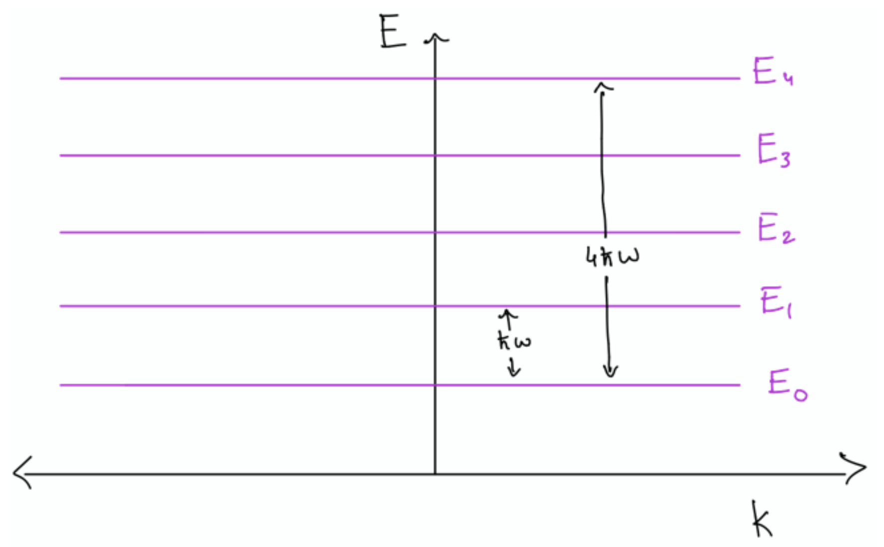
Geometric construction of Flat bands: Magnetic states

Sayantan Roy

Ohio State University

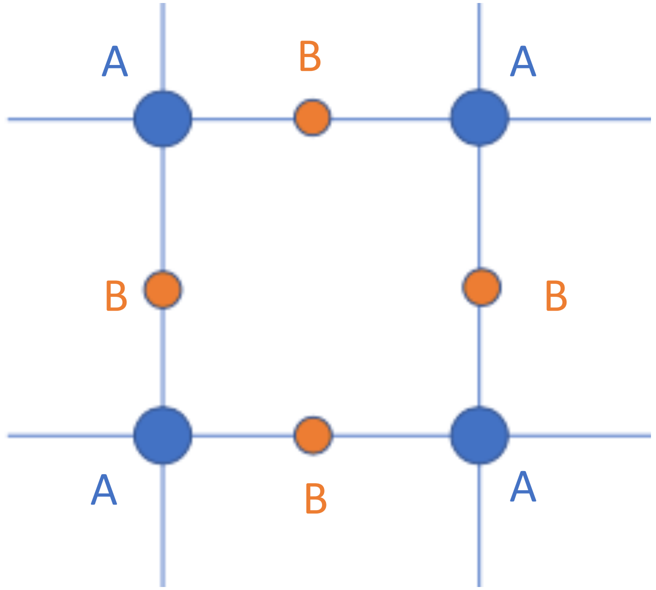
Flat bands – what are they?



- Flat bands – eigenvalues of *H(x)* are independent of *x*.
- Example – Landau level(Quantum Hall effect)
- Flat bands can be trivial(vacuum), non trivial

For translationally invariant systems, $\varepsilon(\vec{k})$ is independent of $\vec{k}$, but $|u_n(\vec{k})\rangle$ is not !

- Geometric construction of Flat bands – Lieb Lattice. Unequal number of orbitals per unit cell in a bipartite lattice



$|N_A - N_B| = 1$ One flat Band!

Geometric construction of Flat bands

- Proof of existence of flat bands - If A and B form bipartite structure, Hamiltonian is of the form

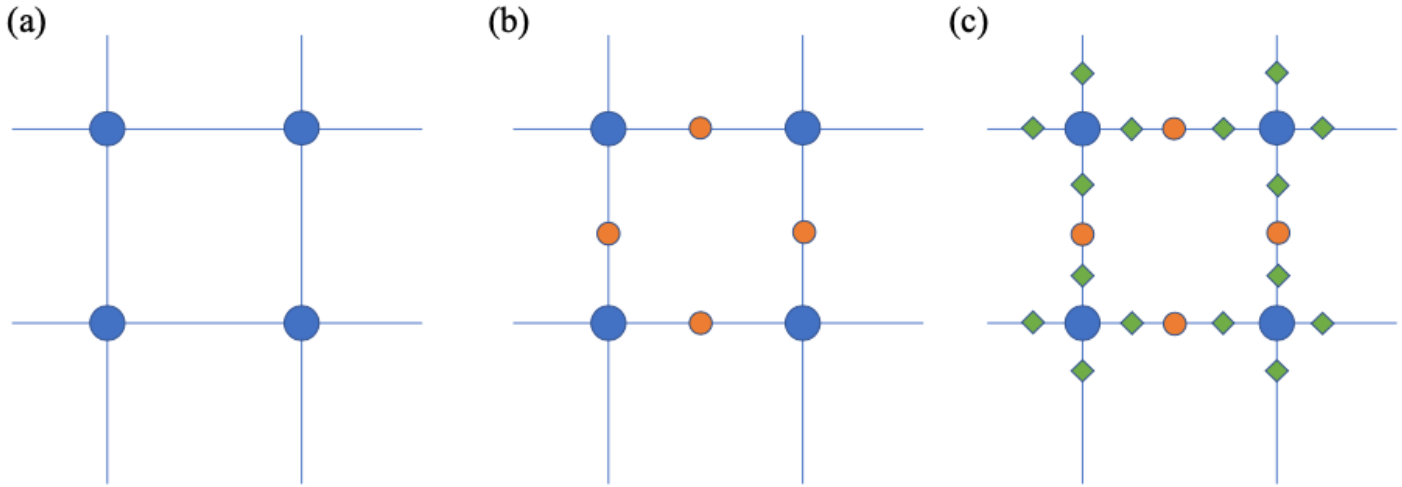
$$\mathcal{H}_{N\times N} = \begin{pmatrix} \mathbb{0}_{N_A\times N_A} & S_{N_A\times N_B} \\ S^{\dagger}_{N_B\times N_A} & \mathbb{0}_{N_B\times N_B} \end{pmatrix}$$ where S is a mapping(hopping process), $S : \mathrm{R}^{N_B} \rightarrow \mathrm{R}^{N_A}$

- If $|N_A| \neq |N_B|$ this will have $\{\psi_i\}_{i=1}^{|N_B-N_A|}$, such that $\hat{H}|\psi_i\rangle = 0$

$\rightarrow$ Flatbands with zero energy

- Recipe for flat bands -

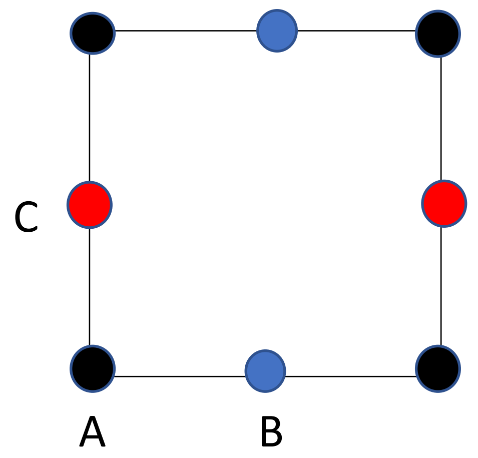
Start with square lattice, add intermediate sites recursively!

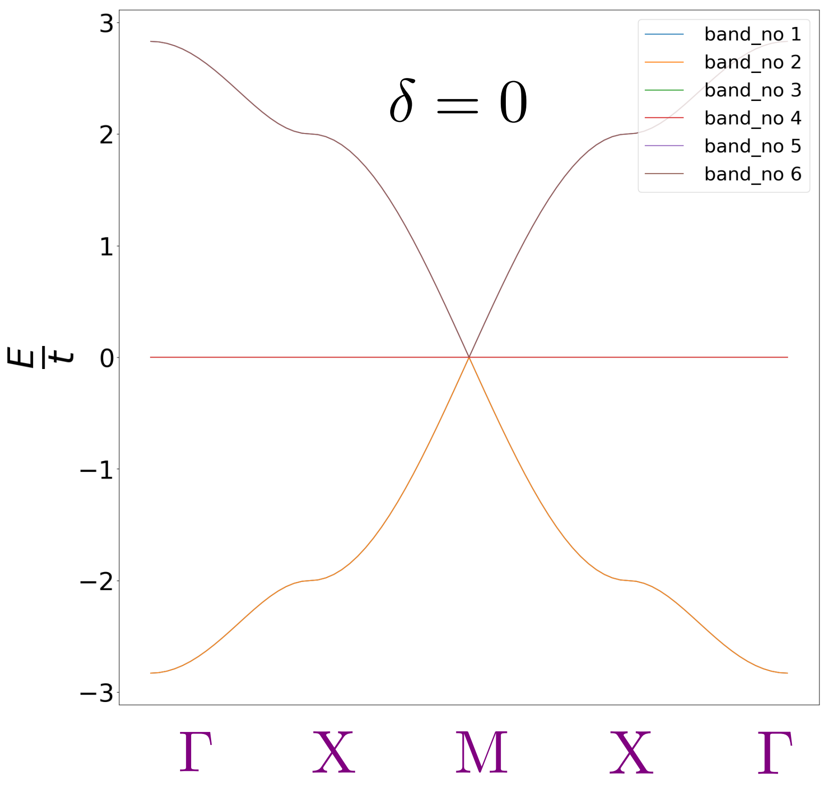


Geometric construction of Flatbands

- Bipartite Lieb Lattice with $|N_A - N_B| = 1$

$$\hat{H} = -t\sum_i c^{\dagger}_{iA}(d_{iB} + c^{\dagger}_{iA}c_{i-a_1,B} + c^{\dagger}_{iA}c_{iC} + c^{\dagger}_{iA}c_{i-a_2,C} + hc)$$





1 flatband, bands are degenerate at (π, π)

Chiral symmetry, bands occur in $\pm E$

$$H = \begin{pmatrix} 0 & S(k) \\ S^{\dagger}(k) & 0 \end{pmatrix}, \quad C = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \{H, C\} = 0$$

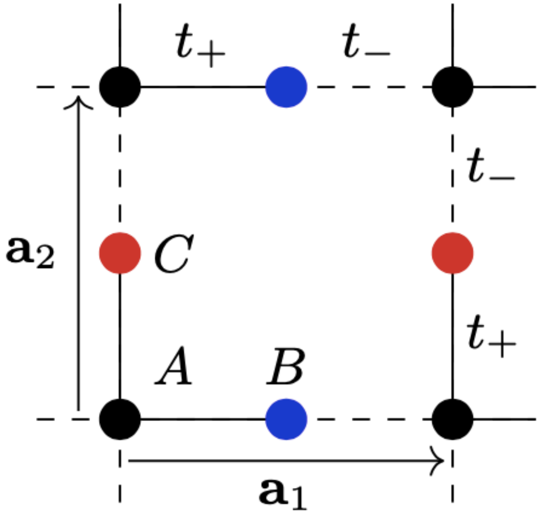
Geometric construction of Flatbands

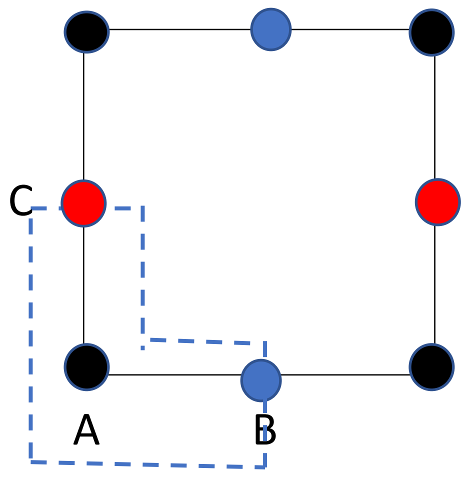
- Staggering breaks inversion symmetry

- Break degeneracy by staggered hopping

$$t_{\pm} = t \pm \delta$$

- Staggering preserves chiral symmetry!



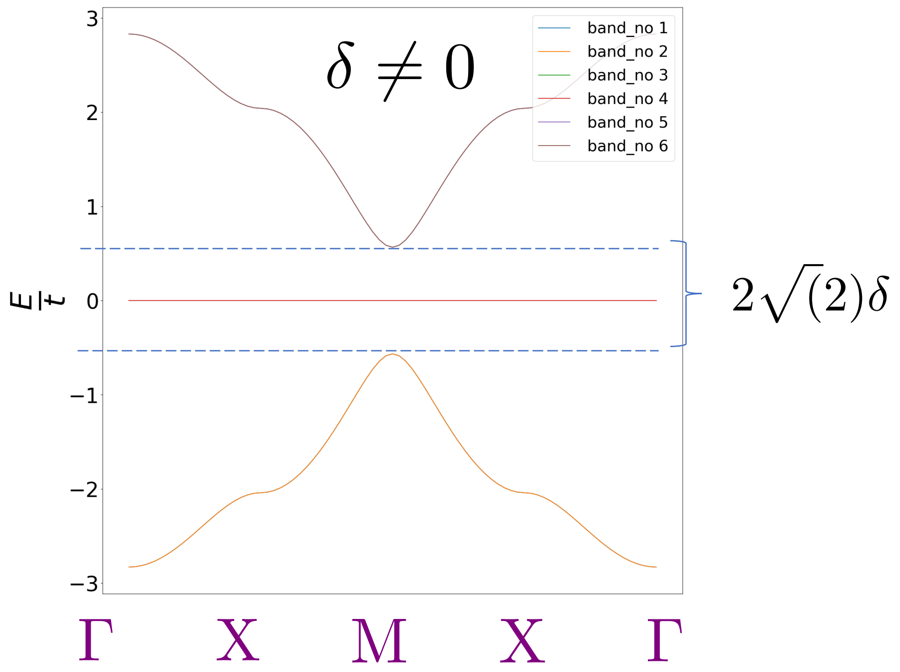


- If interaction strength lower than δ, project into the flatband degree of freedom.

$$\hat{H}_{flat}(k) = 1 - 2\hat{P}(k)$$

- Projection operator for a band l,

$$\langle u_m(k)|\hat{P}_l(k)|u_m(k)\rangle = \delta_{m,l}$$



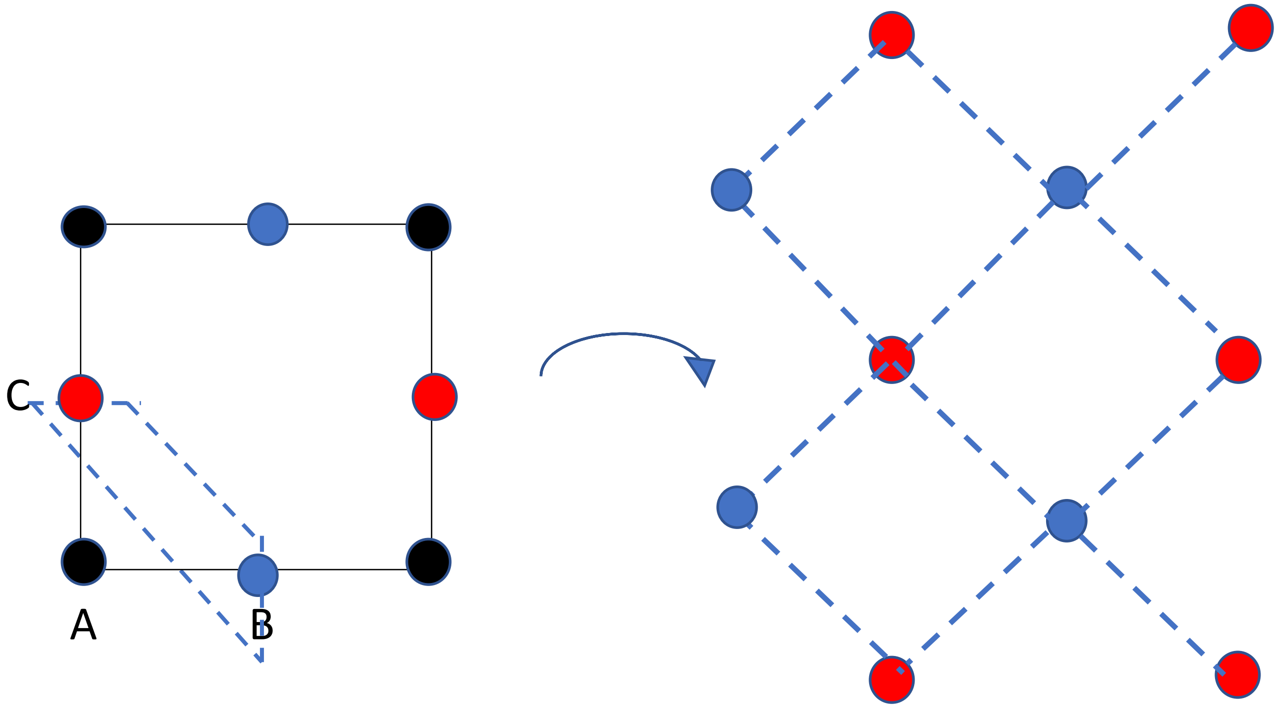
Effective low energy hamiltonian

- For Lieb lattice, flatbands live on B,C only

$$|\psi_{flat}(k)\rangle = c_1|\psi_B(k)\rangle + c_2|\psi_C(k)\rangle$$

- Projection turns Lieb lattice into square lattice

- Projected Hubbard interaction



$$U\sum_{i,\alpha} n_{i,\alpha,\uparrow}n_{i,\alpha,\downarrow}$$

$$P_l(k)c_{km}P_l(k) = c_{kl}\delta_{m,l}$$

$$-J\sum_{i,j}\hat{S}_{i,l}\cdot\hat{S}_{j,l} + \frac{J}{2}\sum_{i,j} n_{i,l}n_{j,l} + \sum_{i,j,\sigma,\sigma'} n_{i,l,\sigma}(c^\dagger_{i,l,\sigma'}c_{j,l,\sigma'} + hc) + \tilde{U}\sum_i n_{i,l,\uparrow}n_{i,l,\downarrow}$$

Lieb's theorems for Hubbard model on bipartite lattices

- E.H. Lieb proposed two theorems for Hubbard model in bipartite lattices (Phys. Rev. Lett. **62**, 1201 (1989))

$$H = -t \sum_{i\in A, j\in B} (c_i^\dagger c_j + hc) + U \sum_{k\in\Lambda} n_{k\uparrow} n_{k\downarrow}$$

- Theorem 1 – Attractive Hubbard model (U<0), for even no of electrons

$|\psi_{GS}\rangle$ is unique, has $S = 0$

- Theorem 2 – Repulsive Hubbard model (U>0), at half filling,

$|\psi_{GS}\rangle$ is unique(apart from spin degeneracy) and has $S = \frac{1}{2}|N_B - N_A|$

$\longrightarrow$ Ferromagnetic order – Strong coupling expansion can give ferromagnets.
(Opposed to traditional anti ferromagnetism on non bipartite lattices)

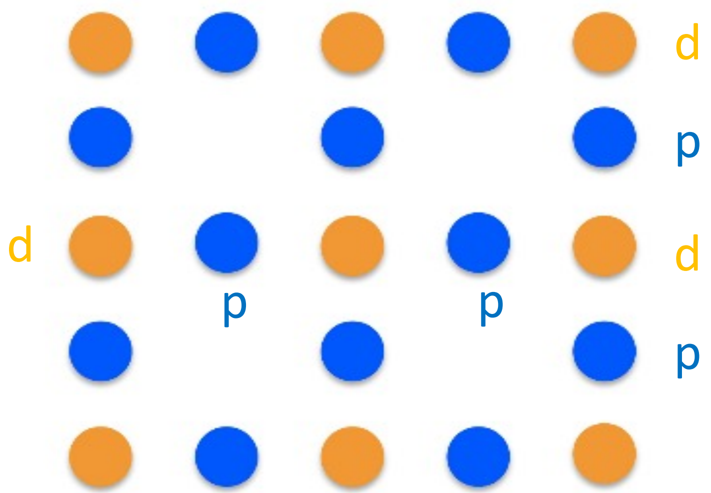
Is Lieb lattice actually ferromagnetic?

- Ferromagnetic order in Lieb lattice is actually site dependent (Phys. Rev. Lett. **72**, 1280 – 1994)

$$\langle S_i^{\dagger} S_j^{-} \rangle \begin{cases} \geq 0, \text{when}(i,j) \in A \text{ or } B \\ \leq 0, \text{when } i \in A \text{ (or } B) \text{ and } j \in B \text{ (or } A) \end{cases}$$

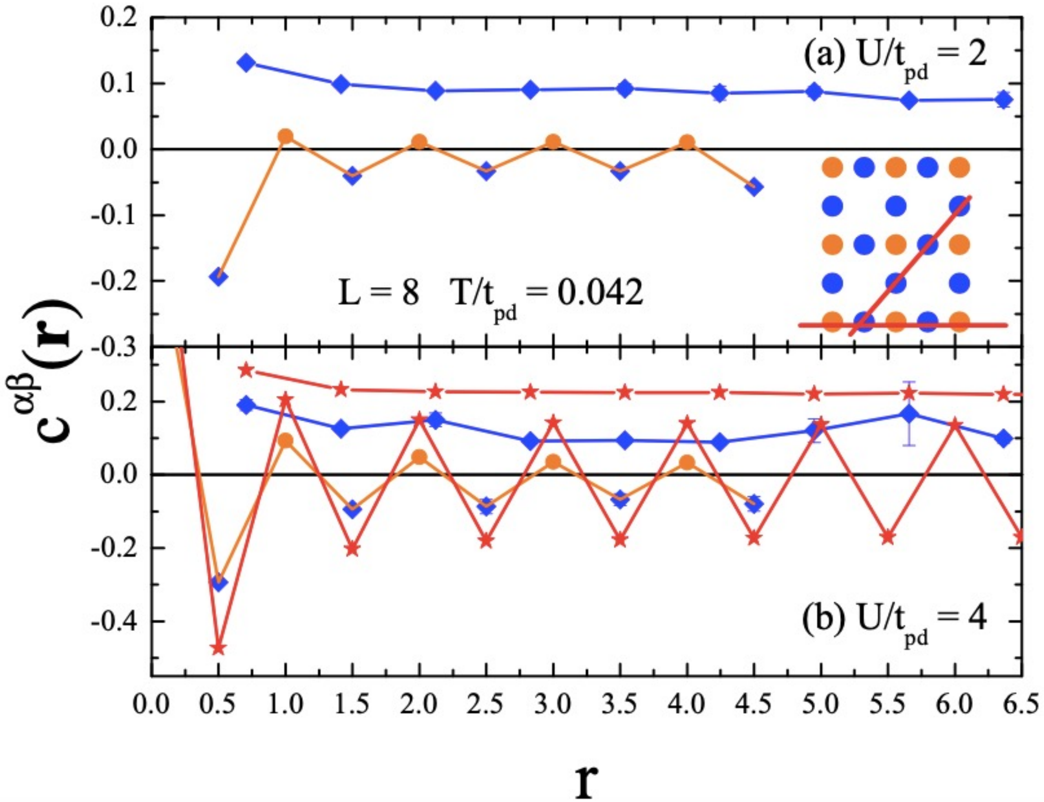
Ferrimagnetism?

- DQMC study of CuO_2 (bipartite lattice of p and d orbitals)



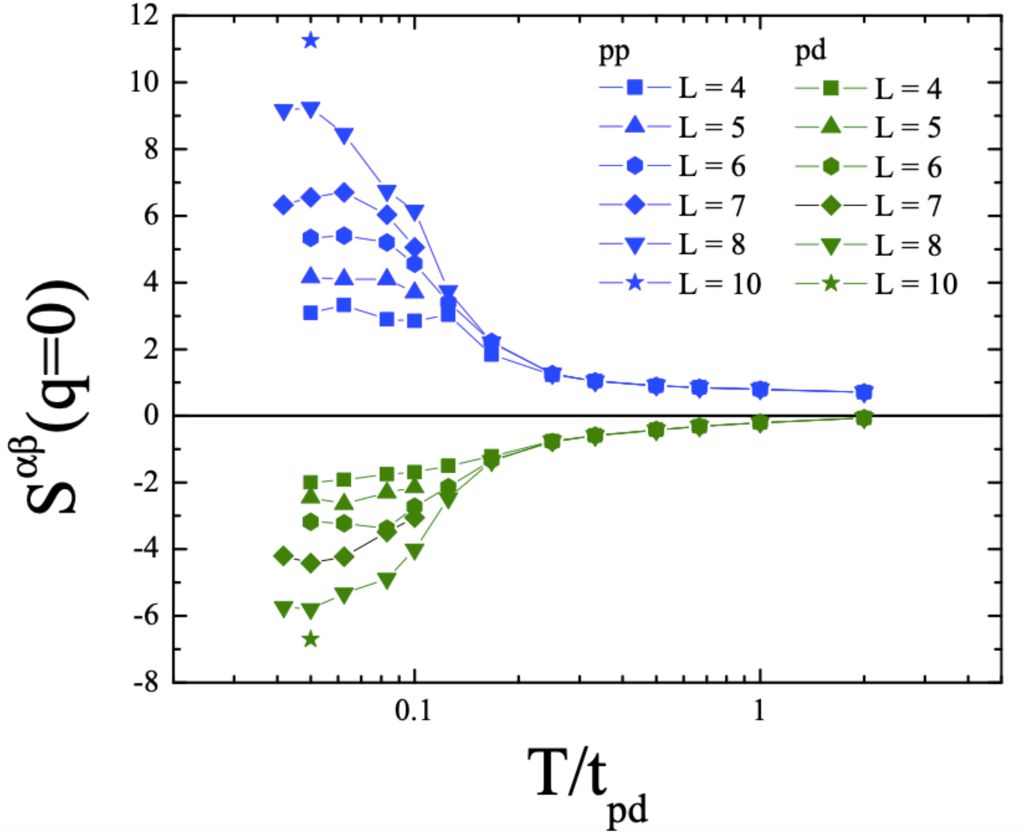
Magnetic correlations,

$$c^{\alpha\beta}(r) = \langle S^{-}_{\alpha, r_0+r} S^{\dagger}_{\beta, r_0} \rangle$$

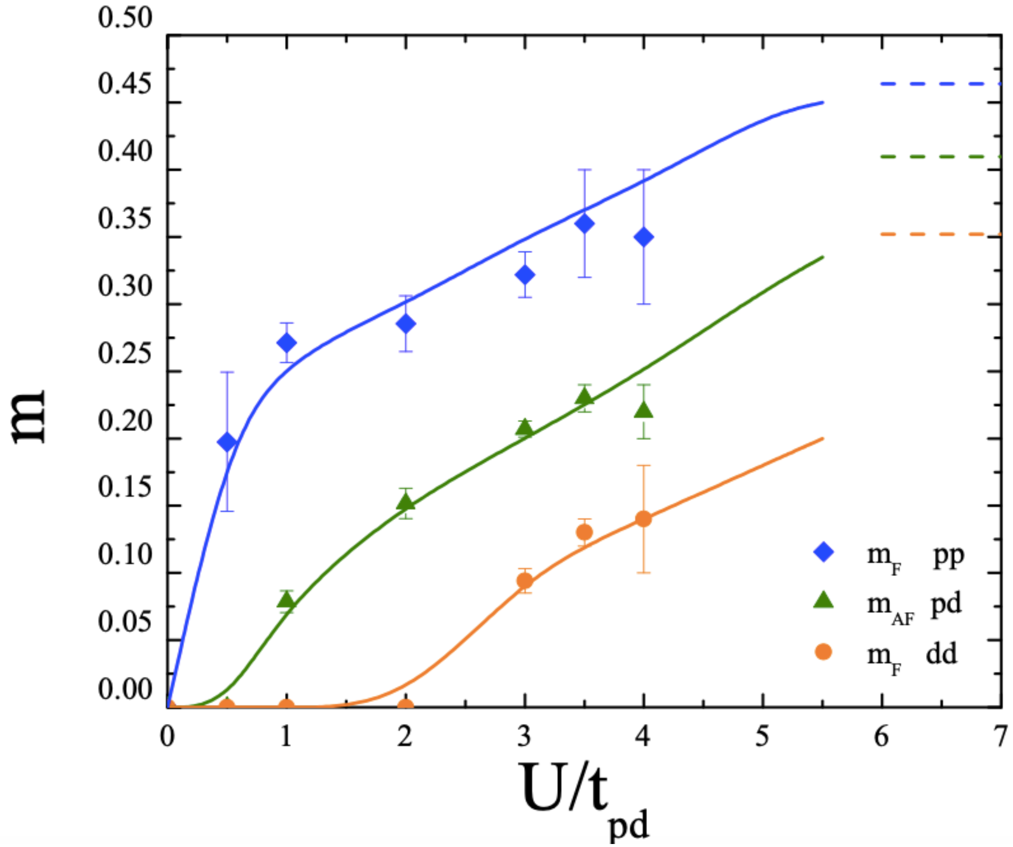


Ferrimagnetic order beyond Lieb lattice

- Structure factor shows Long Range(LR) Ferrimagnetic order



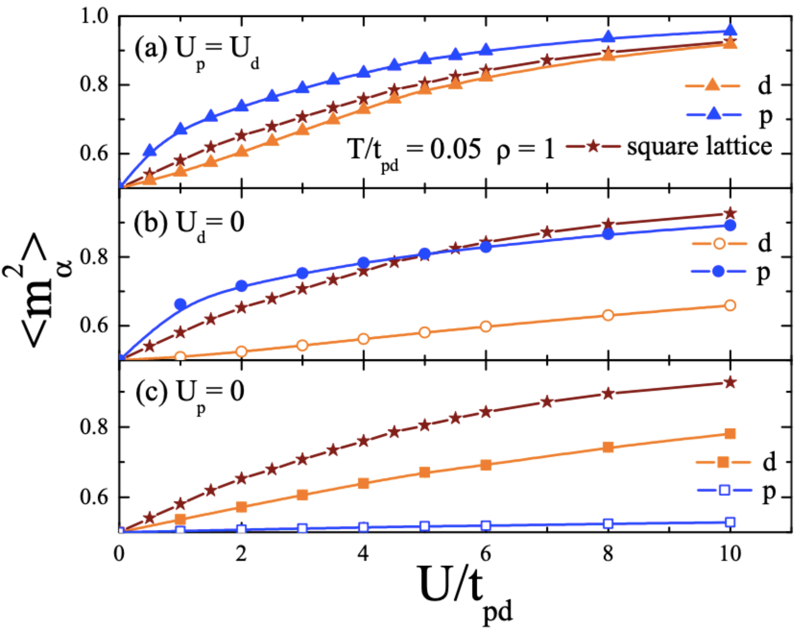
- pp ferromagnetism stronger than dd ferromagnetism(due to difference in co-ordination no)



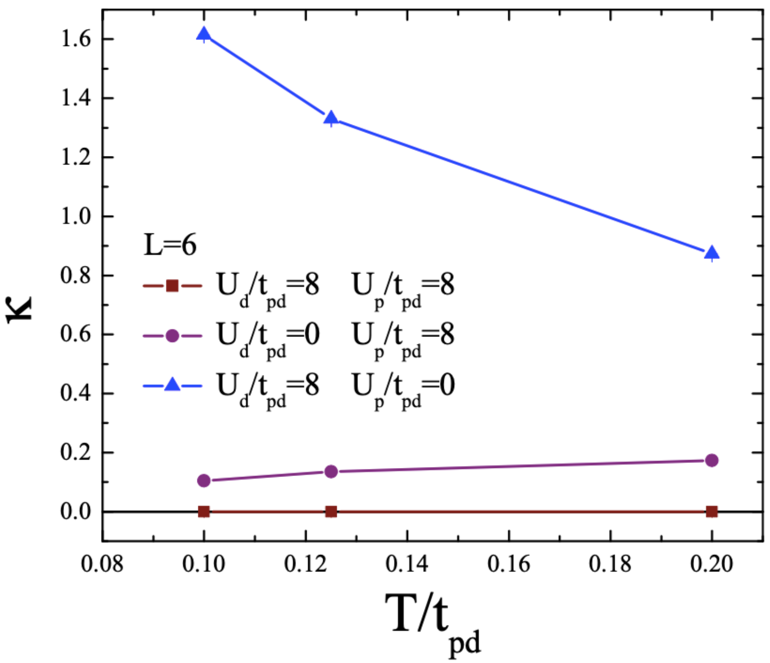
Ferrimagnetism in inhomogeneous Lieb Lattice

- Inhomogenous Lieb lattice gives Heisenberg interaction with strength $\tilde{J} = \dfrac{4t^2(U_p + U_d)}{2U_pU_d}$
- Which sublattice is dominant for ferrimagnetic order? Switch off U_p or U_d

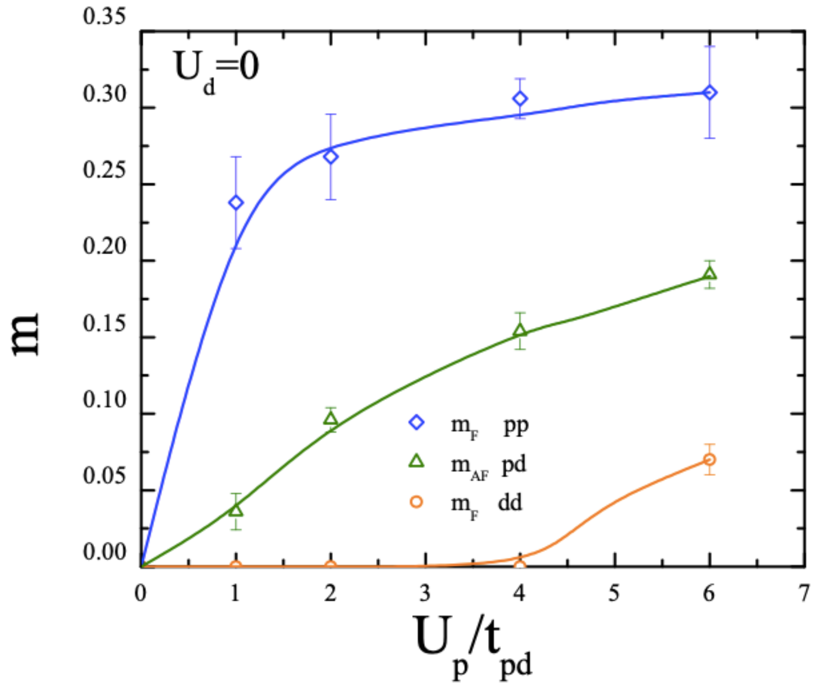
Moment suppression only when $U_p = 0$



Itinerant electrons only when $U_p = 0$!

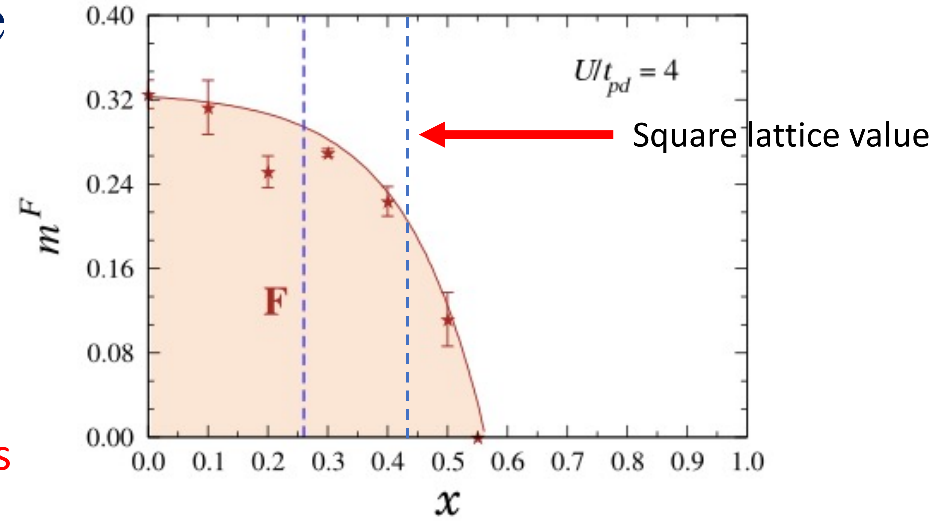


$U_d = 0$ doesn't affect single occupancy of d sites. Long range FM order through U_p



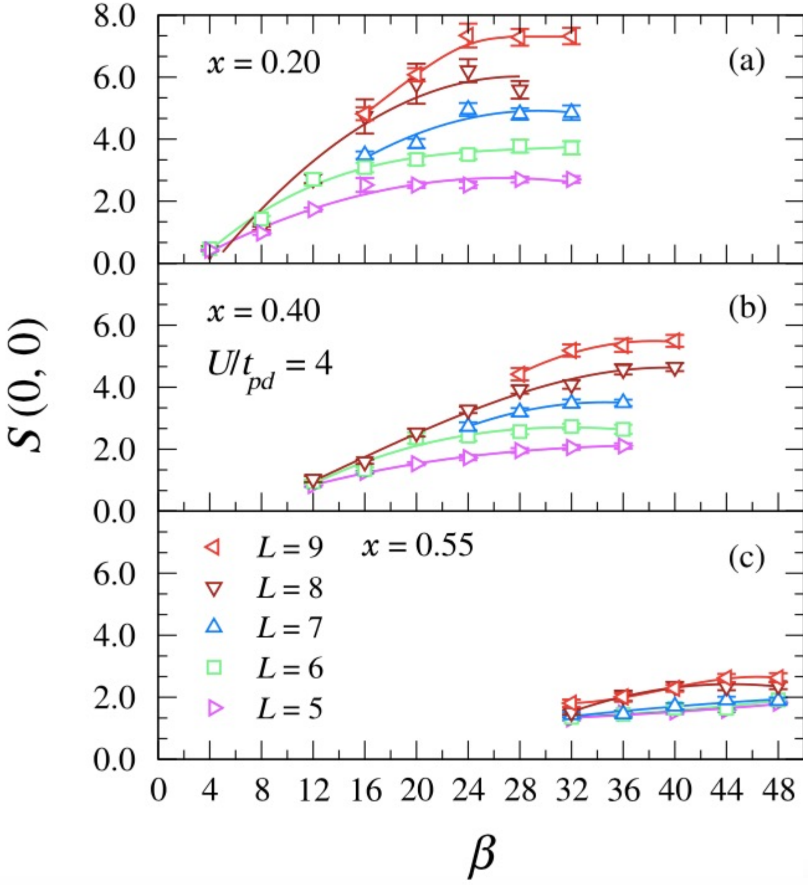
p sublattice has dominant role in long range ferromagnetic order!

Resilience to disorder for the Lieb Lattice

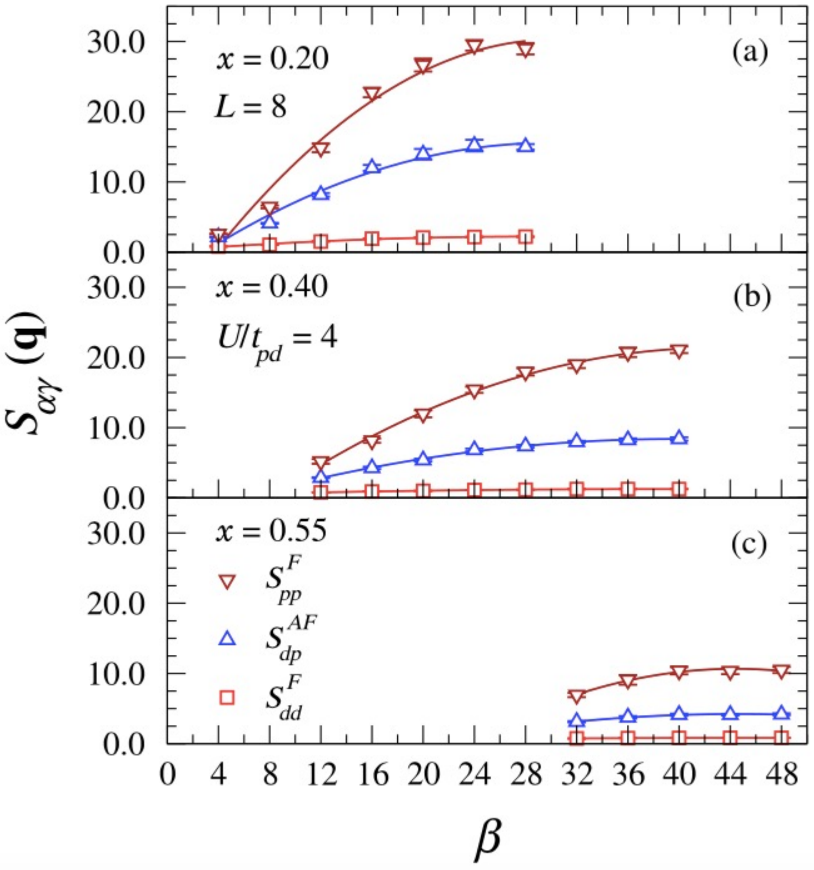


- Bond/site dilution can destroy LRO in Hubbard models! Classical 2d percolation problem.
- Site percolation threshold x_c lowered in Lieb lattice.

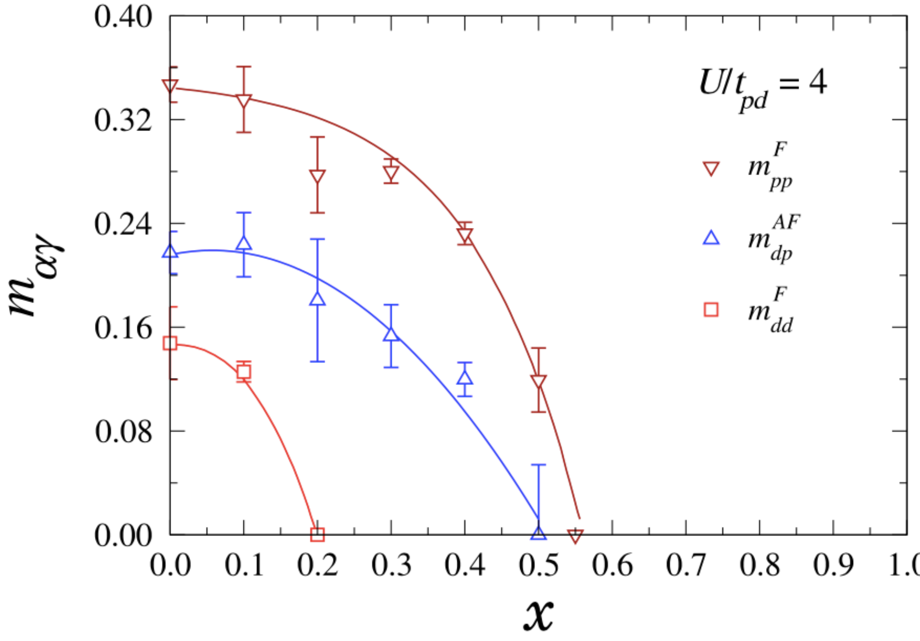
Global FM order parameter



Order resolved spin correlations



p orbitals push threshold beyond classical value



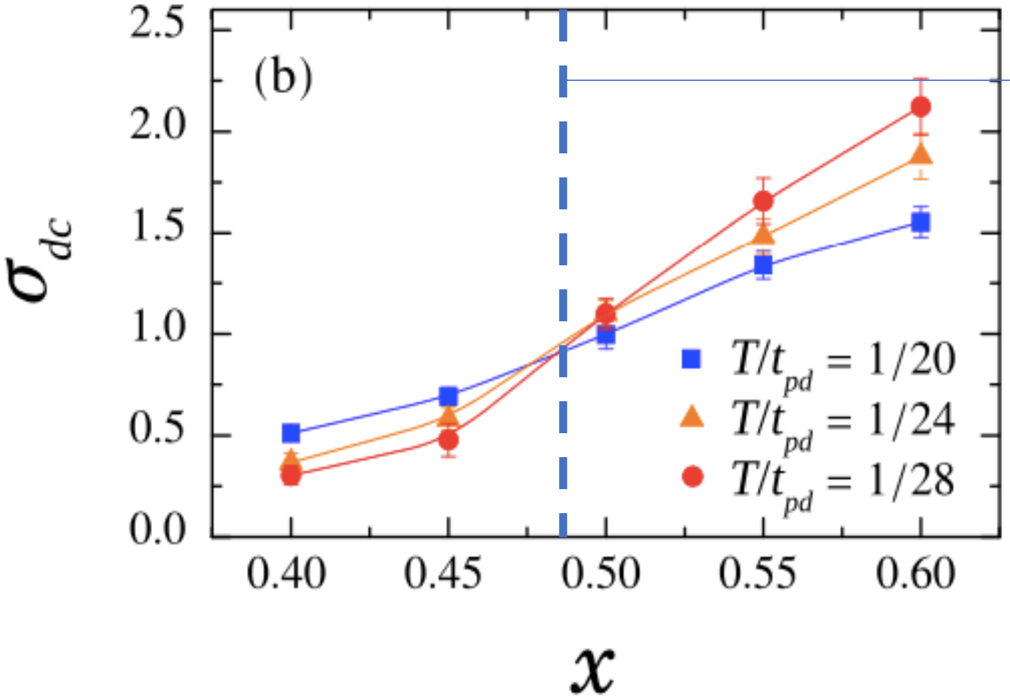
Resilience to disorder for the Lieb Lattice

- Removing U increases itinerancy. Signature in σ_{DC} and κ

→ κ_p high due to flat p bands, dominates global compressibility. Sets x_c

→ System metallic above this due to itinerancy of electrons

- Threshold also determined by crossover in behavior of resistivity vs T



$x_c(\sigma_{DC}) \sim 0.53$