

Anti ferromagnetism

$$H = \sum_{x,y \in \Lambda} t_{xy} c_x^\dagger c_y + \sum_x U_x n_{x\uparrow} n_{x\downarrow}$$

$x \in \Lambda$ (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

$t_{xy} = t_{yx} = \text{real hopping matrix}$ 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 $U \rightarrow 0$ this is true, since we have discrete levels from the band structure $\epsilon(k)$ 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 $U \rightarrow -\infty$ it is true since the ground state is constructed out of the band $\uparrow\downarrow$ 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 $\binom{2n}{n} = m$ 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. $W_{\alpha\beta} = W_{\beta\alpha}^*$

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

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

↑ Hermiticity

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

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

$$= \sum_{\alpha\beta\gamma\delta} \left[W_{\alpha\beta}^* \langle \psi_{\uparrow}^{\alpha} | \sum_{xy} t_{xy} c_{x\uparrow}^{\dagger} c_{y\uparrow} | \psi_{\uparrow}^{\gamma} \rangle W_{\gamma\delta} \delta_{\beta\delta} + W_{\alpha\beta}^* \langle \psi_{\downarrow}^{\beta} | \sum_{xy} t_{xy} c_{x\downarrow}^{\dagger} c_{y\downarrow} | \psi_{\downarrow}^{\delta} \rangle W_{\gamma\delta} \delta_{\alpha\gamma} \right]$$

Define $K_{\alpha\beta} = \langle \psi_{\uparrow}^{\alpha} | \sum_{xy} t_{xy} c_{x\uparrow}^{\dagger} c_{y\uparrow} | \psi_{\uparrow}^{\beta} \rangle$ then K is real & symmetric because t and ψ are

$$\langle \psi | \hat{T} | \psi \rangle = \sum_{\alpha\beta\gamma} \left(W_{\alpha\beta}^* K_{\alpha\gamma} W_{\gamma\beta} + W_{\alpha\beta}^* K_{\beta\gamma} W_{\alpha\gamma} \right)$$

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

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

$$\begin{aligned} \langle \psi | G | \psi \rangle &= \sum_x U_x \sum_{\alpha\beta\gamma\delta} (\psi_\uparrow^\alpha \otimes \psi_\downarrow^\beta)^\dagger W_{\alpha\beta}^* \mathcal{N}_{x\uparrow} \mathcal{N}_{x\downarrow} \psi_\uparrow^\gamma \otimes \psi_\downarrow^\delta W_{\gamma\delta} \\ &= \sum_x U_x \sum_{\alpha\beta\gamma\delta} W_{\alpha\beta}^* \langle \psi_\uparrow^\alpha | \mathcal{N}_{x\uparrow} | \psi_\uparrow^\gamma \rangle \langle \psi_\downarrow^\beta | \mathcal{N}_{x\downarrow} | \psi_\downarrow^\delta \rangle W_{\gamma\delta} \end{aligned}$$

Define $(L_x)_{\alpha\beta} = \langle \psi_\uparrow^\alpha | \mathcal{N}_{x\uparrow} | \psi_\uparrow^\beta \rangle$ $(L_x)_{\alpha\beta} = (L_x)_{\beta\alpha}$ since ψ 's are all real

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

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

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

$$E(w) = \langle \psi | H | \psi \rangle = 2 \text{Tr} [K w^2] + \sum_x U_x \text{Tr} (W L_x W L_x)$$

when $\text{Tr} w^2 = 1$

Now consider a positive semidefinite matrix $|W|$

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

determined by diagonalizing W^2

$$\begin{pmatrix} w_1 & 0 & 0 & 0 \\ 0 & w_2 & & \\ 0 & & w_3 & \\ 0 & & & \ddots \end{pmatrix}$$

and forming

$$|W| = \begin{pmatrix} |w_1| & 0 & 0 & \\ 0 & |w_2| & & \\ 0 & 0 & |w_3| & \\ & & & \ddots \end{pmatrix} = \text{matrix square root}$$

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

$$\text{obviously } \text{Tr} K w^2 = \text{Tr} K |w|^2$$

$$\text{and } \text{Tr} W L_x W L_x = \sum_{ij} w_i w_j (L_x)_{ij} (L_x)_{ji}$$

$$= \sum_{ij} w_i w_j |(L_x)_{ij}|^2 \leq \sum_{ij} |w_i| |w_j| |(L_x)_{ij}|^2$$

$$\leq \text{Tr} |W| L_x |W| L_x$$

since $U_x \leq 0$, we have

$$E(|w\rangle) \leq E(w)$$

\Rightarrow among all ground states, there is one with

$$W = |w\rangle$$

Note that normalization says

$$\text{Tr } W^2 = \sum_{i=1}^{\infty} w_i^2 = 1 \Rightarrow \text{Tr } |w\rangle = \sum_i |w_i| \neq 0$$

So we work in the x -space basis for ψ_x

$$\psi_x = c_{x_1}^+ c_{x_2}^+ \dots |0\rangle$$

$$\text{Then } \text{Tr } |w\rangle = \sum_x w_x \neq 0$$

\Rightarrow the vector $\psi_{\uparrow}^{\dagger} \otimes \psi_{\downarrow}^{\dagger}$ 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 straight forward, 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 $U \rightarrow -U$ $N_{\uparrow} \rightarrow |\Lambda| - N_{\uparrow}$ $N_{\downarrow} \rightarrow N_{\downarrow}$

$$N_{\uparrow} + N_{\downarrow} = |\Lambda| \Rightarrow |\Lambda| - N_{\uparrow} + N_{\downarrow} = |\Lambda| \Rightarrow N_{\uparrow} = N_{\downarrow}$$

but $G=0$ for attractive case with $N_{\uparrow} = N_{\downarrow}$ has $S=0$ and

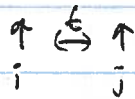
is unique ~~for~~ by theorem 1, $\Rightarrow S=0$ is unique ground state for repulsive case.

Consider the case of U very large.

No double occupancy is allowed

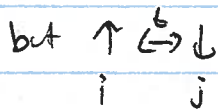
\Rightarrow at $U \rightarrow \infty$ all spin configurations are degenerate

What about finite but large U ?



no shift to second order

since cannot have $\begin{array}{cc} \uparrow \uparrow & 0 \\ i & j \end{array}$



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

In general find Hamiltonian for large U maps onto

$$H = \sum_U \sum_{xy} t_{xy}^2 (\vec{S}_x \cdot \vec{S}_y - \frac{1}{4})$$

for large U at half filling

ground state of this Hamiltonian is known to have

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

\Rightarrow ^{since} ground state is non degenerate, S cannot change

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