Phys 506 lecture 41: Antiferromagnetism

1 Introduction

Recall the general Hubbard Hamiltonian

$$H = \sum_{xy\sigma} t_{xy} \hat{c}^{\dagger}_{x\sigma} \hat{c}_{y\sigma} + \sum_{x} U_x \hat{n}_{x\uparrow} \hat{n}_{x\downarrow}$$

where $x \in \Lambda$ where Λ is a collection of points, like lattice sites. Then $|\Lambda|$ is the number of points in Λ (what we used to call N). Note that U_x can now depend on the lattice site.

Further note that $t_{xy} = t_{yx}$ are elements of a real hopping matrix which is also *connected*. This means that there is a path of bonds $t_{xy} \neq 0$ between any two points in Λ.

2 Attractive case

Theorem 1: (Attractive Case) Assume $U_x \leq 0$ for all $x \in \Lambda$ and M is an even number of electrons. Then, the ground state includes one with $s = 0$. If $U_x < 0$ for all $x \in \Lambda$, then the ground state is unique.

Some comments: Note, as $U \to 0$ 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 spins states if the band structure has degeneracies at the Fermi level.

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 $N_\uparrow = N_\downarrow = \frac{M}{2}$. Then, 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

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

where W is an $m \times m$ matrix. Without loss of generality, we can say W is Hermitian so that $W_{\alpha\beta} = W^*_{\beta\alpha}$.

$$\begin{aligned}\langle\psi|\psi\rangle &= \sum_{\alpha\beta\gamma\delta} (\psi^\alpha_\uparrow \otimes \psi^\beta_\downarrow)^\dagger\, W^*_{\alpha\beta} W_{\gamma\delta}\, (\psi^\gamma_\uparrow \otimes \psi^\delta_\downarrow) \\ &= \sum_{\alpha\beta} |W_{\alpha\beta}|^2 = \sum_{\alpha\beta} W_{\alpha\beta} W_{\beta\alpha} = \mathrm{Tr}(W^2)\end{aligned}$$

where we made use of orthonormality of the basis functions and the Hermiticity of W. Then,

$$\begin{aligned}\left\langle \psi \middle| \hat{T} \middle| \psi \right\rangle &= \sum_{\alpha\beta\gamma\delta} W^*_{\alpha\beta} (\psi^\alpha_\uparrow \otimes \psi^\beta_\downarrow)^\dagger \sum_{xy} t_{xy} (\hat{c}^\dagger_{x\uparrow}\hat{c}_{y\uparrow} + \hat{c}^\dagger_{x\downarrow}\hat{c}_{y\downarrow}) W_{\gamma\delta} (\psi^\alpha_\uparrow \otimes \psi^\beta_\downarrow) \\ &= \sum_{\alpha\beta\gamma\delta} \left(W^*_{\alpha\beta} \left\langle \psi^\alpha_\uparrow \middle| \sum_{xy} t_{xy} \hat{c}^\dagger_{x\uparrow}\hat{c}_{y\uparrow} \middle| \psi^\gamma_\uparrow \right\rangle W_{\gamma\delta}\delta_{\beta\delta} + W^*_{\alpha\beta} \left\langle \psi^\beta_\downarrow \middle| \sum_{xy} t_{xy} \hat{c}^\dagger_{x\downarrow}\hat{c}_{y\downarrow} \middle| \psi^\delta_\downarrow \right\rangle W_{\gamma\delta}\delta_{\alpha\gamma} \right)\end{aligned}$$

Define:

$$K_{\alpha\beta} = \left\langle \psi^\alpha \middle| \sum_{xy} t_{xy} \hat{c}^\dagger_x \hat{c}_y \middle| \psi^\beta \right\rangle$$

Then,

$$\begin{aligned}\left\langle \psi \middle| \hat{T} \middle| \psi \right\rangle &= \sum_{\alpha\beta\gamma} \left(W^*_{\alpha\beta} K_{\alpha\gamma} W_{\gamma\beta} + W^*_{\alpha\beta} K_{\beta\gamma} W_{\alpha\gamma} \right) \\ &= \mathrm{Tr}(KW^2) + \mathrm{Tr}(W^2 K^T) = 2\mathrm{Tr}(KW^2)\end{aligned}$$

since $K^T = K^\dagger$ and $W^2 K^\dagger = (KW^{\dagger 2}) = (KW^2)^\dagger$. We can also calculate

$$\begin{aligned}\left\langle \psi \middle| \hat{U} \middle| \psi \right\rangle &= \sum_x U_x \sum_{\alpha\beta\gamma\delta} (\psi^\alpha_\uparrow \otimes \psi^\beta_\downarrow)^\dagger W^*_{\alpha\beta} \hat{n}_{x\uparrow}\hat{n}_{x\downarrow} (\psi^\gamma_\uparrow \otimes \psi^\delta_\downarrow) W_{\gamma\delta} \\ &= \sum_x U_x \sum_{\alpha\beta\gamma\delta} W^*_{\alpha\beta} \left\langle \psi^\alpha_\uparrow \middle| \hat{n}_{x\uparrow} \middle| \psi^\gamma_\uparrow \right\rangle \left\langle \psi^\beta_\downarrow \middle| \hat{n}_{x\downarrow} \middle| \psi^\delta_\downarrow \right\rangle W_{\gamma\delta}.\end{aligned}$$

Define $(L_x)_{\alpha\beta} = \left\langle \psi^\alpha \middle| \hat{n}_x \middle| \psi^\beta \right\rangle$. Note $(L_x)_{\alpha\beta} = (L_x)_{\beta\alpha}$ since all ψ's are real.

$$\begin{aligned}\left\langle \psi \middle| \hat{U} \middle| \psi \right\rangle &= \sum_x U_x \sum_{\alpha\beta\gamma\delta} W^*_{\alpha\beta} (L_x)_{\alpha\gamma} W_{\gamma\delta} (L_x)_{\beta\delta} \\ &= \sum_x U_x \sum_{\alpha\beta\gamma\delta} W_{\beta\alpha} (L_x)_{\alpha\gamma} W_{\gamma\delta} (L_x)_{\delta\beta} \\ &= \sum_x U_x\ \mathrm{Tr}(W L_x W L_x).\end{aligned}$$

So $E(W) = \langle\psi|H|\psi\rangle = 2\mathrm{Tr}(KW^2) + \sum_x U_x\ \mathrm{Tr}(W L_x W L_x)$ when $\mathrm{Tr}(W^2) = 1$. Now consider a positive semidefinite matrix $|W|$ where $|W| = \sqrt{W^2}$, which is determined by diagonalizing W and forming

$$|W| = \begin{pmatrix} |w_1| & 0 & 0 & \\ 0 & |w_2| & 0 & \\ 0 & 0 & |w_3| & \\ & & & \ddots \end{pmatrix}.$$

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 $\text{Tr}(KW^2) = \text{Tr}(K|W|^2)$ and

$$\begin{aligned}\text{Tr}(WL_xWL_x) &= \sum_{ij} W_iW_j(L_x)_{ij}(L_x)_{ji} \\ &= \sum_{ij} W_iW_j|(L_x)_{ij}|^2 \leq \sum_{ij} |W_i||W_j||(L_x)_{ij}|^2 \\ &\leq \text{Tr}(|W|L_x|W|L_x).\end{aligned}$$

Since $U_x \leq 0$, we have $E(|W|) \leq E(W)$. Among all ground states, there is one with $W = |W|$. Note that normalization says

$$\text{Tr}(W^2) = \sum_{i=1}^{\infty} W_i^2 = 1 \implies \text{Tr}|W| = \sum_i |w|_i \neq 0,$$

so we work in coordinate representation for ψ_α

$$\psi_\alpha = \hat{c}^\dagger_{x1}\hat{c}^\dagger_{x2}\cdots|0\rangle\,.$$

Then $\text{Tr}(W) = \sum_\alpha W_{\alpha\alpha} \neq 0$. Therefore, the vector $\psi^\alpha_\uparrow \otimes \psi^\alpha_\downarrow$ is in the ground state expansion. But $S = 0$ for this state so the ground state has a spin singlet state.

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

3 Proof in the repulsive case

Theorem 2: Assume $U_x = U > 0$ is independent of x. Assume $|\Lambda|$ is even 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 $U \mapsto -U$, $N_\uparrow \mapsto |\Lambda| - N_\uparrow$, $N_\downarrow \mapsto N_\downarrow$. This gives us $N_\uparrow + N_\downarrow = |\Lambda| \implies |\Lambda| - N_\uparrow + N_\downarrow = |\Lambda| \implies N_\uparrow = N_\downarrow$ but the ground state for the attractive case with $N_\uparrow = N_\downarrow$ has $S = 0$ and is unique by theorem 1. Hence $J = 0$ is the unique ground state for the repulsive case.

Consider the case of a very large U. No double occupancy is allowed. Then, at $U = \infty$ all spin configurations are degenerate. But what about finite, but large U?

The singlet state is shifted down in energy proportional to t^2/U. In general, we find that the Hamiltonian for large U maps onto

$$\hat{H}(U \to \infty) \to \frac{2}{U}\sum_{xy} t_{xy}^2 \left(\mathbf{S}_x \cdot \mathbf{S}_y - \frac{1}{4}\right)$$

for large U at half filling. The ground state of this Hamiltonian is known to have $S = \frac{1}{2}(|B| - |A|)$ and since the ground state is nondegenerate, S cannot change.

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

at half-filling for the Hubbard model!