Antiferromagnetism

$$H = \sum_{xy\sigma} t_{xy} c^\dagger_{x\sigma} c_{y\sigma} + \sum_x U_x n_{x\uparrow} n_{x\downarrow}$$

$x \in \Lambda$ (a collection of points, could be a lattice)
$|\Lambda|$ = # of sites in Λ (our old N)

Note, now U_x can depend on the lattice site
$t_{xy} = t_{yx}$ = real hopping matrix and connected $\Rightarrow$ there is a path of bonds $t_{xy} \neq 0$ between any two points in Λ.

Theorem 1: attractive case Assume $U_x \leq 0$ for all x and M = # of electrons and is even
Then the ground state includes one with $S=0$
If $U_x < 0$ for all x, then the ground state is unique.

Note, as $U \to 0$ this is true, since we have discrete levels from the band structure $\varepsilon(k)$ and we fill with $\uparrow\downarrow$ in each level. We only have degeneracies with higher spin states if the band structure has degeneracies at the fermi energy.

As $U \to -\infty$ it is true since the ground state is constructed out of the bound $\uparrow\downarrow$ states on each site which are lowest in energy.

Proof: since S^2 and S^z are conserved, we can work in the $S^z = 0$ subspace with $N_\uparrow = N_\downarrow = M/2$.

Let $\{\psi_\alpha\}$ be basis functions for n spinless electrons. There are $\binom{|\Lambda|}{n} = m$ such basis functions. We choose these basis functions to all be real.

The ground state $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_{\alpha\beta} W_{\alpha\beta}\, \psi_\uparrow^\alpha \otimes \psi_\downarrow^\beta$$

with $W_{\alpha\beta}$ an $m\times m$ matrix, that we can assume without loss of generality, to be Hermitian. $W_{\alpha\beta} = W^*_{\beta\alpha}$

$$\langle\psi|\psi\rangle = \sum_{\alpha\beta\gamma\delta} \underbrace{(\psi_\uparrow^\alpha \otimes \overbrace{\psi_\downarrow^\beta)^\dagger W^*_{\alpha\beta} W_{\gamma\delta} (\psi_\uparrow^\gamma}_{\delta_{\alpha\gamma}} \otimes \psi_\downarrow^\delta)}^{\delta_{\beta\delta}}$$

$$= \sum_{\alpha\beta} |W_{\alpha\beta}|^2 = \sum_{\alpha\beta} W_{\alpha\beta} W_{\beta\alpha} = \operatorname{Tr} W^2$$

↑ Hermiticity

$$\langle\psi|\psi\rangle = \operatorname{Tr} W^2 = 1$$

$$\langle\psi|\hat{T}|\psi\rangle = \sum_{\alpha\beta\gamma\delta} W^*_{\alpha\beta} (\psi_\uparrow^\alpha \otimes \psi_\downarrow^\beta)^\dagger \sum_{xy} t_{xy} (c^\dagger_{x\uparrow} c_{y\uparrow} + c^\dagger_{x\downarrow} c_{y\downarrow}) W_{\gamma\delta} (\psi_\uparrow^\gamma \otimes \psi_\downarrow^\delta)$$

$$= \sum_{\alpha\beta\gamma\delta} \Big[W^*_{\alpha\beta} \langle \psi_\uparrow^\alpha | \sum_{xy} t_{xy} c^\dagger_{x\uparrow} c_{y\uparrow} | \psi_\uparrow^\gamma\rangle W_{\gamma\delta} \delta_{\beta\delta}$$
$$+ W^*_{\alpha\beta} \langle \psi_\downarrow^\beta | \sum_{xy} t_{xy} c^\dagger_{x\downarrow} c_{y\downarrow} | \psi_\downarrow^\delta\rangle W_{\gamma\delta} \delta_{\alpha\gamma} \Big]$$

Define $K_{\alpha\beta} = \langle \psi^\alpha | \sum_{xy} t_{xy} c^\dagger_x c_y | \psi^\beta\rangle$ then

K is real & symmetric because t and ψ are

$$\langle\psi|\hat{T}|\psi\rangle = \sum_{\alpha\beta\gamma} \left[W^*_{\alpha\beta} K_{\alpha\gamma} W_{\gamma\beta} + W^*_{\alpha\beta} K_{\beta\gamma} W_{\alpha\gamma} \right]$$

$$= \operatorname{Tr} K W^2 + \operatorname{Tr} W^2 K^T = 2 \operatorname{Tr} K W^2$$

since $K^T = K^\dagger$ $\quad W^2 K^\dagger = (K W^{\dagger 2})^\dagger = (K W^2)^\dagger$ but $\operatorname{Tr} M^\dagger = \operatorname{Tr} M$ for ~~real symmetric~~ Hermitian M.

$$\langle\psi|G|\psi\rangle = \sum_x U_x \sum_{\alpha\beta\gamma\delta} (\psi_\uparrow^\alpha \otimes \psi_\downarrow^\beta)^\dagger W_{\alpha\beta}^* \, n_{x\uparrow} n_{x\downarrow} \, \psi_\uparrow^\gamma \otimes \psi_\downarrow^\delta W_{\gamma\delta}$$

$$= \sum_x U_x \sum_{\alpha\beta\gamma\delta} W_{\alpha\beta}^* \langle\psi_\uparrow^\alpha | n_{x\uparrow} | \psi_\uparrow^\gamma\rangle \langle\psi_\downarrow^\beta | n_{x\downarrow} | \psi_\downarrow^\delta\rangle W_{\gamma\delta}$$

Define $(L_x)_{\alpha\beta} = \langle\psi^\alpha | n_x | \psi^\beta\rangle$ $\quad (L_x)_{\alpha\beta} = (L_x)_{\beta\alpha}$ since ψ's are all real

$$= \sum_x U_x \sum_{\alpha\beta\gamma\delta} W_{\alpha\beta}^* (L_x)_{\alpha\gamma} W_{\gamma\delta} (L_x)_{\beta\delta}$$

$$= \sum_x U_x \sum_{\alpha\beta\gamma\delta} W_{\beta\alpha} (L_x)_{\alpha\gamma} W_{\gamma\delta} (L_x)_{\delta\beta}$$

$$= \sum_x U_x \, \mathrm{Tr}\,[W L_x W L_x]$$

$$E(W) = \langle\psi|H|\psi\rangle = 2\,\mathrm{Tr}\,(K W^2) + \sum_x U_x \,\mathrm{Tr}(W L_x W L_x)$$

when $\mathrm{Tr}\, W^2 = 1$

Now consider a positive semidefinite matrix $|W|$

$$|W| = \sqrt{W^2}$$

determined by diagonalizing W $\quad \begin{pmatrix} W_1 & 0 & 0 & 0 \\ 0 & W_2 & & \\ 0 & & W_3 & \\ 0 & & & \ddots \end{pmatrix}$

and forming

$$|W| = \begin{pmatrix} |W_1| & 0 & 0 & \\ 0 & |W_2| & 0 & \\ 0 & 0 & |W_3| & \\ & & & \ddots \end{pmatrix} = \text{matrix square root}$$

In general, $|W| \neq |W_{\alpha\beta}|$. That holds only in the basis where $|W|$ is diagonal.

Let's examine $E(W)$ in the diagonal basis

obviously $\mathrm{Tr}\, K W^2 = \mathrm{Tr}\, K |W|^2$

and $\mathrm{Tr}\, W L_x W L_x = \sum_{ij} W_i W_j (L_x)_{ij} (L_x)_{ji}$

$$= \sum_{ij} W_i W_j |(L_x)_{ij}|^2 \leq \sum_{ij} |W_i||W_j| \, |(L_x)_{ij}|^2$$

$$\leq \mathrm{Tr}\, |W| L_x |W| L_x$$

since $U_x \le 0$, we have

$$E(|W|) \le E(W)$$

$\Rightarrow$ among all ground states, there is one with

$$W = |W|$$

Note that normalization says

$$\mathrm{Tr}\, W^2 = \sum_{i=1}^{\infty} w_i^2 = 1 \Rightarrow \mathrm{Tr}\,|W| = \sum_i |w_i| \neq 0$$

so we work in the x-space basis for ψ_α

$$\psi_\alpha = c^+_{x_1} c^+_{x_2} \cdots |0\rangle$$

Then $\mathrm{Tr}\,|W| = \sum_\alpha W_{\alpha\alpha} \neq 0$

$\Rightarrow$ the vector $\psi^\alpha_\uparrow \otimes \psi^\alpha_\downarrow$ is in the ground state expansion

but $S=0$ for this state $\Rightarrow$ projection onto $S=0$

So the ground state has a spin singlet state.

Proof of uniqueness is straightforward, but we don't have enough time to do so here.

Theorem 2: Assume $U_x = U > 0$ independent of x.

Assume $|\Lambda|$ is even and Λ is bipartite. Let $M = |\Lambda| =$ half-filled band. Then $S = \frac{1}{2}(|B| - |A|) = 0$ for most bipartite lattices

proof: Need to do the partial particle-hole transformation which changes $U \to -U$ $\quad N_\uparrow \to |\Lambda| - N_\uparrow \quad N_\downarrow \to N_\downarrow$

$N_\uparrow + N_\downarrow = |\Lambda| \Rightarrow \quad |\Lambda| - N_\uparrow + N_\downarrow = |\Lambda| \Rightarrow N_\uparrow = N_\downarrow$

but GS for attractive case with $N_\uparrow = N_\downarrow$ has $S=0$ and is unique ~~for~~ by theorem 1, $\Rightarrow J=0$ is unique ground state for repulsive case.

Consider the case of U very large.

No double occupancy is allowed

$\Rightarrow$ at $U = \infty$ all spin configurations are degenerate

What about finite but large U?

$\uparrow \overset{t}{\leftrightarrow} \uparrow$ (i, j) no shift to second order

since cannot have $\uparrow\uparrow$ (i) 0 (j)

but $\uparrow \overset{t}{\leftrightarrow} \downarrow$ (i, j) $\uparrow\downarrow$ (i) 0 (j) or 0 (i) $\uparrow\downarrow$ (j)

$\Rightarrow$ spin singlet state is shifted down in energy proportional to t^2/U

In general find Hamiltonian for large U maps onto

$$h = \frac{2}{U} \sum_{xy} t_{xy}^2 \left(\vec{S}_x \cdot \vec{S}_y - \frac{1}{4} \right)$$

For large U at half filling

ground state of this Hamiltonian is known to have

$$S = \tfrac{1}{2}(|B| - |A|)$$

$\Rightarrow$ since ground state is non degenerate, S cannot change

$\Rightarrow$ $S = \frac{1}{2}(|B| - |A|)$ at half filling for the Hubbard model!