Phys 506 lecture 40: Nagaoka ferromagnetism

1 Nagaoka ferromagnetism

We begin with the general form of the Hubbard model Hamiltonian:

$$H = \sum_{ij} t_{ij}(\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{1\downarrow}\hat{c}_{j\downarrow}) + U\sum_i n_{i\uparrow}n_{i\downarrow}.$$

Note that we now have a hopping matrix. The condition on t_{ij} is that $t_{ij} \geq 0$, otherwise arbitrary and $t_{ij} = t_{ji}$.

Suppose the lattice has N sites. Consider the limit $U \to \infty$ and $N_e = \#$ of electrons $= N - 1$.

With $U = \infty$ there is no double occupancy. So we can use the following set of states as a basis

$$|i,\sigma\rangle = (-1)^i \hat{c}^\dagger_{1\sigma_1}\hat{c}^\dagger_{2\sigma_2}\hat{c}^\dagger_{3\sigma_3}\cdots\hat{c}^\dagger_{i-1,\sigma-1}\hat{c}^\dagger_{i+1,\sigma+1}\cdots\hat{c}^\dagger_{i_N,\sigma_N}|0\rangle$$

This state has spins $\{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ for the $N-1$ electrons and a hole at site i.

Two sites $|i,\sigma\rangle$ and $|j,\tau\rangle$ are said to be connected if $\left\langle j\tau\middle|\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow}\middle|i\sigma\right\rangle \neq 0$. We say $(i\sigma) \longleftrightarrow (j\tau)$ the state $|i\sigma\rangle$ is connected to the state $|j\tau\rangle$.

If $(i\sigma) \longleftrightarrow (j\tau)$ then all $\sigma_\alpha = \tau_\alpha$ except $\alpha = i$ and j

$$\sigma_j = \tau_i \quad \sigma_i = \tau_j = 0$$

In taking $(\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow})|i\sigma\rangle$ into $|j\tau\rangle$ form, we need to move the $\hat{c}^\dagger_{j\sigma_j}$ operator from the j location to the i location. This brings a factor of $(-1)^{j-i+1}$ due to the minus signs on interchanging each creation operator.

So $(\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow})|i\sigma\rangle = (-1)|j\tau\rangle$ hence

$$\left\langle j\tau\middle|t_{ij}(\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow})\middle|i\sigma\right\rangle = -t_{ij}$$

We say a lattice satisfies the *connectivity condition* if for every state $|i\sigma\rangle$ with a fixed value of S_z there is a finite chain

$$(i\sigma_1) \longleftrightarrow (j\sigma_2) \longleftrightarrow (k\sigma_3) \longleftrightarrow \cdots \longleftrightarrow (l,\sigma_n)$$

that connects each state $(i\sigma_1)$ to $(l\sigma_n)$.

This turns out to be true for any lattice where for each site i we have either $t_{ij}t_{jk}t_{ki} \neq 0$ for some jk or $t_{ij}t_{jk}t_{kl}t_{li}$ for jkl and there is at least one site other than site i that is connected to all other sites via a path of t's that does not pass through site i.

We won't prove this here, but the square lattice, triangular lattice, simple cubic, bcc, fcc, etc. all satisfy this. The one-dimensional lattice with nn hopping does not.

2 Variational argument for the ground state

Let $|\psi\rangle = \sum_{(i\sigma)} \psi_{i\sigma} |i\sigma\rangle$ be a unit norm state. $\psi_{i\sigma}$ are numbers and $\langle\psi|\psi\rangle = \sum_{(i\sigma)} |\psi_{i\sigma}|^2 = 1$.

Choose

$$|\phi\rangle = \sum_i \phi_i \, |i\{\sigma\}\rangle$$

where all spins are up except for a hole at site i. $|\phi\rangle$ has $s = s_{max} = \frac{N-1}{2}$. Let $\phi_i = (\sum_\sigma |\psi_{i\sigma}|^2)^{1/2}$ be real. Then $\langle\phi|\phi\rangle = 1$. Also

$$\begin{aligned}\left\langle \psi \middle| \sum_{ij} t_{ij}(\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow}) \middle| \psi \right\rangle &= \sum_{\sigma\tau}\sum_{ij}(-t_{ij})\psi^*_{j\tau}\psi_{i\sigma} \geq \sum_{ij}(-t_{ij})\phi^*_j\phi_i \\ &= \left\langle \phi \middle| \sum_{ij} t_{ij}(\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow}) \middle| \phi \right\rangle .\end{aligned}$$

The inequality comes from the Schwartz inequality

$$\langle a|b\rangle = \sum_\alpha a^*_\alpha b_\alpha \leq \sqrt{\sum_\alpha |a_\alpha|^2}\sqrt{\sum_\beta |b_\beta|^2}$$

$$a \cdot b \leq |a||b|$$

Proof:

$$\langle a - \lambda b | a - \lambda b\rangle \geq 0$$

$$|a|^2 - 2\lambda a \cdot b + \lambda^2 |b|^2 \geq 0$$

$$a \cdot b \leq \frac{1}{2\lambda}|a|^2 + \frac{\lambda}{2}|b|^2$$

which is true for all λ. Let's choose $\frac{|a|}{|b|}$. Then,

$$a \cdot b \leq \frac{1}{2}|a||b| + \frac{1}{2}|a||b| = |a||b|$$

For us, choose $a_\sigma = \psi_{j\tau}$ and $b_\tau = \psi_{i\sigma}$. Then,

$$\sqrt{\sum_\sigma |a_\sigma|^2} = \phi_j \quad \sqrt{\sum_\sigma |b_\sigma|^2} = \phi_i.$$

If $|\psi\rangle$ is a ground state

$$\left\langle \psi \middle| \sum_{ij} t_{ij}(\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow}) \middle| \psi \right\rangle = E_{gs}.$$

But, then $|\phi\rangle$ has energy

$$\left\langle \phi \middle| \sum_{ij} t_{ij}(\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow}) \middle| \phi \right\rangle \leq E_{gs},$$

so we must have equality. If $|\psi\rangle$ is a ground state, then $|\phi\rangle$ is also a ground state. Hence, the system has a ferromagnetic ground state. There is an alternate proof using the Perron-Frobenius theorem.

3 Frobenius-Perron-theorem-based proof

Let M be a matrix with $M_{ij} \geq 0$ for $i \neq j$ (M_{ii} can be anything). If M_{ij} is connected, then the eigenstate of M with maximal eigenvalue is unique and has all basis vectors with strictly positive coefficients.

Proof: Let m be the smallest diagonal element $M_{ij} \geq m$. Then, consider $M'_{ij} = M_{ij} + |m|\delta_{ij}$. This matrix has $M'_{ij} \geq 0$ for all i and j and $E' = E + |m|$.

Suppose ψ_i is an eigenvector of M' and some ψ_1 are less than zero and E' is the largest eigenvalue. Then,

$$\sum_j M'_{ij}\psi_j = E'\psi_i$$

Now consider $\phi_i = |\psi_i|$. It can be shown that

$$\sum_j M'_{ij}\phi_j \leq E'\phi_i$$

because all $m'_{ij} \geq 0$ and $\phi_j \geq 0$ so all terms on the LHS are greater than 0 but not necessarily so for $\sum_j M'_{ij}\psi_j$ since ψ_j could be less than zero $\implies$ ϕ_i would have a larger eigenvalue than E' which is a contradiction so we must have $\phi_i \geq 0$ for the largest eigenvalue.

Furthermore, if M'_{ij} is connected, then $\phi_i \geq 0$ for all i. Consider

$$\sum_j M'_{ij}\phi_j = E'\phi_i$$

and suppose $\phi_k = 0$. But k is connected to some k' by a nonzero $M'_{kk'}$

$$\implies (pos) + M'_{kk'}\phi_{k'} = E'\phi_k$$

since $E' \neq 0 \implies \phi_k \neq 0$. To prove the Nagaoka theorem we apply to $M = -H$.

4 Summary

For $U = \infty$ and $M = N-1$ and t_{ij} all nonnegative, the ground state includes a state with $s = \frac{N-1}{2}$. If lattice is connected, the ground state is unique so the ground state is $s = \frac{N-1}{2}$.

For a bipartitite lattice, result holds for both signs of t, since we can change the sign of t with a unitary transformation.

Find result (ferromagnet) holds also for U finite but U_{crit} can be very large.

If $M = N - 2$, the ground state is usually a spin singlet (not proven in general).

Important question: Does ferromagnetism survive a finite density away from half-filling?

For 1D it never does for finite U. For $d \to \infty$ unsaturated-ferromagnetism appears to be present.