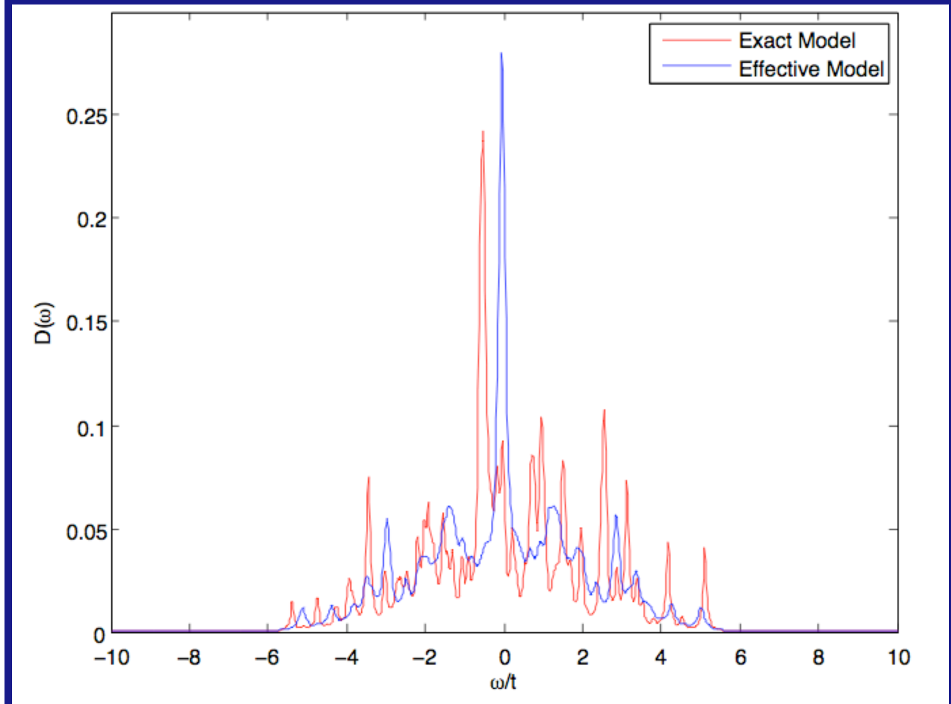
[9] C. Lanczos J. Res. Natl. Bur. Stand. **45**, 255 (1950)

How good is the model?

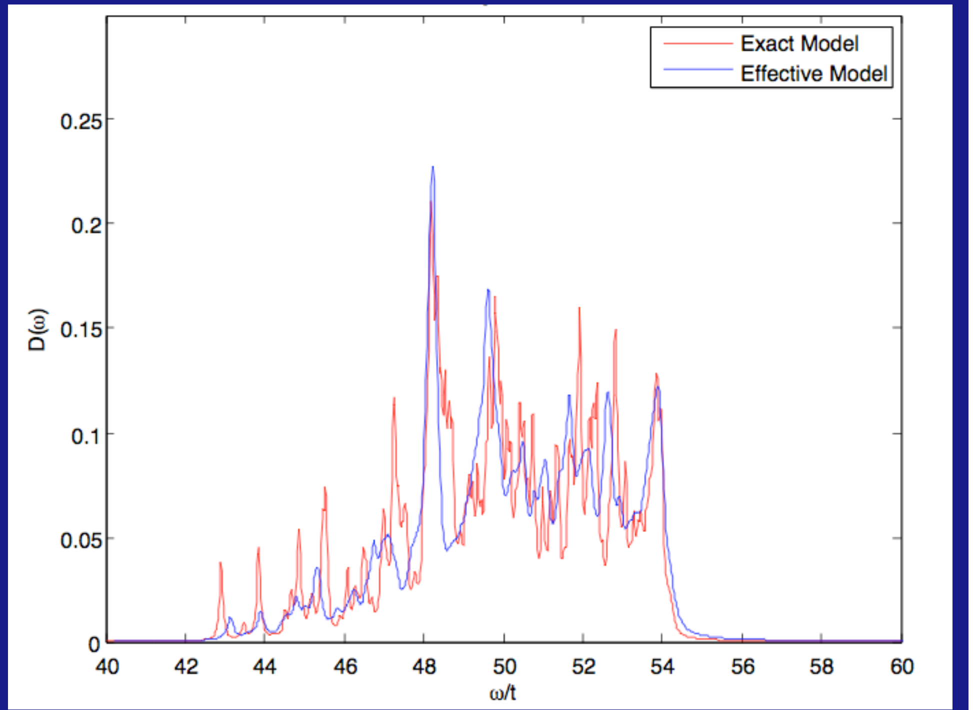
- Exact and effective models on a 27-site cluster are compared…

Density of States - a comparison

Hole contribution



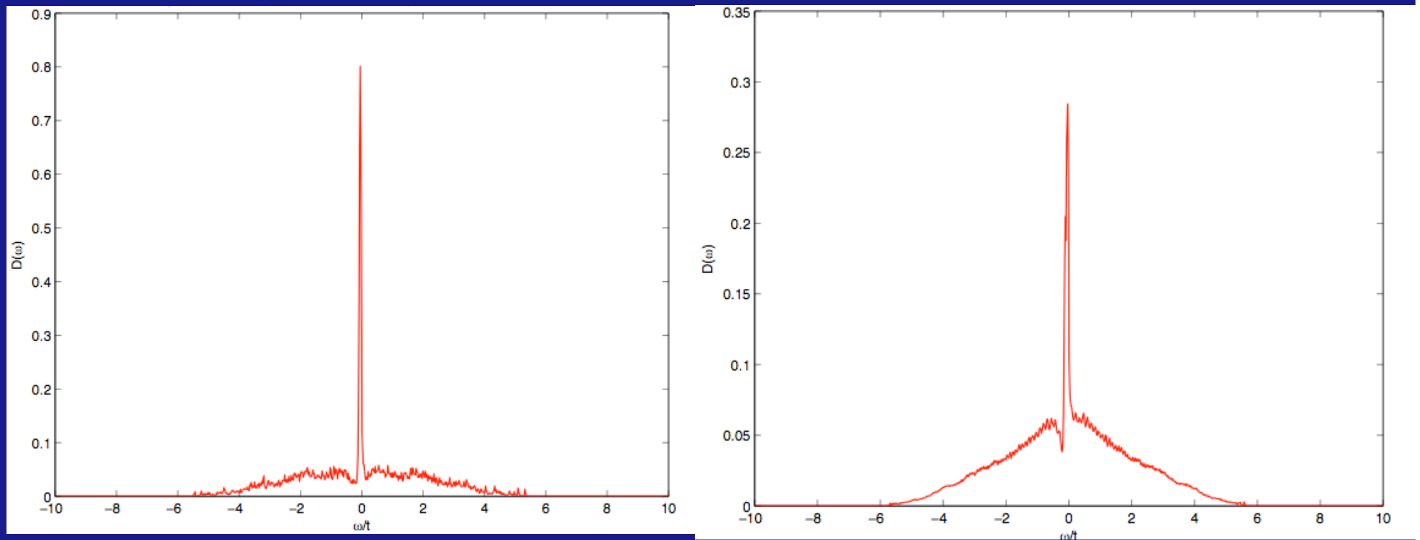
Particle contribution



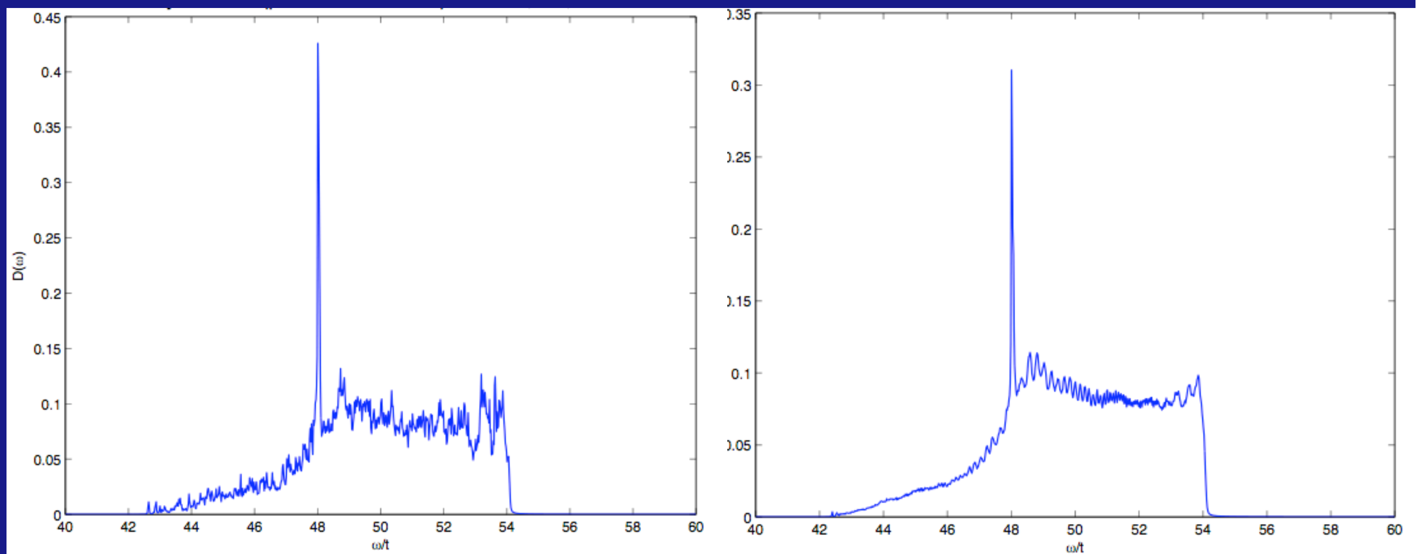
Results

48-site cluster 75-site cluster

Hole contribution



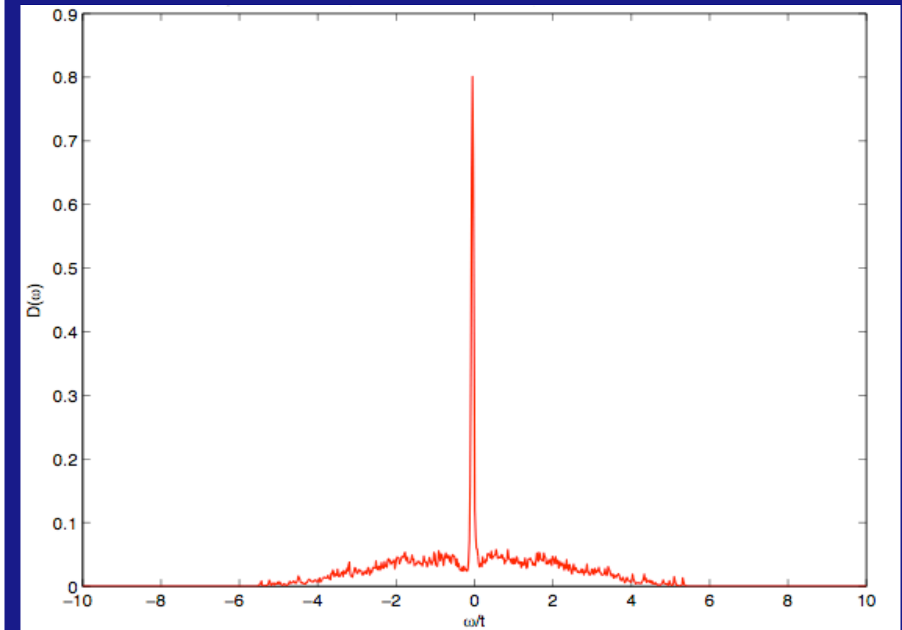
Particle contribution



Density of states figures show that finite-size effects decrease markedly with system size:

Results

- Hole contribution is symmetric; the eigenspectrum for the 1/3 filled system in the presence of one hole defect is symmetric:



Hole contribution to the density of states

⟶ Underlying **bipartiteness** for the particle hopping in the presence of one hole defect!

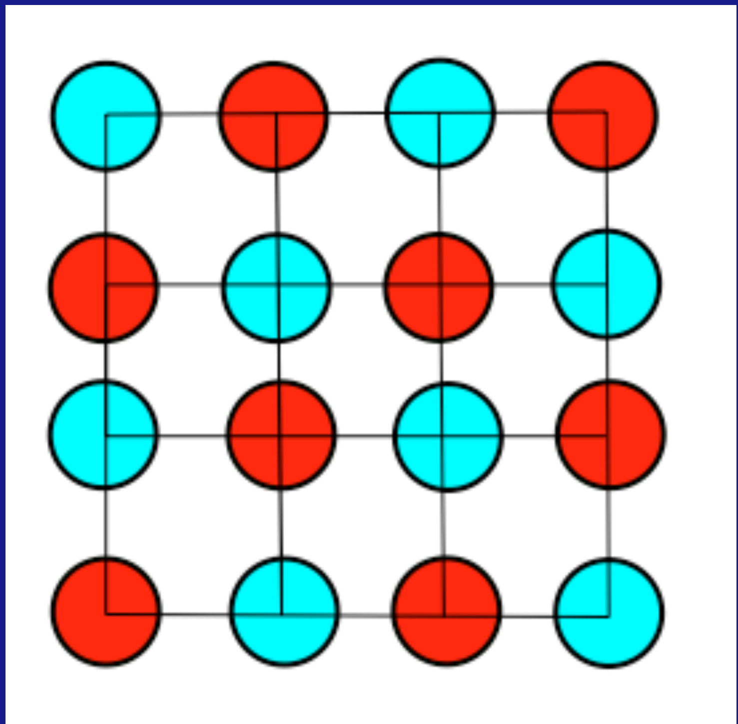
⟶ A **gauge transformation** that changes the sign of each hopping process must exist…!

Results

Eigenspectrum symmetry → **Bipartite hopping** on kagome lattice

Bipartiteness → expressible in terms of a gauge transformation

Example - 2D Square Lattice



A sites

B sites

$$|\tilde{b_i}\rangle = (-1)^{\sum_A n_i} |b_i\rangle$$

$$\Longrightarrow \quad \tilde{H}_{hop} = -H_{hop}$$

$$\Longrightarrow Eig[H_{hop}] = Eig[-H_{hop}]$$

Results

- Large peak in particle contribution - at zero momentum- full spectral weight of flat band contained in a single delta peak:

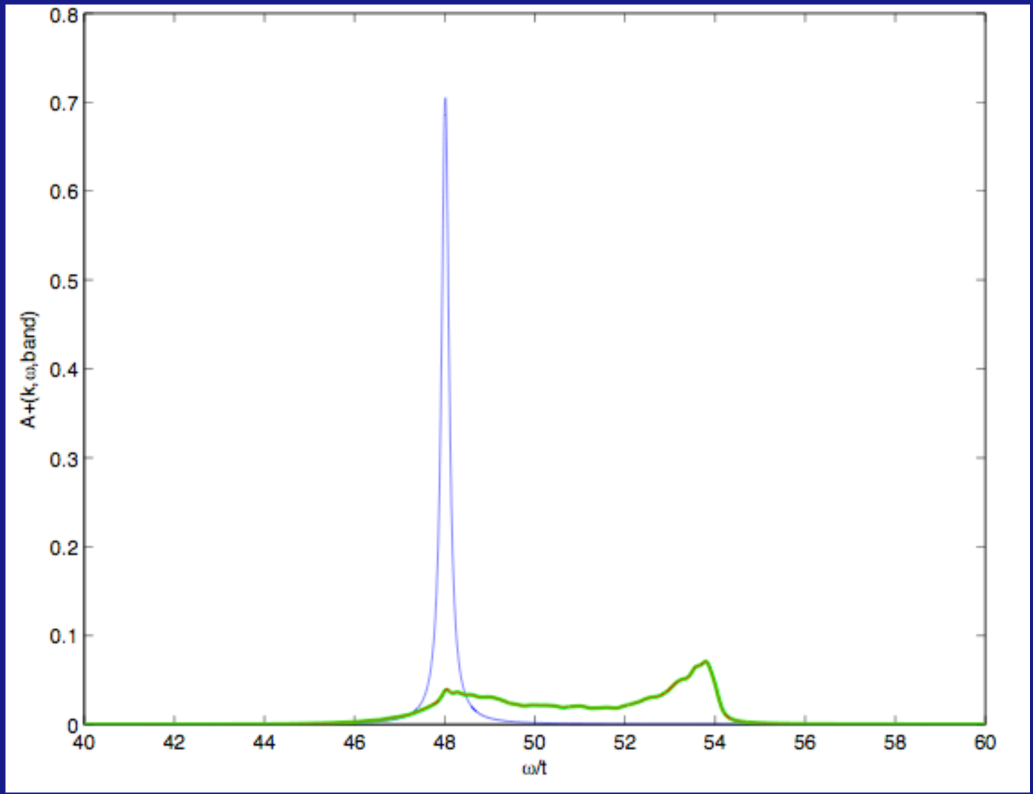
→ GS wavefunction exact eigenfunction of the $\tilde{H}|\tilde{\psi}^{N+1}\rangle = \tilde{E}|\tilde{\psi}^{N+1}\rangle$ effective Hamiltonian, in the limit of $t/V \rightarrow 0$.

→ This can be shown analytically…

$$|\tilde{\psi}^{N+1}\rangle = c^{\dagger}_{\mathbf{k}=0,\mathrm{band}\ 1}|\psi_0\rangle$$

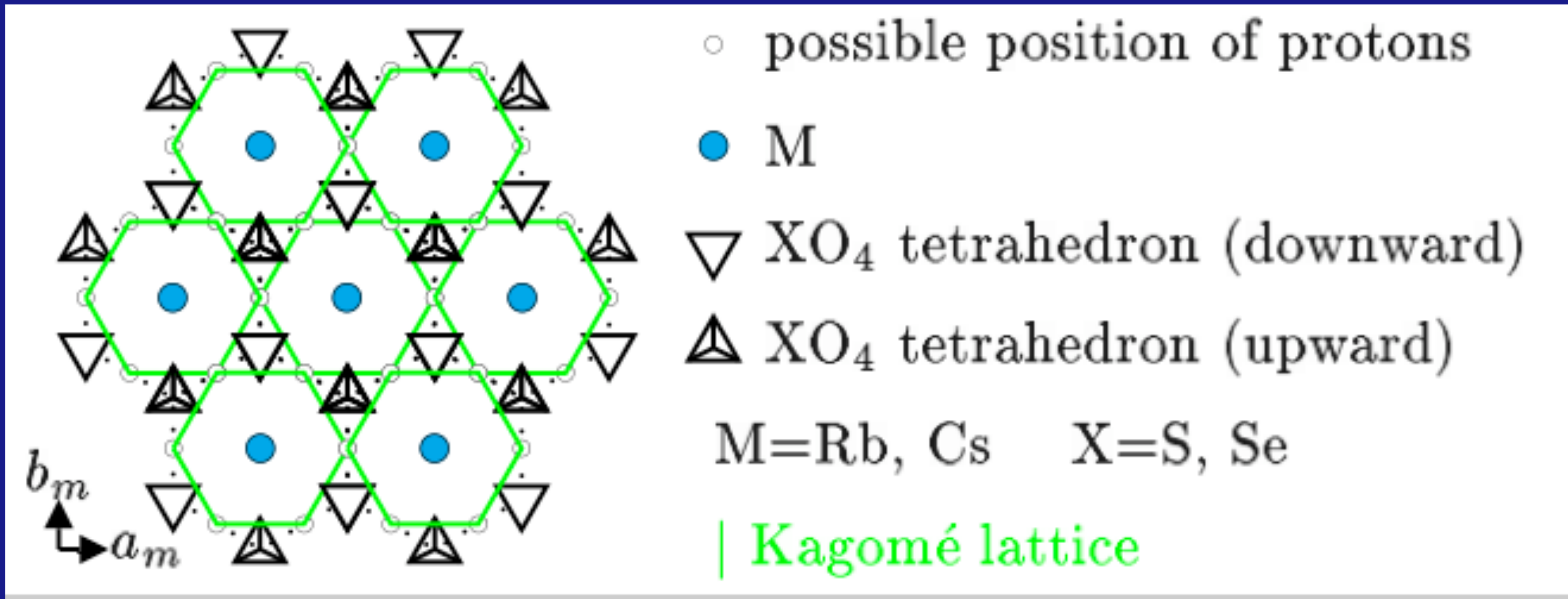
$$H|\tilde{\psi}^{N+1}\rangle = (\epsilon(\mathbf{k}=0,\mathrm{band}\ 1) + 2V + E_0)|\tilde{\psi}^{N+1}\rangle$$

Particle contribution to the spectral function for the three energy bands at **k**=(0,0), 75- site cluster



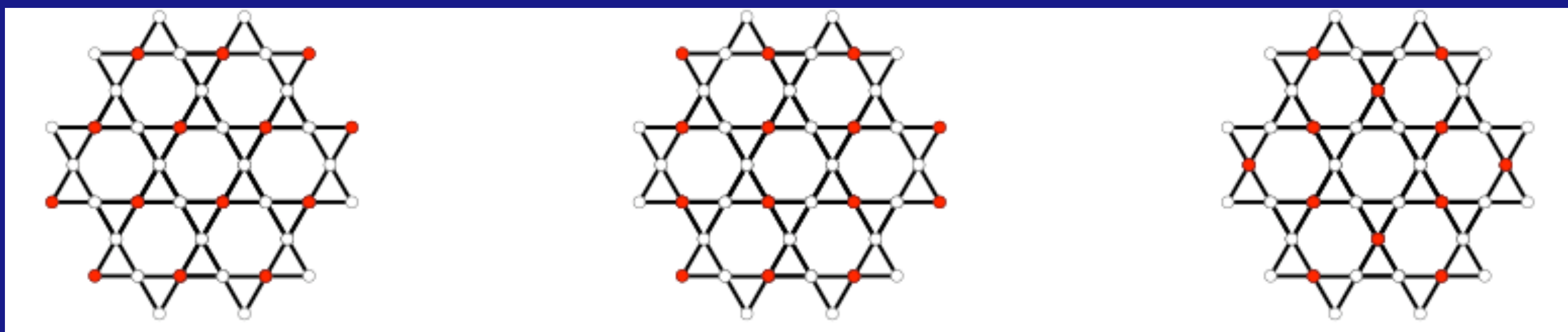
Do such models model real systems?

- Materials which may provide the answer…$MH_3(XO_4)_2$
- Here protons act as particles at 1/3 filling



Do such models model real systems?

- Model gives three possible charge-ordered states - material shows just two of these at different temperatures!
- Goal-to obtain a **phase diagram** of the model to compare with that of corresponding real materials
- Apply Random Phase Approximation to calculate charge susceptibities; calculate spectral functions in the limit of small *V*



Conclusion and Outlook

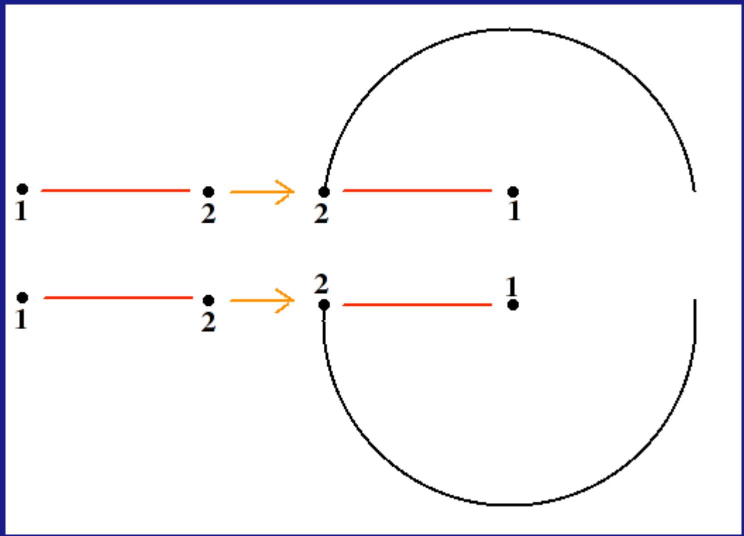
- With exact diagonalisation on finite size clusters we are able to analyse the dynamics of kagome lattice models at specific fillings
  - Understand most prominent features of spectrum - what is the physical interpretation?
  - Compare -bosonic and fermionic dynamics
  - Effective model is bipartite in nature-how can we understand this through a gauge transformation?
  - QDM mapping -> we have a confined ground state- evidence of this in the spectral function results?
- RPA treatment of Hubbard model/spectral function calculations - hope to compare the results of our theoretical model with real materials

Thank you!

Fractionalization

$\Delta\varphi = -\pi$

- Fractional excitations exhibit **fractional statistics** [a]:



$\Delta\varphi = \pi$

$$\psi(1,2) \rightarrow \psi'(1,2) = e^{i\nu\Delta\varphi}\psi(1,2)$$

3D -> **fermionic/bosonic** statistics

2D -> possibility of **anyonic** statistics!

[a]D.Arovas,J.R.Schrieffer, and F. Wilczek, Phys. Rev. Lett. 53 ,722-723 (1984)