Theory in Materials Science

8th lecture

Ferromagnetism in the Hubbard model II

The Nagaoka ferromagnetism

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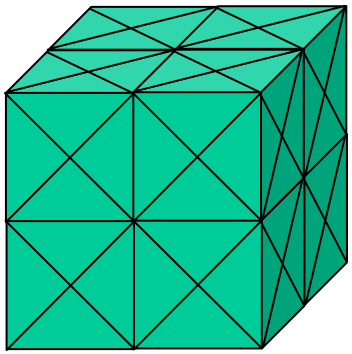
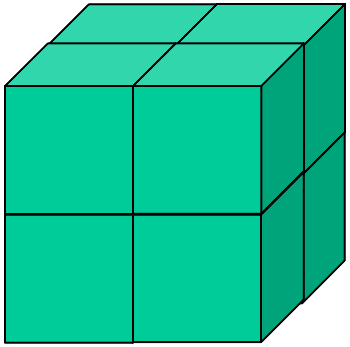
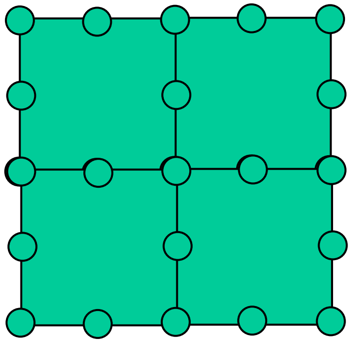
The Hubbard models with various lattice structures



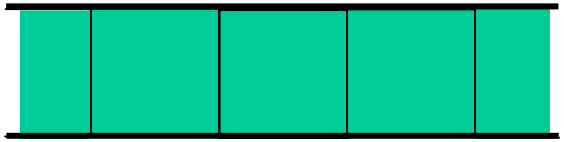
Kanamori theory
at low density
Kanamori (1963)



Nagaoka theory
for 1 hole from h.f.
Kanamori (1963)

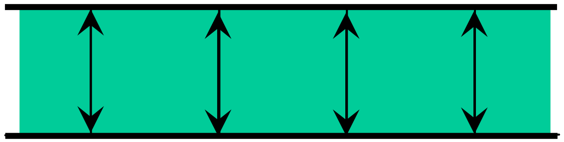


Ferimagnetism
Lieb(1989)

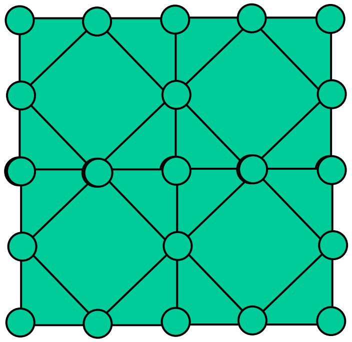


Nagaoka ferromagnetism at finite density
Kohno (1997)

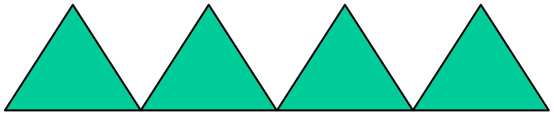
Flatband ferromagnetism
Mielke(1991)
Tasaki(1992).



Double exchange & Nagaoka
Kubo, Tsunetsugu, Yanagisawa&Shimoi



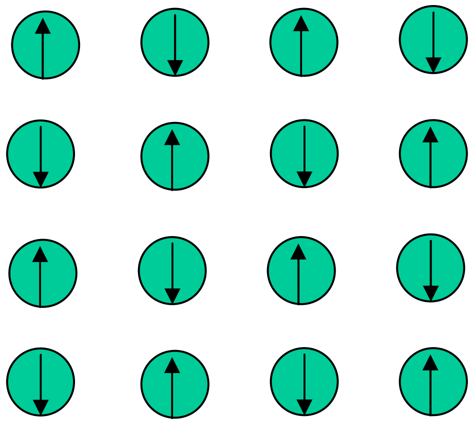
Ferromagnetism in
Multi-band models
Tanaka & Idogaki



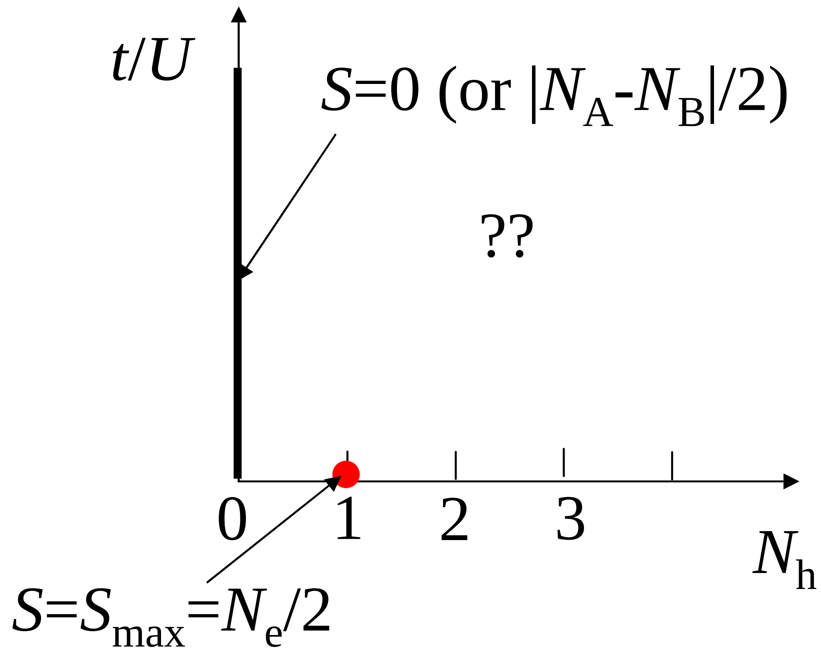
Flatband ferromagnetism to Nagaoka F
Penc. et al. Sakamoto&Kubo
Watanabe&Miyashita, Daul&Noak

Phase diagram of the Hubbard model in the strong-correlation limit

- Lieb's theorem ⇒ S=0 (or $|N_A$-$N_B|/2$) for bipartite lattices.
- Nagaoka's theorem ⇒ $S=S_{max}=N_e/2$ for $U=\infty$



The half filling



N_h : number of holes in a half-filled system

Stability of ferromagnetic phase in the Hubbard model

Hanish, Uhrig & Muller-Hartmann, PRB 56 (1997) 13960.

2D t-t'-U model

HM on FCC

Deleted based on copyright concern.

Ferromagnetic phase of the t-J model

Putikka-Luchini-Ogata PRL 69 (1992) 2288.

Deleted based on copyright concern.

The result of the high-temperature expansion method concludes that the fully polarized ferromagnetic phase is limited to the Nagaoka state.

The Nagaoka theorem

- Consider a Hamiltonian for the Hubbard model with $U=\infty$.

$$H = \sum_{\langle ij \rangle \sigma} t_{ij} P_G (c_{i\sigma}^{\dagger} c_{j\sigma} + h.c.) P_G$$

Here, N, N_e and S denote the total number of sites, the total number of electrons and the total spin. P_G is the Gutzwiller projection. $P_G = \prod_k (1 - n_{k\uparrow} n_{k\downarrow})$

1. Theorem 1
   - If $t_{ij} \geqq 0$ and if $N_e = N-1$, one of the lowest energy eigen states is a fully spin-polarized state with $S=S_{max}=N_e/2$.
2. Theorem 2
   - Furthermore, if a graph defined by t_{ij} satisfy the connectivity condition, the lowest state given by the theorem 1 is the unique ground state up to trivial $(2S+1)$-fold degeneracy.

1. If one finds a proper unitary transformation, these theorems are applicable for models with $t_{ij} \leqq 0$.
2. The connectivity condition guarantees that every possible spin configuration within S_z=constant is generated by motion of a hole.

Tasaki's proof of theorem 1

1. Definition of the problem

- Consider a Hubbard model with N atomic sites.
- The transfer integrals $t_{i,j}$ give a graph whose edges are the sites and whose bonds represents non-zero $t_{i,j}$.
- A condition $t_{i,j} > 0$ is assumed.
- The Hubbard interaction is assumed to be $U = \infty$.
- The number of electrons is $N_e = N - 1$.

2. Choice of the basis set

- We may determine the index $x = 1, \cdots, N$ of the sites.
- A state is characterized by the position of a hole x and the spin configuration specified by the direction of a spin $\tau_s = \pm$ on a site $s \neq x$. We may use an index $\tau = \{\tau_1, \cdots, \tau_N\}$.
- Choose a phase factor of the basis function so that the Hamiltonian matrix becomes a non-positive matrix.

$$|x, \tau\rangle = (-1)^x c^\dagger_{1,\tau_1} c^\dagger_{2,\tau_2} \cdots c^\dagger_{x-1,\tau_{x-1}} \cdot c^\dagger_{x+1,\tau_{x+1}} \cdots c^\dagger_{N,\tau_N} |0\rangle \ . \qquad (1)$$

- An example of motion of a hole at the 5-th site may be,

$$\begin{aligned} & t_{5,2} c^\dagger_{5,\uparrow} c_{2,\uparrow} \times (-1)^5 c^\dagger_{1,\downarrow} c^\dagger_{2,\uparrow} c^\dagger_{3,\downarrow} c^\dagger_{4,\uparrow} \times c^\dagger_{6,\downarrow} |0\rangle \\ = & (-1)^5 t_{5,2} c^\dagger_{1,\downarrow} \left(c^\dagger_{5,\uparrow} c_{2,\uparrow} \right) c^\dagger_{2,\uparrow} c^\dagger_{3,\downarrow} c^\dagger_{4,\uparrow} \times c^\dagger_{6,\downarrow} |0\rangle \\ = & (-1)^5 t_{5,2} c^\dagger_{1,\downarrow} c^\dagger_{5,\uparrow} c^\dagger_{3,\downarrow} c^\dagger_{4,\uparrow} \times c^\dagger_{6,\downarrow} |0\rangle \\ = & (-1)^5 t_{5,2} (-1)^{5-2+1} c^\dagger_{1,\downarrow} \times c^\dagger_{3,\downarrow} c^\dagger_{4,\uparrow} c^\dagger_{5,\uparrow} c^\dagger_{6,\downarrow} |0\rangle \\ = & (-1) t_{5,2} (-1)^2 c^\dagger_{1,\downarrow} \times c^\dagger_{3,\downarrow} c^\dagger_{4,\uparrow} c^\dagger_{5,\uparrow} c^\dagger_{6,\downarrow} |0\rangle \ . \end{aligned}$$

- The matrix element satisfies the following equation.

$$\langle y, \tau | H | x, \sigma \rangle = \begin{cases} -t_{x,y} & \text{if } \tau_z = \sigma_z \text{ for } z \neq x, y \text{ and } \tau_x = \tau_y, \\ 0 & \text{otherwise.} \end{cases} \tag{2}$$

3. The ground state may be written as,

$$|\Psi\rangle = \sum_{x,\sigma} \psi_{x,\sigma} |x, \sigma\rangle \ . \tag{3}$$

4. Let us consider a trial state,

$$|\Phi\rangle = \sum_{x,\sigma} \phi_{x,\sigma} |x, \sigma\rangle \ , \tag{4}$$

$$\phi_{x,\sigma} = \left(\sum_{\sigma} |\psi_{x,\sigma}|^2 \right)^{\frac{1}{2}} \ . \tag{5}$$

5. We have the next inequality, which is shown by the Schwarz inequality.

$$\begin{aligned} & \langle\Psi|t_{x,y}\left(c^\dagger_{x,\uparrow}c_{y,\uparrow}+c^\dagger_{x,\downarrow}c_{u,\downarrow}\right)|\Psi\rangle \\ = \ & (-t_{x,y})\sum_\sigma\left(\psi_{y,\tau}\right)^*\psi_{x,\sigma} \\ \geq \ & (-t_{x,y})\sqrt{\sum_\tau|\psi_{y,\tau}|^2\sum_\sigma|\psi_{x,\sigma}|^2} \\ = \ & -t_{x,y}\phi_y\phi_x \\ = \ & \langle\Phi|t_{x,y}\left(c^\dagger_{x,\uparrow}c_{y,\uparrow}+c^\dagger_{x,\downarrow}c_{u,\downarrow}\right)|\Phi\rangle \ . \end{aligned}$$

Here we should note that τ and σ is identified if $\tau_z=\sigma_z$ for $z\neq x,y$ and $\tau_x=\tau_y$ in the first equation.

6. Due to the variational principle, we have an inequality for the energy of the ground state E_{GS} as,

$$E_{GS}=\langle\Psi|H|\Psi\rangle\geq\langle\Phi|H|\Phi\rangle\geq E_{GS}\ . \tag{6}$$

Thus Φ is also a ground state.

7. The total spin of Φ is $S = S_{max} = N_e/2$, since the next state with $S = S_{max} = N_e/2$ has a finite amplitude on Ψ.

$$|\Phi_0\rangle \equiv \left(S^-_{\rm tot}\right) c^\dagger_{1,\uparrow} \cdots c^\dagger_{N-1,\uparrow}|0\rangle \ . \tag{7}$$

Note that the ground state is an eigen state of the total spin $\vec{S}$, since the operator $\vec{S}$ commutes with H.

Uniqueness of the ground state in Theorem 2 is shown by the Perron-Frobenius theorem for the non-positive matrix in stead of the Schwarz inequality.