High Temperature Cuprate Superconductors

Theoretical Physics Year 4 Project

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Outline

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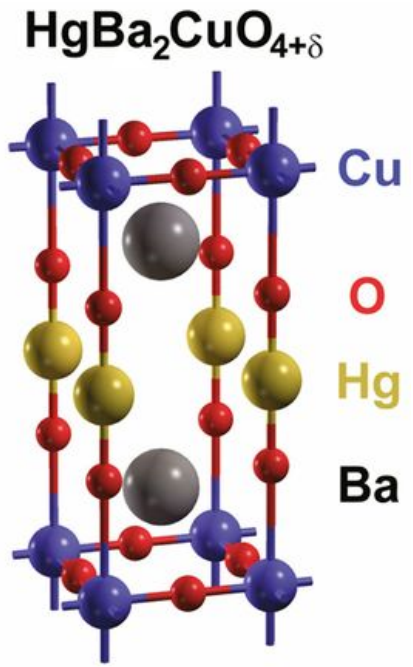
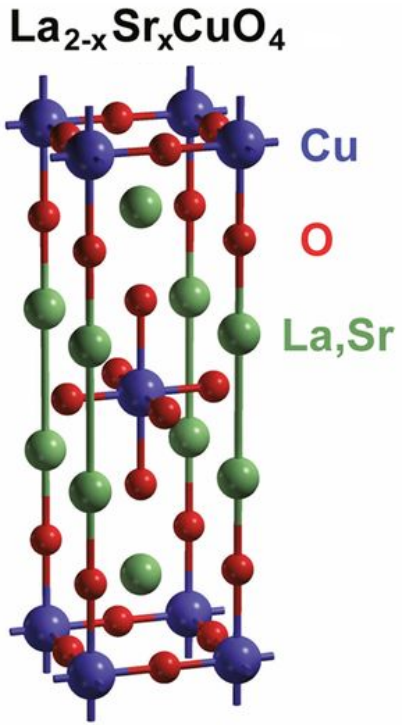
High TC Cuprates - General Structure

Cuprate superconductors have a layered structure.

- We introduce extra atoms - **doping**.
- Additional electrons or holes are released.
- A change in the overall charges occurs.
- The copper oxide layers become doped.



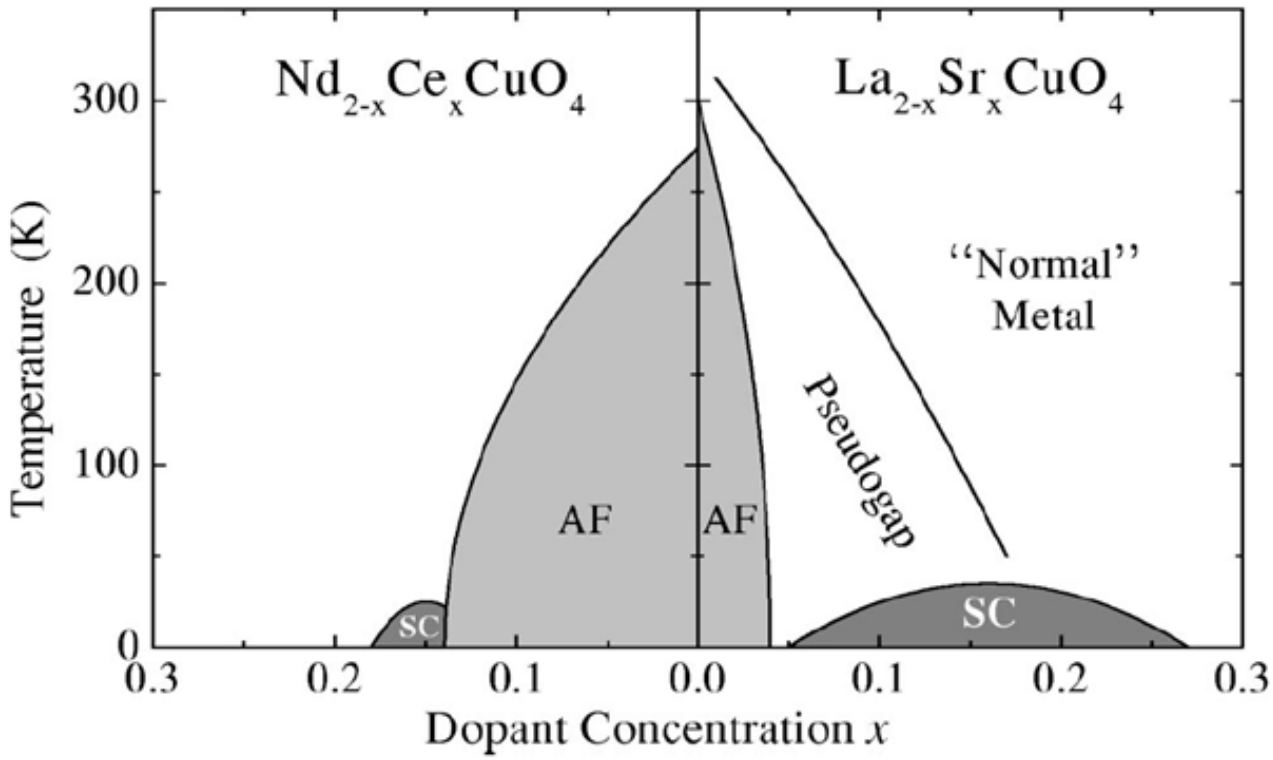
N. Barišić et. al, Proc. Natl. Acad. Sci. U.S.A. 110, 12 235 (2013)



The key to the universal properties are the layers of copper oxide.

Phase Diagram

- Cuprate superconductors can either be electron or hole doped.
- Experiments show a big difference between the two types.



Lee, P., N. Nagaosa, and X.-G. Wen, 2006, Rev. Mod. Phys. 78, 17.

- Why is there an asymmetry in the phase diagram ?

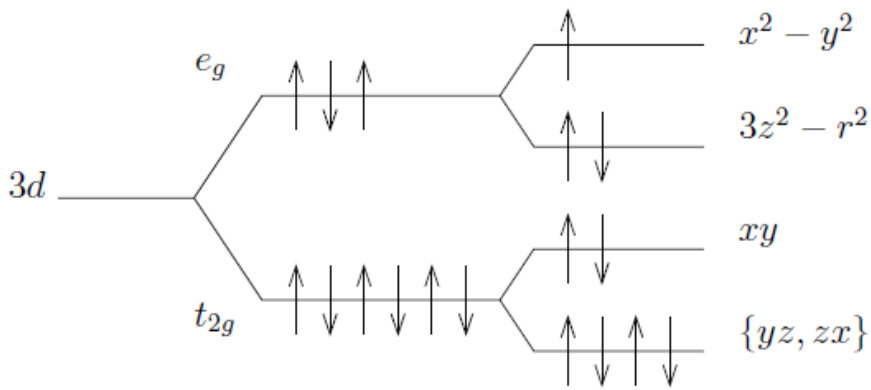
Relevant Orbitals

Consider the parent compound La_2CuO_4 - from $La_{2-x}Sr_xCuO_4$
Charges on the copper and oxygen ions are,

$$Cu^{2+} = 1s^2 2s^2 2p^6 3s^2 3p^6 3d^9$$
$$O^{2-} = 1s^2 2s^2 2p^6$$

3d and 2p orbitals are further split by La_2CuO_4 structure

- Key Cu orbital: $3d_{x^2-y^2}$
- Key O orbitals: $2p_x$,$2p_y$



3 Band Model

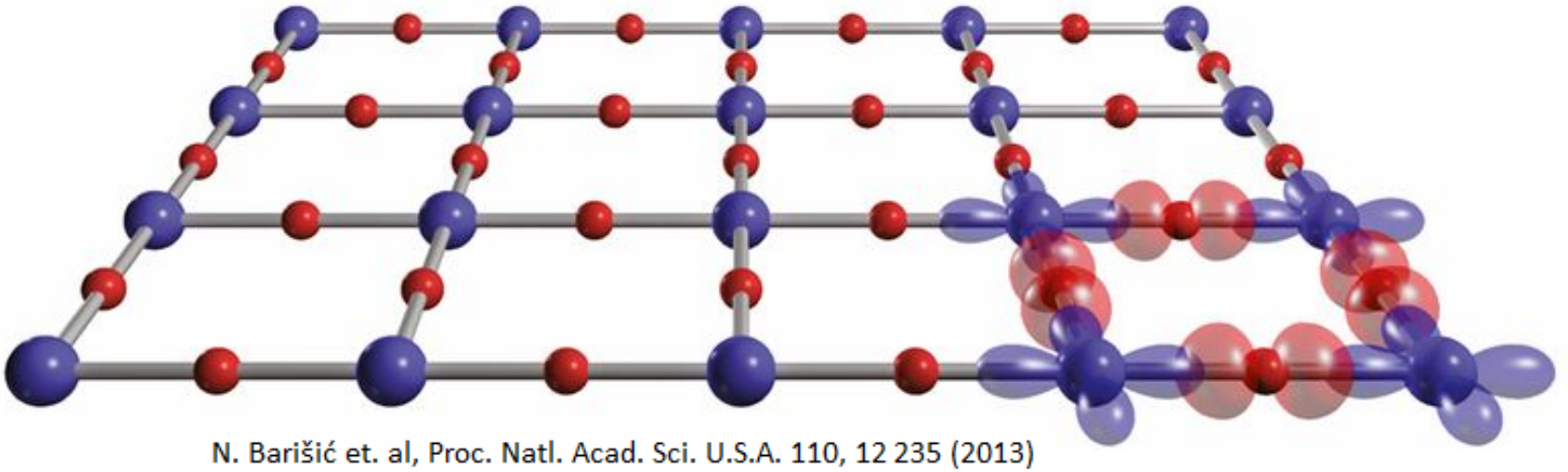


Figure: A 3 band model of CuO_2 square plane.

Key Points

- Every copper site is occupied by a single hole.
- Every oxygen site is unoccupied by holes.
- Doped electrons form $3d^{10}$ orbitals.
- Doped holes form $2p^5$ orbitals.

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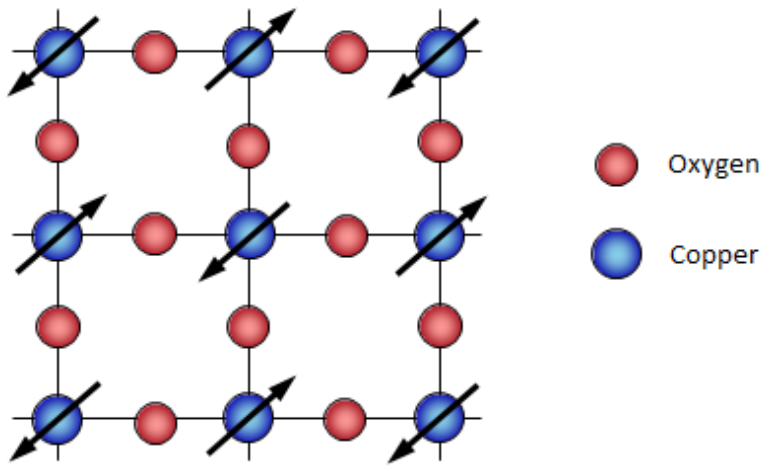
Hamiltonian

We propose a model for the ground state of the copper oxide layer.

$$\mathcal{H}_0 = -\Delta \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma} + U \sum_i d^\dagger_{i\sigma} d_{i\sigma} d^\dagger_{i\bar{\sigma}} d_{i\bar{\sigma}}$$

- Δ = the energy needed to place a single hole on a copper site
- U = the energy needed to place a a second hole on a copper site



Lee, P., N. Nagaosa, and X.-G. Wen, 2006, Rev. Mod. Phys. 78, 17.

Higher Order Contributions

- We have a degenerate ground state that we wish to maintain.
- We want to exclude terms of order V and include order V^2.

$$\mathcal{H}_0 = -\Delta \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma} + U \sum_i d^\dagger_{i\sigma} d_{i\sigma} d^\dagger_{i\bar{\sigma}} d_{i\bar{\sigma}}$$

$$\mathcal{H}_1 = V \sum_{<ij>\sigma} (d^\dagger_{i\sigma} p_{j\sigma} + p^\dagger_{j\sigma} d_{i\sigma})$$

$$\mathcal{H}_2 = ?$$

- How do we obtain a form for $\mathcal{H}_2$?

Canonical Transformation

This is the canonical transformation, a rotation in Hilbert space.

$$f(\lambda) = e^{\lambda S}(H_0 + H_1)e^{-\lambda S}$$

Evaluating out we get,

$$f(1) = H_0 + (H_1 + [S, H_0]) + ([S, H_1] + \frac{1}{2}[S, [S, H_0]]) + \dots$$

Eliminating the order V dependence gives us,

$$\mathcal{H}_1 + [S, H_0] = 0 \Rightarrow \mathcal{H}_1 = [H_0, S]$$

As a result we get that the new Hamiltonian is,

$$\mathcal{H}_2 = \frac{1}{2}[S, H_1]$$

Hopping Hamiltonian

The extension to the Hamiltonian contains two separate terms,

$$H_2 = +\frac{V^2}{\Delta} \sum_{<im>\sigma} \sum_{<ij>} p^\dagger_{j\sigma} p_{m\sigma}$$
$$- \frac{UV^2}{\Delta(U-\Delta)} \sum_{<im>} \sum_{<ij>} (d^\dagger_{i\uparrow} p^\dagger_{j\downarrow} - d^\dagger_{i\downarrow} p^\dagger_{j\uparrow})(p_{m\downarrow} d_{i\uparrow} - p_{m\uparrow} d_{i\downarrow})$$

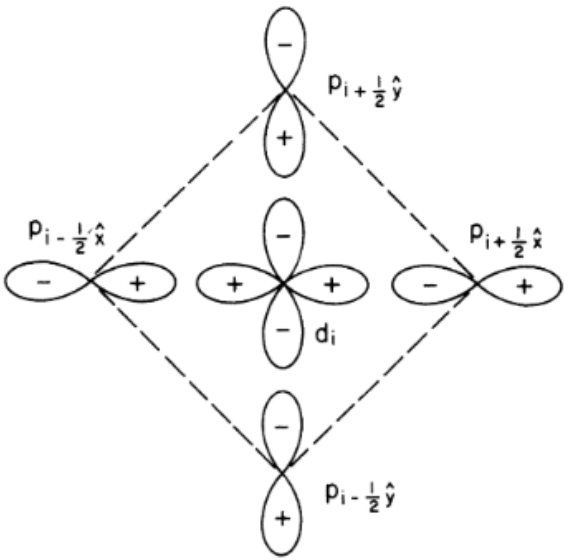
- Term 1 is an oxygen hopping term.
- Term 2 is a singlet hopping term.

Note

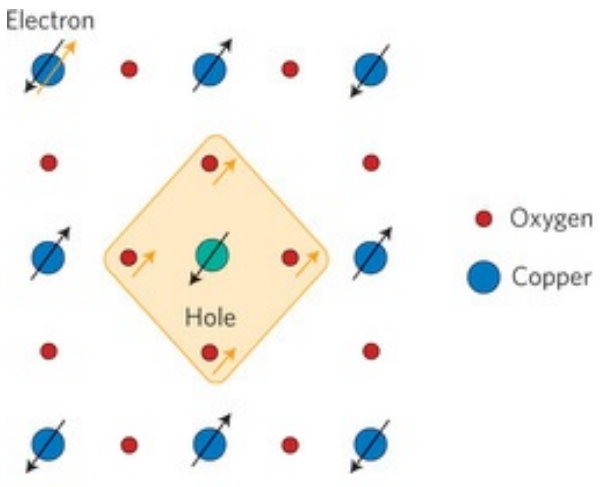
- Valid for both electron and hole doping.

Physical Interpretation

- Our Hamiltonian also describes a singlet and a triplet solution.
- The lowest energy solution is the Zhang-Rice Singlet.



Zhang, F. C. & Rice, T. M.
Phys. Rev. B 37, 3759–3761 (1988)



J. Orenstein and A. Vishwanath,
Nat. Phys. 6, 566 (2010)

- A doped hole resonates around an adjacent copper hole.
- Have been observed experimentally.

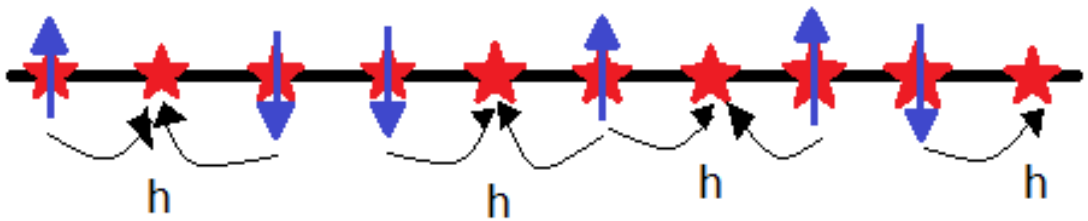
Outline

Hubbard Model Limit

For electron doping, our model reduces to the Hubbard model.

$$\mathcal{H}_2 = -\frac{V^2}{\Delta} \sum_{<il>\sigma} d^\dagger_{l\sigma} d_{i\sigma}$$

- Doped electrons will reside on copper sites e.g. removes holes.
- We want to try and solve this model on various geometries.



- Spin order maintained $\Rightarrow$ concertina effect

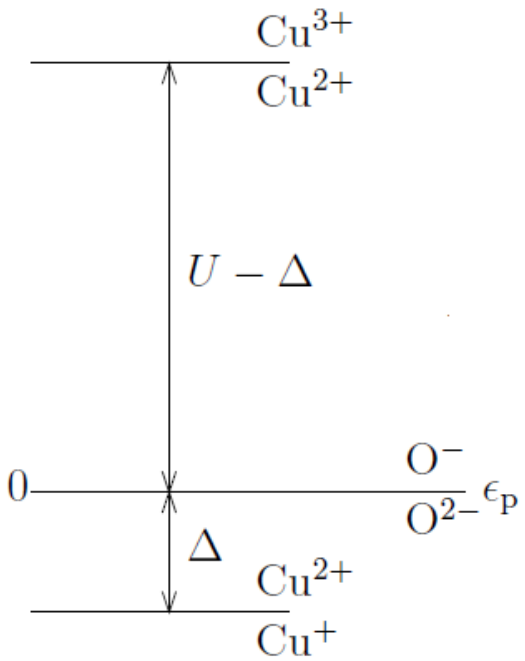
$$\mathcal{E}_k = -\frac{2V^2}{\Delta} \cos k$$

Outline

Limiting Cases

There are two possibilities we need to explore for hole doping:

- Produces Cu^{3+} ions: $\Delta \approx U$
  - Easy to double occupy sites.
  - Easier to solve.
  - Unphysical limit.
- Produces Cu^{+} ions: $\Delta \ll U$
  - Never double occupy sites.
  - Harder to solve.
  - Physical limit.



Line

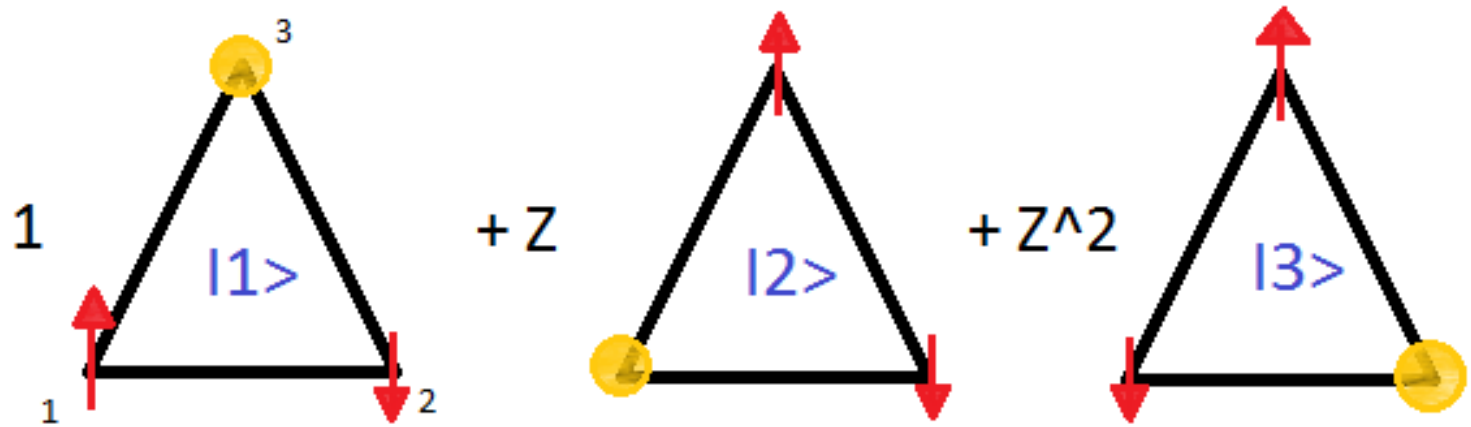
- In the Cu^{3+} limit our Hamiltonian turns into the form of a singlet.

$$\mathcal{H}_2 = -X \sum_{<im>} \sum_{<ij>} (d^\dagger_{i\uparrow} p^\dagger_{j\downarrow} - d^\dagger_{i\downarrow} p^\dagger_{j\uparrow})(p_{m\downarrow} d_{i\uparrow} - p_{m\uparrow} d_{i\downarrow})$$

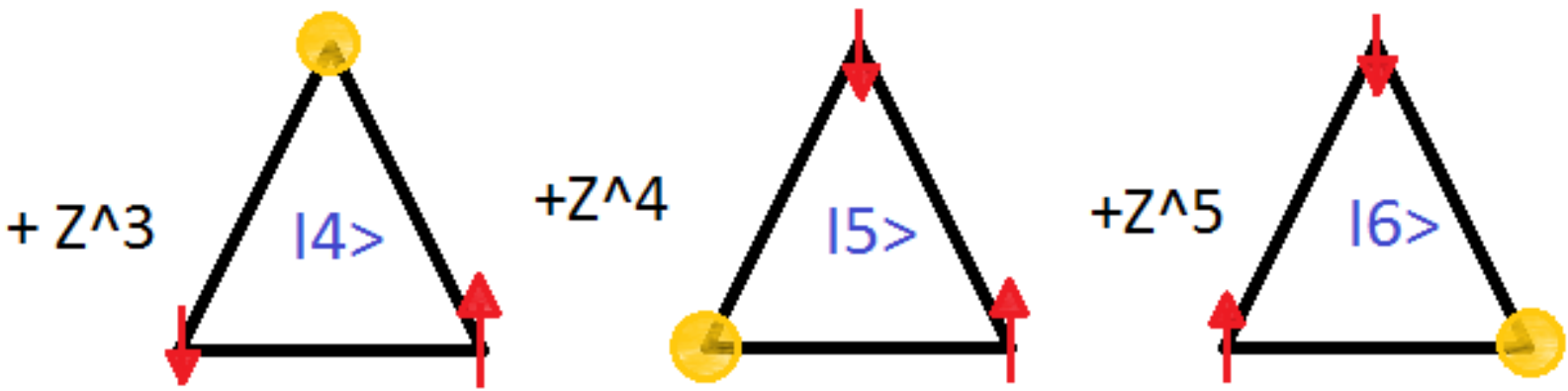
- Solving for the linear chain we get a Hubbard like solution.
- What happens if we solve on more complicated geometries?

Triangles

Consider 1 hole and 2 electrons forming the corners of a triangle.

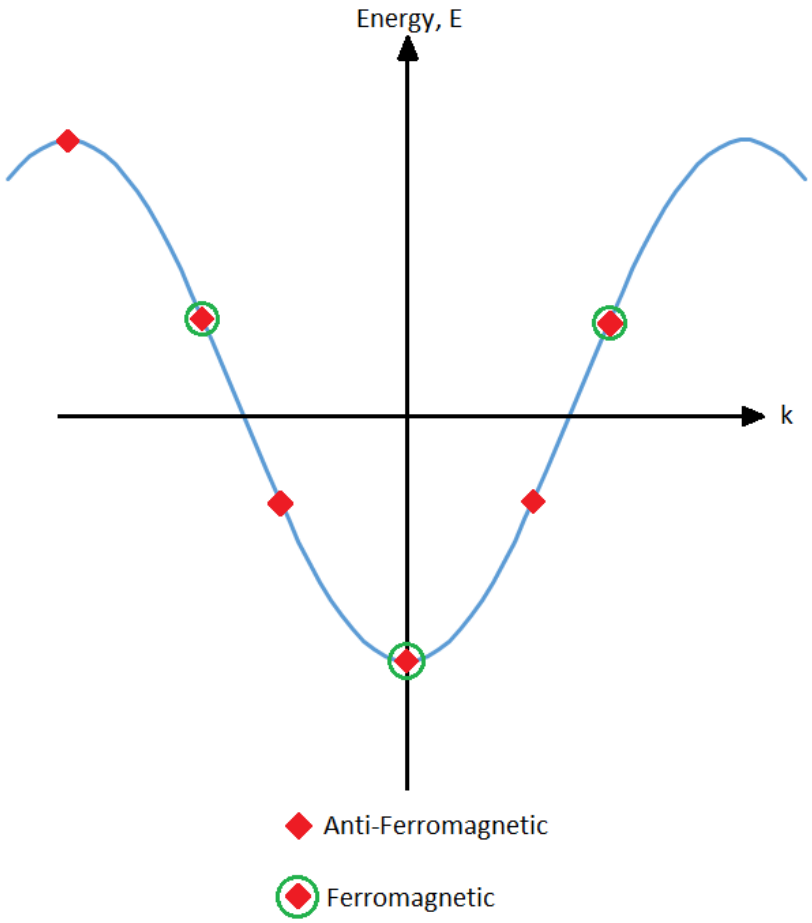


The holes (yellow) move anti-clockwise



Energy Values - Triangles

Solving for the eigenvalues of the triangular system.

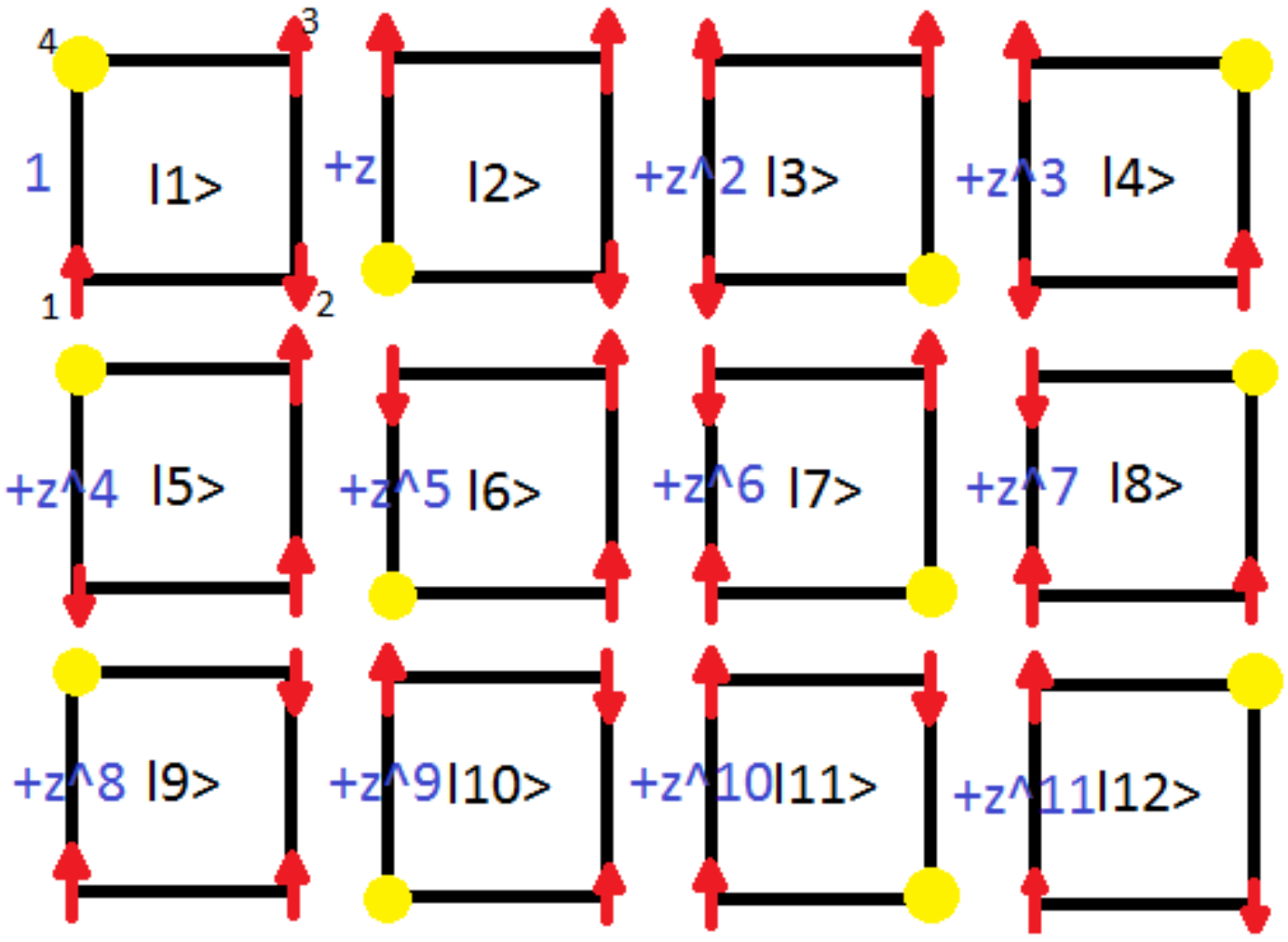


$$\mathcal{E}_k \propto \frac{2V^2}{\Delta} \cos k$$

- Need to combine 2 spin-$\frac{1}{2}$ particles - spin physics
- Either ferromagnetic or anti-ferromagnetic ground state

Squares

Consider 1 hole and 3 electrons forming the corners of a square.



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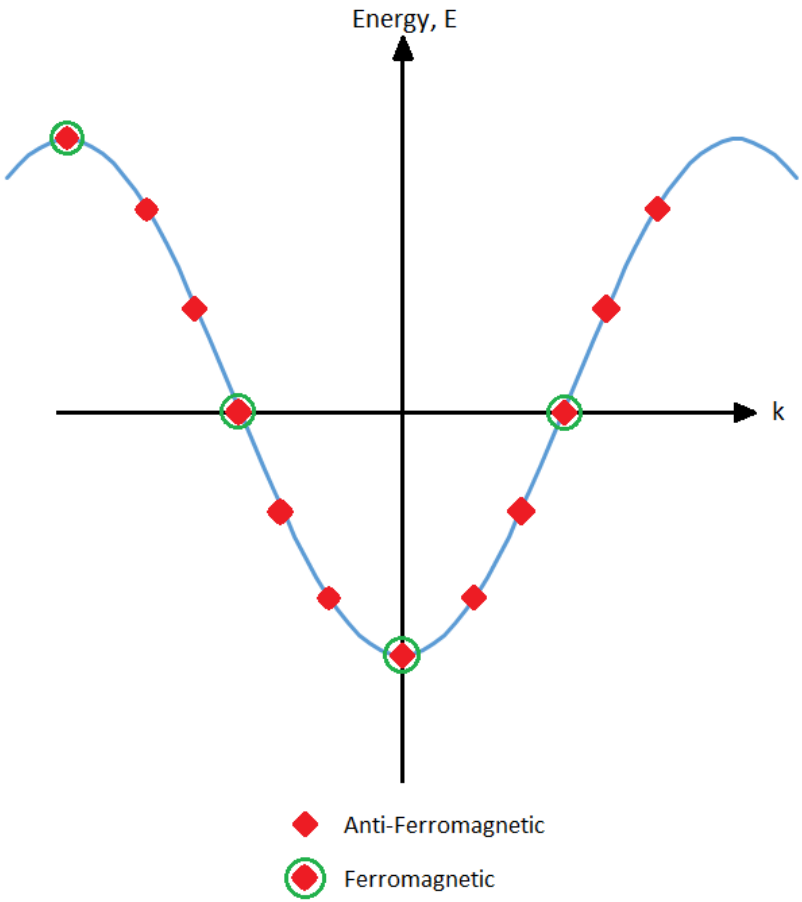


$$\mathcal{E}_k \propto \frac{2V^2}{\Delta} \cos k$$

- Need to combine 3 spin-$\frac{1}{2}$ particles - spin physics
- Always ferromagnetic ground state
- Differs from the triangle case

Nagoaka's Theorem

The results we have seen for squares and triangles have been solved in general for even bigger number of sites.

The conditions required are:

- Requires exactly one doped hole
- Sites form a closed loop

Nagoaka's Theorem - Implications

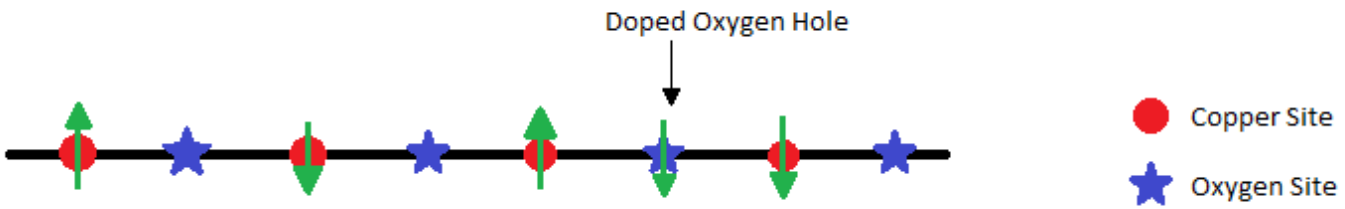
- Even number of sites $\Rightarrow$ ground state is always ferromagnetic.
- Odd number of sites $\Rightarrow$ ground state is either of maximum or minimum total spin.

Cu^+ Limit

- In the physical limit we have both hopping and singlet terms.

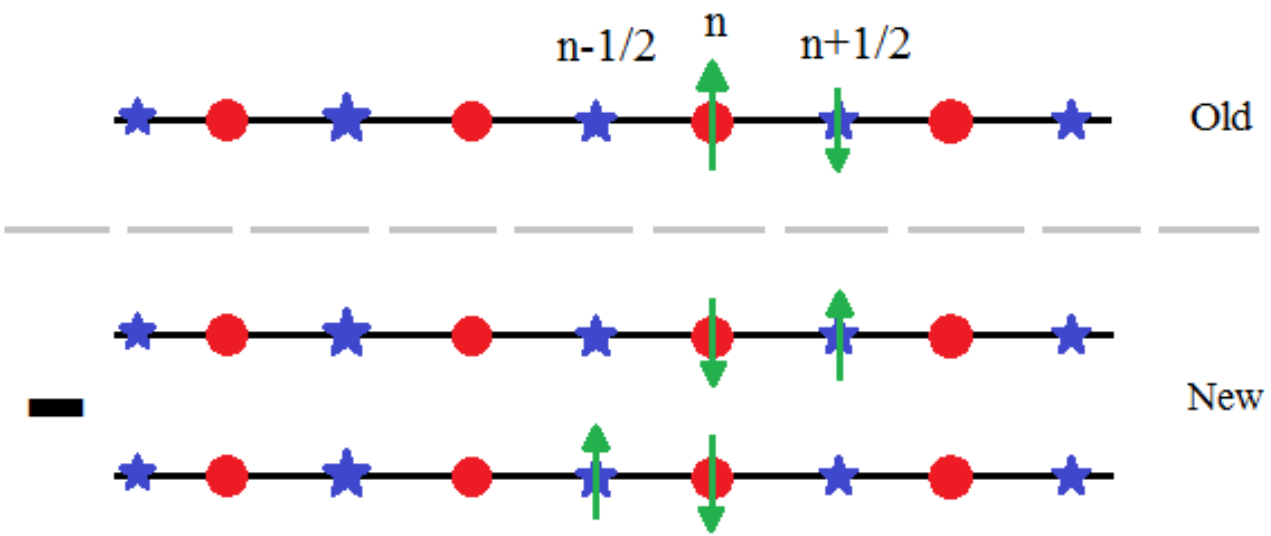
$$\mathcal{H}_2 = T \sum_{<jm>\sigma} p^\dagger_{j\sigma} p_{m\sigma} - T \sum_{<im>} \sum_{<ij>} (d^\dagger_{i\uparrow} p^\dagger_{j\downarrow} - d^\dagger_{i\downarrow} p^\dagger_{j\uparrow})(p_{m\downarrow} d_{i\uparrow} - p_{m\uparrow} d_{i\downarrow})$$

- Difficulty is increased as we have two competing interactions.
- We shall illustrate this on a linear chain - surprising result !



Illustrating the Mechanism

- Consider a doped spin which is anti-parallel to its neighbour.



- The holes hop along preserving the spin order - shuffling
- The spin order can be altered - 1st appearance so far !

Summary

We have proposed a Hamiltonian for our 3 band model.

- Electron doping and Cu^{3+} limit both yield Hubbard model.
- Cu^{+} limit provides something different.

Our Cu^{+} limit can provide a mechanism for spin exchange.

- Could provide a answer for asymmetry in phase diagram.

Can we find an answer for the linear chain ground state to test experimentally ?