Nagaoka Ferromagnetism

$$H = \sum_{ij} t_{ij} \left(c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

↑ note hopping matrix (used to be $-t$)

condition on t_{ij} is $t_{ij} \geq 0$, otherwise arbitrary and $t_{ij} = t_{ji}$.

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

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

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

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 $\langle j\tau | c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow} | i\sigma\rangle \neq 0$

we say $(i\sigma) \leftrightarrow (j\tau)$ the state $|i\sigma\rangle$ is connected to $|j\tau\rangle$

If $(i\sigma) \leftrightarrow (j\tau)$ then

all $\sigma_\alpha = \tau_\alpha$ except $\alpha = i$ and j

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

In taking $(c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow})|i\sigma\rangle$ into $|j,\tau\rangle$ form, we need to move the $c^\dagger_{j\sigma_j}$ 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 $(c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}) |i\sigma\rangle = (-1) |j\tau\rangle$

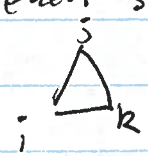
hence $\langle j\tau | t_{ij} (c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}) |i\sigma\rangle = -t_{ij}$

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

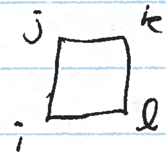
$$(i\sigma_1) \leftrightarrow (j\sigma_2) \leftrightarrow (k,\sigma_3) \ldots \leftrightarrow (l,\sigma_n)$$

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 $t_{ij} t_{jk} t_{kl} t_{li} \neq 0$



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.

let $|\psi\rangle = \sum_{(i\sigma)} \psi_{i\sigma} |i\sigma\rangle$ be a unit norm state

$\psi_{i\sigma}$ are numbers $\langle\psi|\psi\rangle = \sum_{(i\sigma)} |\psi_{i\sigma}|^2 = 1.$

choose $|\phi\rangle = \sum_i \phi_i |i\{\uparrow\}\rangle$ where all spins are up except for a hole at site i.

$|\phi\rangle$ has $S = S_{max} = \frac{N-1}{2}$

let $\phi_i = \left(\sum_\sigma |\psi_{i\sigma}|^2\right)^{1/2}$ = real. Then $\langle\phi|\phi\rangle = 1$

Also $\langle\psi| \sum_{ij} t_{ij} (c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}) |\psi\rangle$

$$= \sum_{\sigma\tau} \sum_{ij} (-t_{ij}) \psi^*_{j\tau} \psi_{i\sigma} \geq \sum_{ij} (-t_{ij}) \phi_j^* \phi_i$$

$\hookrightarrow$ τ is config connected to σ $= \langle\phi| \sum_{ij} t_{ij} (c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}) |\phi\rangle$

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

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

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

true for all λ. Choose $\lambda = \frac{|a|}{|b|}$

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

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

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

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

$$\langle\psi| \sum_{ij} t_{ij} (c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}) |\psi\rangle = E_{gs}$$

But then $|\phi\rangle$ has energy

$$\langle\phi| \sum_{ij} t_{ij} (c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}) |\phi\rangle \leq E_{gs}$$

$\Rightarrow$ must have $=$ since gs. So if $|\psi\rangle$ is a gs

$|\phi\rangle$ is also a gs.

$\Rightarrow$ system has a ferromagnetic gs.

There is an alternate proof using the Perron-Frobenius theorem

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

$M_{ii} \geq m$

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_i are less than zero and E' is the largest eigenvalue, then

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

Now consider $\phi_i = |\psi_i|$

box on right shows $\sum_j M'_{ij}\phi_j \geq E'\phi_i$

$$\Rightarrow \Big|\sum_j M'_{ij}\psi_j\Big| = |E'\psi_i| \qquad E'>0$$
$$= E'|\psi_i|$$
$$\text{but } \Big|\sum_j M'_{ij}\psi_j\Big| \leq \sum_j |M'_{ij}\psi_j|$$
$$\leq \sum_j M'_{ij}|\psi_j|$$
since $M'_{ij} \geq 0$

because all $M'_{ij} \geq 0$ and $\phi_j \geq 0$

all terms on LHS ≥ 0

but not necessarily so for $\sum_j M'_{ij}\psi_j$ since ψ_j could be <0

$\Rightarrow \sum_{ij} \phi_i M'_{ij} \phi_j \geq E' \sum_i \phi_i^2$

$\Rightarrow \phi_i$ 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 $\phi_i > 0$ for all i

Consider

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

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

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

since $E' \neq 0 \Rightarrow \phi_k \neq 0$

To prove the Nagaoka theorem we apply to

$M = -H$.

<u>Summary</u>

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

For bipartite 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 (see HW12 for an example)

If $M=N-2$, GS is usually a spin singlet (not proven in general)

Important question: does ferromagnetism survive a finite density <u>away</u> from half filling

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