Introduction to kinetic frustration

~~Magnetism is~~
Magnetic correlations typically come from magnetic exchange interactions, i.e. explicit spin-spin interactions such as Ising or Heisenberg interactions. However, magnetic correlations can also arise ~~from~~ purely from the motion of electrons. This is ~~the~~ what we will focus on in this lecture.

Hubbard model:

$$H = -t \sum_{\langle ij \rangle \sigma} \tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + \text{h.c.} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

electron hopping — on-site Coulomb repulsion

Atomic limit: $U >> t$ $\quad U \to \infty$

* no double occupancy

$$H = -t \sum_{\langle ij \rangle \sigma} P c^{\dagger}_{i\sigma} c_{j\sigma} + \text{h.c.}$$

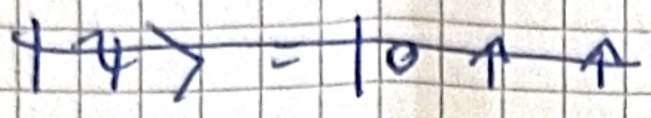
↑ no-double occupancy built in

$\left(c_{j\sigma} = \tilde{c}_{j\sigma} P_{j\sigma} = \tilde{c}_{j\sigma} (1 - n_{j\bar{\sigma}}) \right)$

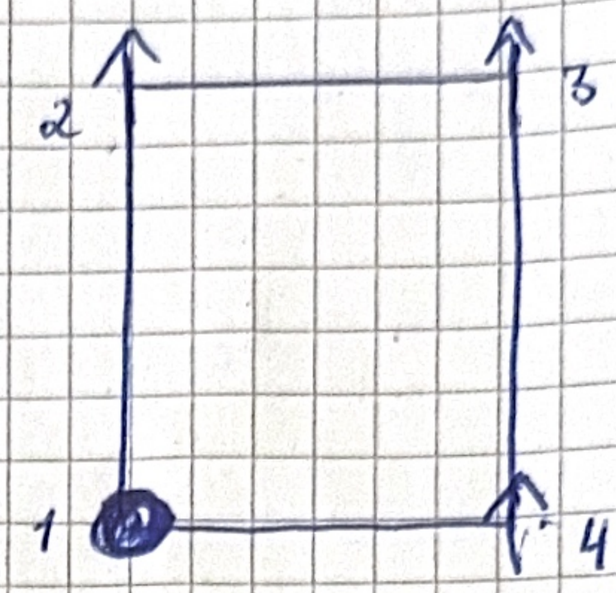
$$\boxed{\{ c^{\dagger}_{i\sigma}, c^{\dagger}_{j\sigma'} \} = 0} \quad \Rightarrow \quad c^{\dagger}_{i\sigma} c^{\dagger}_{j\sigma'} = - c^{\dagger}_{j\sigma'} c^{\dagger}_{i\sigma}$$

Single square

× 1 hole



$$H = -t\sum_{\sigma}\left(c^{+}_{10}c_{20} + c^{+}_{20}c_{10} + c^{+}_{20}c_{30} + c^{+}_{30}c_{20} + c^{+}_{30}c_{40} + c^{+}_{40}c_{30} + c^{+}_{40}c_{10} + c^{+}_{10}c_{40} \right)$$



$$c^{+}_{1\uparrow}c_{4\uparrow}\; c^{+}_{2\uparrow}c^{+}_{3\uparrow}c^{+}_{4\uparrow}|0\rangle$$

$$(-1)^2 = (-1)^2 = c^{+}_{4\uparrow}c^{+}_{2\uparrow}c^{+}_{3\uparrow}$$

$E \geq -2t$

$$|4\rangle = \left(|\circ\uparrow\uparrow\uparrow\rangle + |\uparrow\circ\uparrow\uparrow\rangle + |\uparrow\uparrow\circ\uparrow\rangle + |\uparrow\uparrow\uparrow\circ\rangle \right)/2$$

$$H|4\rangle = -t\left(|\uparrow\circ\uparrow\uparrow\rangle + (-1)^2|\uparrow\uparrow\uparrow\circ\rangle + |\circ\uparrow\uparrow\uparrow\rangle + |\uparrow\uparrow\circ\uparrow\rangle + |\uparrow\circ\uparrow\uparrow\rangle + |\uparrow\uparrow\uparrow\circ\rangle + |\uparrow\uparrow\circ\uparrow\rangle + (-1)^2|\circ\uparrow\uparrow\uparrow\rangle \right)/2$$

$$= -2t\left(|\circ\uparrow\uparrow\uparrow\rangle + |\uparrow\circ\uparrow\uparrow\rangle + |\uparrow\uparrow\circ\uparrow\rangle + |\uparrow\uparrow\uparrow\circ\rangle \right)/2 = -2t|4\rangle$$

$|4\rangle$ is a GS!

And the kinetic energy of the hole is minimized by a ferromagnetic spin background!

(Nagaoka effect).

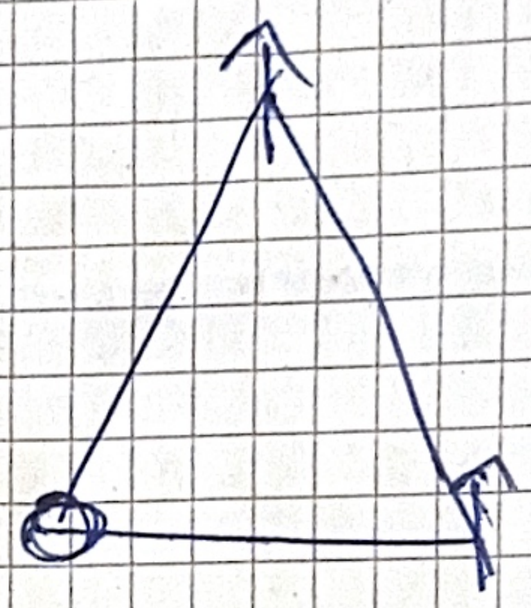
What was special about the square? Always an even # of fermion interchanges! (0 or 2), so fermionic statistics effectively did not matter.

Reason: even ↔ odd (bipartite)

Let us look at a system where this is no longer the case:

<u>Single triangle</u>

$E \geq -2t$.



Try fully delloc eq. amp.

$|4\rangle = (|\circ\uparrow\uparrow\rangle + |\uparrow\circ\uparrow\rangle + |\uparrow\uparrow\circ\rangle)/\sqrt{3}$

$H|4\rangle = -t(|\uparrow\circ\uparrow\rangle - |\uparrow\uparrow\circ\rangle + |\circ\uparrow\uparrow\rangle + |\uparrow\uparrow\circ\rangle - |\circ\uparrow\uparrow\rangle + |\uparrow\circ\uparrow\rangle)/\sqrt{3}$

$= -2t\,|\uparrow\circ\uparrow\rangle/\sqrt{3}$ ← Not an eigenstate!

$\langle 4|H|4\rangle = -\frac{2}{3}t \ldots > -2t$

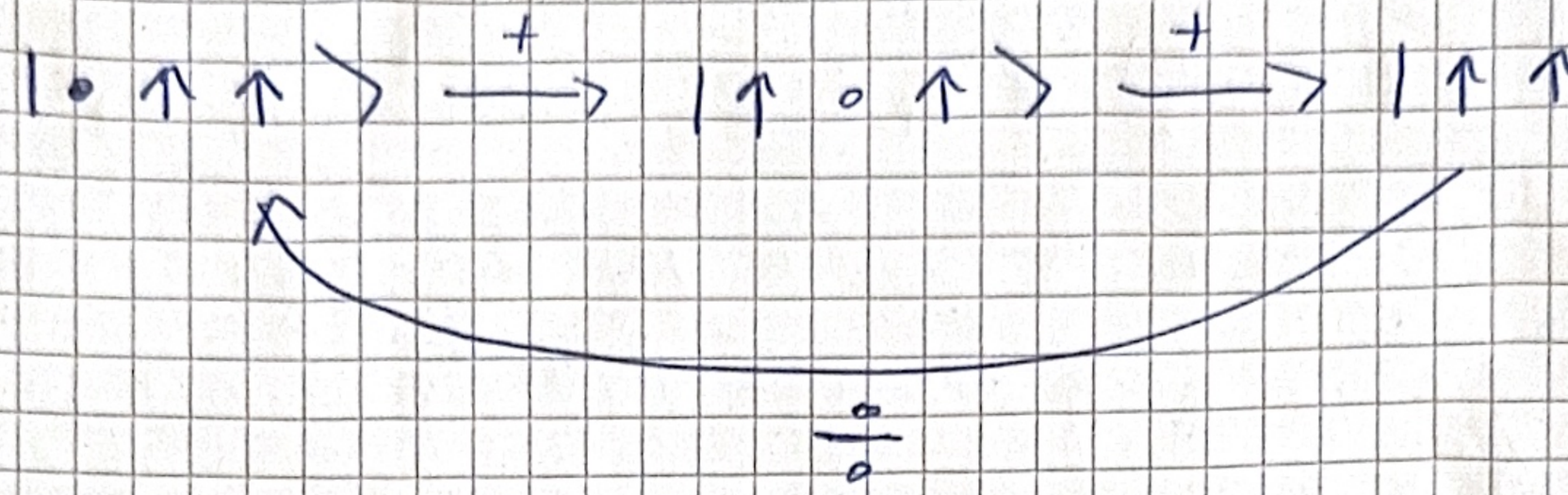
$H(|\uparrow\circ\uparrow\uparrow\rangle + |\uparrow\circ\uparrow\rangle)/\sqrt{2} = -t(|\circ\uparrow\uparrow\rangle + |\uparrow\circ\uparrow\rangle)/\sqrt{2}$

$E = -t > -2t$.

Hole resonating on one bond.

Why can the hole not fully delocalise?

Answer: frustration from ferm. stat.
(kinetic frustration!)



$$|\Psi\rangle = |\bullet\uparrow\uparrow\rangle + |\uparrow\circ\uparrow\rangle + |\uparrow\uparrow\circ\rangle$$

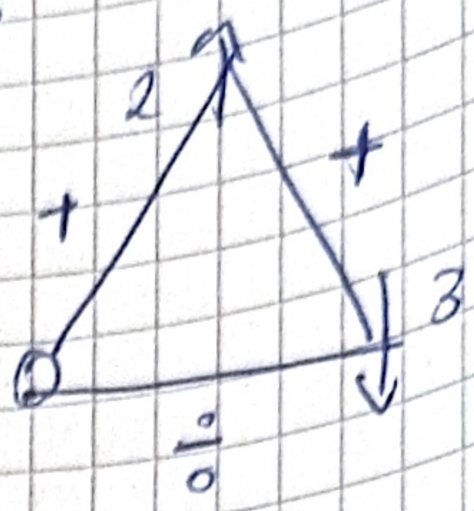
MAXIMISED

Impossible to write down a state that minimises the kinetic energy on all three bonds simultaneously.

Reason: odd number of fermion signs as we work through all the basis states.

BUT: We assumed an FM spin background.

What about the AF sector?



Basis:

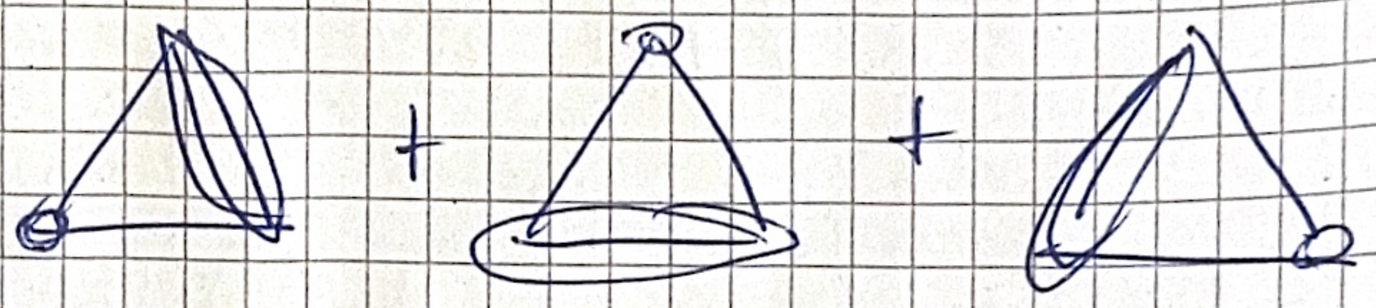
$|1\rangle = |\circ\uparrow\downarrow\rangle$ $|2\rangle = |\uparrow\circ\downarrow\rangle$

$|3\rangle = |\uparrow\downarrow\circ\rangle$ $|4\rangle = |\circ\downarrow\uparrow\rangle$

$|5\rangle = |\downarrow\circ\uparrow\rangle$ $|6\rangle = |\downarrow\uparrow\circ\rangle$

$$|7\rangle = \Big(|\circ\uparrow\downarrow\rangle + |\uparrow\circ\downarrow\rangle + |\uparrow\downarrow\circ\rangle \mp |\circ\downarrow\uparrow\rangle \mp |\downarrow\circ\uparrow\rangle \mp |\downarrow\uparrow\circ\rangle\Big)/\sqrt{6}$$

$$= \Big(|\circ\,\text{⬭}\rangle + |\,\text{⌒}\,\circ\rangle + |\,\text{⬭}\,\circ\rangle\Big)/\sqrt{3}$$



⬭ : spin singlet $(\uparrow\downarrow - \downarrow\uparrow)/\sqrt{2}$.

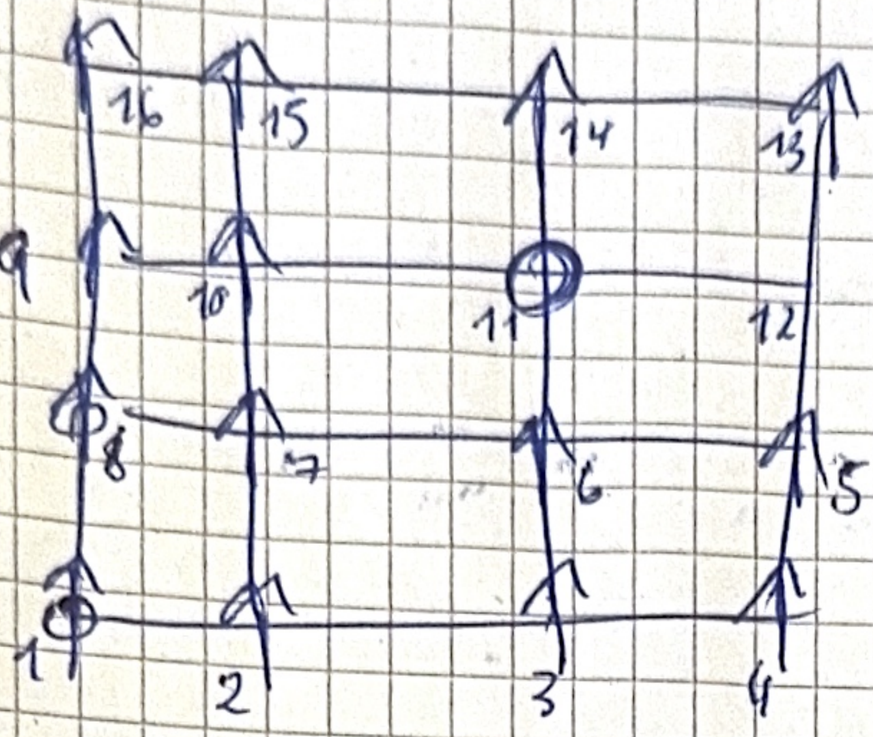
$H|7\rangle = -2t\,|7\rangle$ ⇒ All bonds minimised!

Counter-Nagaoka effect

* non-bipartite
* ⇒ kinetic energy minimised by MINIMISING S^2_{tot} (AFM corr.)

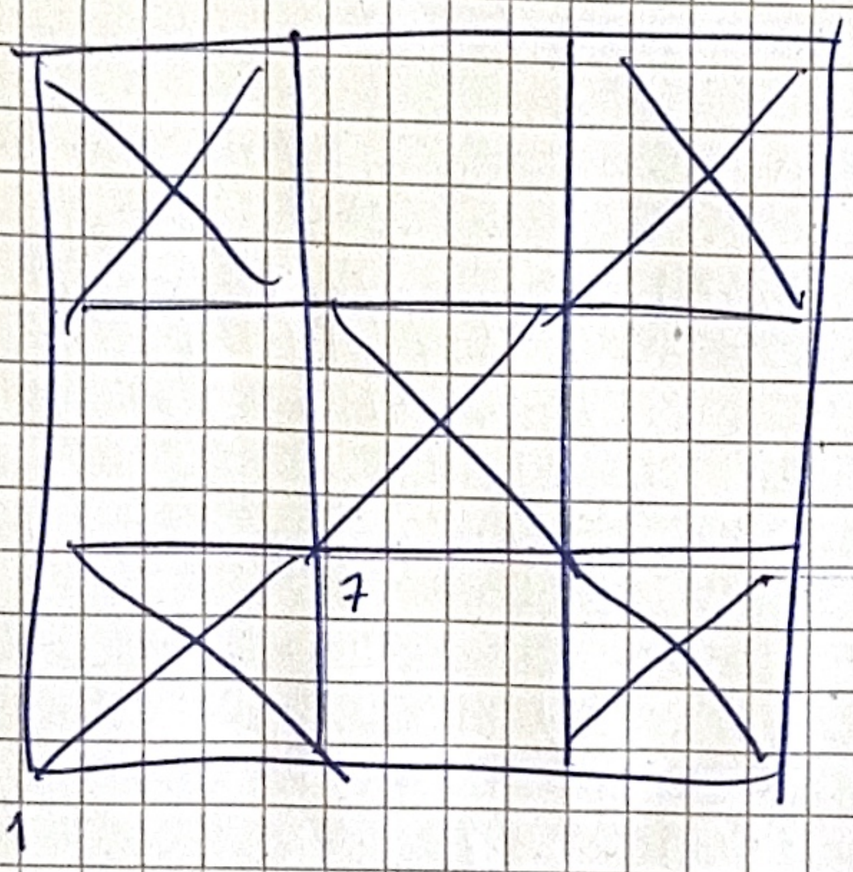
What happens on a full lattice?

Square lattice:



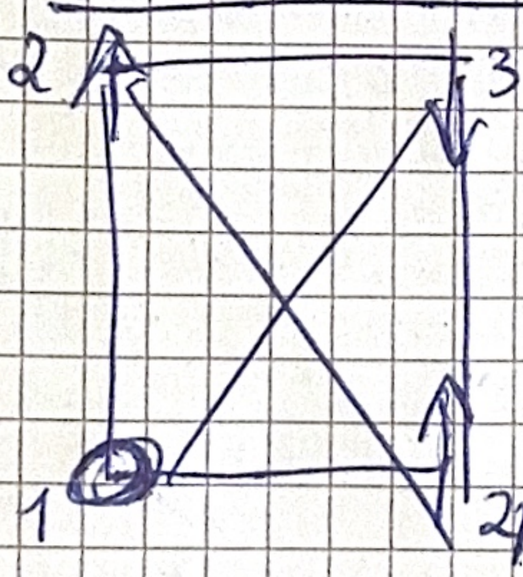
* hole delocalises
* spins ±M.
* (only odd ↔ even even # interchange)

Frustrate the system:

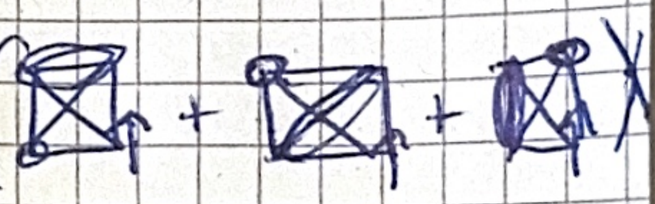


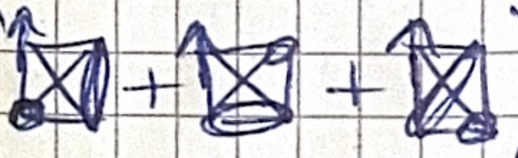
What is the prefered spin config. now, that ~~mini~~ lets the hole deloc. to minimise kinetic energy?

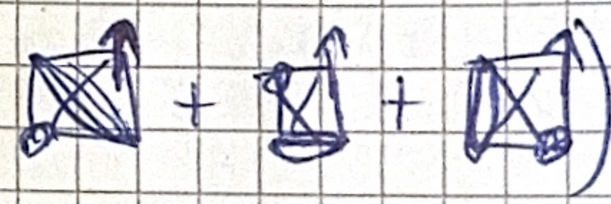
4 sites:



$E_{GS} = -2t$

$|GS_1\rangle = ($  $)$

$|GS_2\rangle = ($  $)$

$|GS_3\rangle = ($  $)$

Hole and singlet resonating on one of the 4 triangles

$|GS_4\rangle = -|GS_1\rangle \mp |GS_2\rangle - |GS_3\rangle$

$$|GS_1\rangle = \frac{1}{\sqrt{3}} c_{10}^{+} (d_{23}^{+} + d_{34}^{+} + d_{42}^{+}) |0\rangle$$

$$|GS_2\rangle = \frac{1}{\sqrt{3}} c_{20}^{+} (d_{13}^{+} + d_{34}^{+} + d_{41}^{+}) |0\rangle$$

$$|GS_3\rangle = \frac{1}{\sqrt{3}} c_{30}^{+} (d_{12}^{+} + d_{24}^{+} + d_{41}^{+}) |0\rangle$$

$$d_{ij}^{+} = \frac{1}{\sqrt{2}} (c_{i\uparrow}^{+} c_{j\downarrow}^{+} - c_{i\downarrow}^{+} c_{j\uparrow}^{+})$$

$$|GS_4\rangle = -(|GS_1\rangle + |GS_2\rangle + |GS_3\rangle)$$

Based on this, we can compute a lower bound on the GS energy of the full checkerboard lattice:

$$H = \sum_{\alpha} H_{\alpha} \qquad \alpha : \boxtimes \text{ unit}$$

$$|\Psi_{GS}\rangle = \sum_{r} |\varphi_r\rangle \qquad r: \text{hole position (arbitary spin config.)}$$

$$\langle \varphi_r | \varphi_{r'} \rangle = \delta_{r,r'} \langle \varphi_r | \varphi_r \rangle$$

$$\langle \Psi_{GS} | \Psi_{GS} \rangle = 1 = \sum_{r'r} \langle \varphi_{r'} | \varphi_r \rangle = \sum_{r} \langle \varphi_r | \varphi_r \rangle$$

Introduce $\boxtimes$ unit states

$$|\chi_{\alpha}\rangle = \sum_{r \in \alpha} |\varphi_r\rangle$$

↑ running over the 4 sites on unit α.

$$E_{GS} = \langle \Psi_{GS} | H | \Psi_{GS} \rangle$$

$$= \sum_{rr'} \langle \varphi_r | H | \varphi_{r'} \rangle$$

$$= \sum_{\langle rr' \rangle} \langle \varphi_r | H | \varphi_{r'} \rangle$$

$$= \sum_{\alpha} \langle \chi_\alpha | H_\alpha | \chi_\alpha \rangle$$

Because $H|\varphi_{r'}\rangle$ only hops the hole ~~from~~ within either of the two α-units containing r', and the overlap is only non-zero with the states in that same unit!

Introduce $p_\alpha = \frac{1}{2} \langle \chi_\alpha | \chi_\alpha \rangle > 0$

$$\sum_\alpha p_\alpha = \frac{1}{2} \sum_\alpha \sum_{r',r \in \alpha} \langle \varphi_{r'} | \varphi_r \rangle$$

$$= \frac{1}{2} \sum_\alpha \sum_{r'r \in \alpha} \delta_{r,r'} \langle \varphi_r | \varphi_r \rangle$$

$$= \frac{1}{2} \cdot 2 \sum_r \langle \varphi_r | \varphi_r \rangle = \sum_r \langle \varphi_r | \varphi_r \rangle$$

$$= \underline{1} \quad \Rightarrow \underline{p_\alpha \text{ is a prob.}}$$

$$E_{GS} = 2 \sum_\alpha p_\alpha \frac{\langle \chi_\alpha | H_\alpha | \chi_\alpha \rangle}{\langle \chi_\alpha | \chi_\alpha \rangle}$$

Assume $E_{GS} < -4t$, then there must exist at least one unit β

$$2 \frac{\langle \chi_\beta | H_\beta | \chi_\beta \rangle}{\langle \chi_\beta | \chi_\beta \rangle} < -\frac{4}{2} t$$

But the unit GS has $E = -2t$.

Thus $\boxed{E_{GS} \geq -4t}$

Can we find an analytical GS meeting $E = -4t$? Yes!

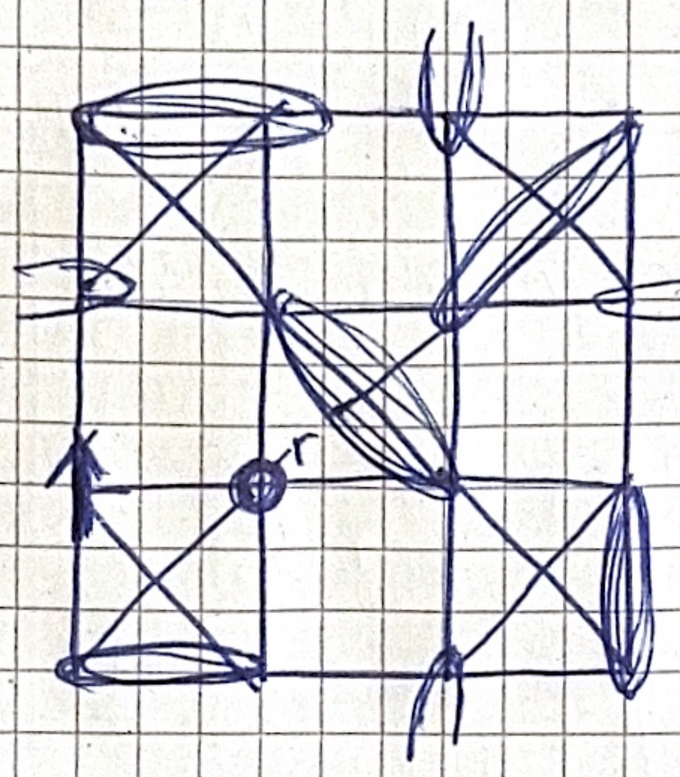
Consider the following wave function:

$$|\Psi_{RVB}\rangle = \frac{1}{\sqrt{\eta N}} \sum_r |\varphi_r^{RVB}\rangle \qquad \eta = \langle \varphi_r^{RVB} | \varphi_r^{RVB} \rangle$$

$$|\varphi_r^{RVB}\rangle = \sum_{a_r} |\Psi_{a_r}\rangle$$

↖ all singlet coverings with one singlet per unit.

a_r :



let $N \to \infty$ # sites so that ↑ can be moved to the boundary.

$$|\Psi_{a_r}\rangle = \prod_{c(ij) \in a_r} d_{ij}^\dagger |0\rangle$$

$$|\Psi_{RVB}^*\rangle = \frac{1}{\sqrt{\eta N}} \sum_r \sum_{a_r} |\Psi_{a_r}\rangle = \frac{1}{\sqrt{\eta N}} \sum_{r,\{a_r\}} \prod_{c(ij) \in a_r} d_{ij}^\dagger |0\rangle$$

$$E_{RVB} = \langle \Psi_{RVB} | H | \Psi_{RVB} \rangle$$

$$= \frac{1}{N} \sum_{\alpha} \langle \chi^{\alpha}_{RVB} | H^{\alpha} | \chi^{\alpha}_{RVB} \rangle$$

$$|\chi^{\alpha}_{RVB}\rangle = \sum_{r \in \alpha} |\varphi_r^{RVB}\rangle = \sum_{r \in \alpha} |\tilde{\psi}_r^{r_1 r_2}\rangle + |\tilde{\psi}_r^{r_2 r_3}\rangle + |\tilde{\psi}_r^{r_1 r_3}\rangle$$

(r_1, r_2, r_3) sites without hole.

$$|\tilde{\psi}_r^{r_i r_j}\rangle = \sum_{ar/de(r_i, r_j)} |\psi_{ar}\rangle$$

↖ dimer cov. with dimer on (r_i, r_j)

$$|\psi^{\alpha}_{RVB}\rangle = \underbrace{\sum_{r \in \alpha, i<j} |\tilde{\psi}_r^{r_i r_j}\rangle}$$

4 . 3 terms = 12 terms

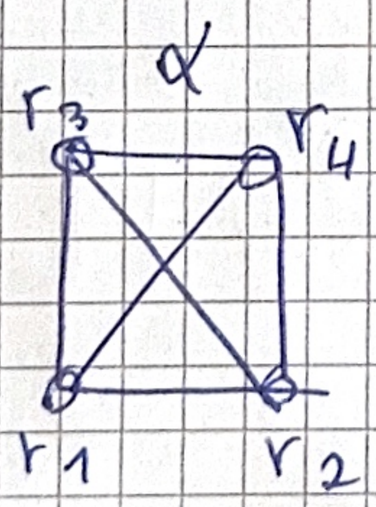
hole pos ↑ ↑ singlets.

Re-group:

$$|\tilde{\psi}_r^{\alpha}\rangle = \underbrace{|\tilde{\psi}_{r_k}^{r_i r_j}\rangle + |\tilde{\psi}_{r_j}^{r_k r_i}\rangle + |\tilde{\psi}_{r_i}^{r_j r_k}\rangle}$$

↑ site without hole or singlet

hole + singlet on (r_i, r_j, r_k) resonating! Eigenstate of a unit!



$$|\chi^{\alpha}_{RVB}\rangle = |\tilde{\psi}^{\alpha}_{r_1}\rangle + |\tilde{\psi}^{\alpha}_{r_2}\rangle + |\tilde{\psi}^{\alpha}_{r_3}\rangle + |\tilde{\psi}^{\alpha}_{r_4}\rangle$$

$$E_{RVB} = \frac{1}{\eta N} \sum_{\alpha} \langle \chi^{\alpha}_{RVB} | H^{\alpha} | \chi^{\alpha}_{RVB} \rangle$$

$$= \frac{1}{\eta N} \sum_{\alpha} \sum_{a_k=1}^{4} \langle \hat{\psi}^{\alpha}_{r_a} | H^{\alpha} | \hat{\psi}^{\alpha}_{r_b} \rangle$$

$$H^{\alpha} | \hat{\psi}^{\alpha}_{r_b} \rangle = -2t | \hat{\psi}^{\alpha}_{r_\alpha} \rangle$$

$$E_{RVB} = \frac{1}{\eta N} \sum_{\alpha} \sum_{a,b=1}^{4} (-2t) \langle \hat{\psi}^{\alpha}_{r_a} | \hat{\psi}^{\alpha}_{r_b} \rangle$$

$$= \frac{-2t}{\eta N} \sum_{\alpha} \underbrace{\langle \chi^{\alpha}_{RVB} | \chi^{\alpha}_{RVB} \rangle}_{\sum_{r \in \alpha} \langle \phi_r^{RVB} | \phi_r^{RVB} \rangle}$$

$$= \eta$$

$$= -4t \frac{1}{N} \sum_{r} 1$$

$$= -4t$$

$\Rightarrow |\Psi_{RVB}\rangle$ is a ground state of H.

This GS is the so-called resonating-valence bond state (RVB)

with one fully delocalised hole

~~spin~~ un-paired spin at boundary

+ thermodyn. Limit

$\Rightarrow$ spin-charge sep.