Spin ordering at weak coupling: spin density waves

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Antiferromagnetism has the remarkable feature of being realizable both in the strong-coupling and in the weak-coupling regimes (needless to say, by 'coupling' we here mean e-e interaction). For comparison, superconductors appear only in the weak-coupling, while crystals are realized only in the strong-coupling regime.

In both cases the starting point is the Hubbard model

$$H = -t \sum_{i,\delta,\sigma} \left(c^{+}_{i\sigma} c_{i+\delta,\sigma} + h.c. \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} .$$

In our treatment of the strong-coupling regime we used a perturbation theory with t/U being the small parameter. Now we want to address the regime where kinetic energy dominates over the interactions (i.e., the weak-coupling regime). We will address this regime using what is called Hartree-Fock mean-field theory.

The existence of Néel order, mathematically expressed as

$$\langle S^{z}_{i} \rangle = \frac{1}{2} \left(\langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle \right) \neq 0 ,$$

is anticipated within this mean-field approach.

We introduce operators $\delta O_{i\sigma} \equiv n_{i\sigma} - \underbrace{\langle n_{i\sigma} \rangle}_{O_{i\sigma}}$

$$\Rightarrow \boxed{n_{i\sigma} = O_{i\sigma} + \delta O_{i\sigma}}$$

Using the Hartree-type decoupling of the interaction term, and to remind you (we already used it in the context of the RPA approximation) this is the decoupling of the type

$$A\,B \longrightarrow \langle A\rangle B + A\langle B\rangle - \langle A\rangle\langle B\rangle ,$$

$A \to a^{+}_{\mu} a_{\mu}$, $B \to b^{+}_{\nu} b_{\nu'}$

we obtain the mean-field Hamiltonian

$$H^{MF} = -t \sum_{i,\delta,\sigma} \left(C^{+}_{i\sigma} C_{i+\delta,\sigma} + h.c. \right)$$

$$+ U \sum_{i} \left(O_{i\uparrow} n_{i\downarrow} + O_{i\downarrow} n_{i\uparrow} - O_{i\uparrow} O_{i\downarrow} \right)$$

the e-e-interaction effects are now absorbed in simple single-electron scattering terms

By introducing $\Omega^{z}_{i} = \frac{1}{2}\left(O_{i\uparrow} - O_{i\downarrow} \right)$

$$\bar{n}_{i} = \frac{1}{2}\left(O_{i\uparrow} + O_{i\downarrow} \right) ,$$

we have $O_{i\uparrow} = \bar{n}_{i} + \Omega^{z}_{i}$,

$O_{i\downarrow} = \bar{n}_{i} - \Omega^{z}_{i}$,

which, when substituted in the last mean-field Hamiltonian leads to

$$H_{MF} = -t \sum_{i,\delta,\sigma} \left(c_{i\sigma}^{\dagger} c_{i+\delta,\sigma} + h.c. \right)$$

$$+ U \sum_i \left[\bar{n}_i (n_{i\uparrow} + n_{i\downarrow}) - \Delta_i^z (n_{i\uparrow} - n_{i\downarrow}) - \bar{n}_i^2 + (\Delta_i^z)^2 \right]$$

Is something perhaps wrong with the last mean-field Hamiltonian?

When doing mean-field theory we would ideally want our mean-field Hamiltonian to obey the same symmetries as the original Hubbard Hamiltonian.
One of these symmetries is the spin-rotational symmetry which we discussed before. H'_{MF} breaks this symmetry!

When we are decoupling a quartic (interaction) term with all four operators of the same type (i.e., describing interactions between the same kind of particles) then another decoupling (known as Fock-type) has to be taken into account:

$$U \sum_i n_{i\uparrow} n_{i\downarrow} \longrightarrow -U \sum_i \underbrace{c_{i\uparrow}^{\dagger} c_{i\downarrow}}_{S_i^+} \underbrace{c_{i\downarrow}^{\dagger} c_{i\uparrow}}_{S_i^-}$$

$$= -U \sum_i (\Delta_i^+ + \delta\Delta_i^+)(\Delta_i^- + \delta\Delta_i^-)$$

All in all, the interaction term in the Hartree-Fock mean-field theory becomes

$$U \sum_i n_{i\uparrow} n_{i\downarrow} \longmapsto U \sum_i \Big[\bar{n}_i (n_{i\uparrow} + n_{i\downarrow}) - \Omega_i^z (n_{i\uparrow} - n_{i\downarrow}) - \Omega_i^+ c_{i\downarrow}^+ c_{i\uparrow} - \Omega_i^- c_{i\uparrow}^+ c_{i\downarrow} - \bar{n}_i^2 + (\Omega_i^z)^2 + \Omega_i^+ \Omega_i^- + \text{fluct.} \Big]$$

Having arrived at this Hartree-Fock mean-field Hamiltonian, the further procedure entails the following:

1) Choose a set of classical variables $\bar{n}_i$ and Ω_i (they can in principle be different on each lattice site)

2) Each set of these variables defines an <u>independent-electron</u> problem, which we want to solve.

3) Find the <u>minimum classical energy</u> in the classical configuration space. This is the sum of the Ne (= total electron number) lowest single-particle energies (found in step 2)), plus the potential energy

$$U(-\bar{n}_i^2 + \Omega_i^2)$$

We illustrate this for the half-filled Hubbard model on a cubic lattice.

Assuming that the ground state corresponds to the Néel state with a uniform charge density, we adopt

$$\bar{n}_i = \bar{n} \quad (\forall i) \,,$$
$$\Omega_i = (0,0,\Omega) \quad (i \in A) \,,$$
$$\Omega_i = (0,0,-\Omega) \quad (i \in B) \,,$$

where $\bar{n}$ and Ω are still to be determined.

From our mean-field Hamiltonian we can see that spin-↑ electrons experience potential $U*(\bar{n}-\Omega)$ on the A sublattice and $U*(\bar{n}+\Omega)$ on the B sublattice. For spin-↓ electrons, the role of the A and B sublattices is reversed:

$$H^{MF}_{Neel} = -t \sum_{i,\delta,\sigma} \left(c^{\dagger}_{i\sigma} c_{i+\delta,\sigma} + h.c. \right)$$

sign here depends on the sublattice!

$$+ U \sum_{i \in A,B} \left\{ \bar{n} \left(n_{i\uparrow} + n_{i\downarrow} \right) \mp \Omega \left(n_{i\uparrow} - n_{i\downarrow} \right) - \bar{n}^2 + \Omega^2 \right\}$$

The last Hamiltonian defines a "band-structure-like" problem on a lattice with <u>two inequivalent sites per unit cell.</u>

To solve such a problem, we first perform a Fourier transformation to momentum space. We obtain the Hamiltonian

$$H^{MF}_{Néel} = \sum_{K} \Big[2t\cos\left(\tfrac{K}{2}\right) \sum_{\delta}^{\rightarrow} \left(c^{+}_{A,K\delta} c_{B,K\delta} + h.c. \right)$$
$$+ U(\bar{n} - \Omega)\left(c^{+}_{AK\uparrow} c_{A,K\uparrow} + c^{+}_{BK\downarrow} c_{B\bar{K}\downarrow} \right)$$
$$+ U(\bar{n} + \Omega)\left(c^{+}_{AK\downarrow} c_{AK\downarrow} + c^{+}_{BK\uparrow} c_{BK\uparrow} \right)$$
$$+ U(\Omega^2 - \bar{n}^2) \Big] ,$$

where we introduced "A" and "B" fermions (that is, fermions living on two different sublattices).

Through a fermion Bogoliubov transformation

$$\gamma^{+}_{K\uparrow} = \cos\phi_K \, c^{+}_{AK\uparrow} + \sin\phi_K \, c^{+}_{BK\uparrow} ,$$
$$\bar{\gamma}^{+}_{K\uparrow} = \sin\phi_K \, c^{+}_{AK\uparrow} - \cos\phi_K \, c^{+}_{BK\uparrow} ,$$
$$\gamma^{+}_{K\downarrow} = \cos\phi_K \, c^{+}_{BK\downarrow} + \sin\phi_K \, c^{+}_{AK\downarrow} ,$$
$$\bar{\gamma}^{+}_{K\downarrow} = \sin\phi_K \, c^{+}_{BK\downarrow} - \cos\phi_K \, c^{+}_{AK\downarrow} ,$$

where $\gamma^{+}_{K\delta}$ are the low-lying bonding states (lower-band states) and $\bar{\gamma}^{+}_{K\delta}$ higher-lying unoccupied states, after diagonalization we obtain

$$H^{MF}_{Néel} = \sum_{K\delta} \left[\omega^{-}_{K}(\bar{n}, \Omega) \gamma^{+}_{K\delta} \gamma_{K\delta} + \omega^{+}_{K}(\bar{n}, \Omega) \bar{\gamma}^{+}_{K\delta} \bar{\gamma}_{K\delta} \right]$$
$$+ NU(\Omega^2 - \bar{n}^2)$$

with $\boxed{\omega_k^{\pm} = U\bar{n} \pm \sqrt{U^2\Omega^2 + 4t^2\cos^2\frac{k}{2}}\ .}$ (**)

For large $\frac{U\Omega}{t}$ the lower band corresponds to the up- (down-) electrons being predominantly on the A- (B) sublattice.

In accordance with the "prescription" given above the classical energy is given by

$$E(\bar{n},\Omega) = \frac{\langle H_{MF}\rangle}{N} = \frac{1}{N}\sum_{k=-\pi}^{\pi} \omega_k^-(\bar{n},\Omega) + U(\Omega^2 - \bar{n}^2)\ .$$

Minimization with respect to $\bar{n}$ and Ω leads to the equations

$$\frac{\partial E}{\partial \bar{n}} = -2\bar{n}U + \frac{1}{N}\sum_k \frac{\partial}{\partial \bar{n}}\omega_k^-(\bar{n},\Omega) = 0$$

$$\frac{\partial E}{\partial \Omega} = 2\Omega U + \frac{1}{N}\sum_k \frac{\partial}{\partial \Omega}\omega_k^-(\bar{n},\Omega) = 0$$

Combining this last equation with Eq. (**) above we get an implicit equation for the order parameter amplitude Ω: $\frac{1}{2N}\sum_k \frac{1}{\sqrt{U^2\Omega^2 + 4t^2\cos^2\frac{k}{2}}} = \frac{1}{U}$,

or, equivalently,

$$(\Delta) \qquad \boxed{\frac{1}{2\pi}\int_0^{\pi}\frac{dk}{\sqrt{1+\left(\frac{2t}{U\Omega}\right)^2\cos^2\frac{k}{2}}} = \Omega\,.}$$

Such an equation can be solved by iteration.

Let us consider the limit $\frac{U}{t} \to 0$ in one dimension. It can be expected that only the electron states close to ε_F are affected; accordingly, their dispersion can be linearized

$$\omega_k = 2t\cos\left(\frac{k}{2}\right) \longrightarrow \omega_k = v_F(k-k_F)$$

k_F here is $k_F = \frac{\pi}{2a}$

Fermi momentum of the folded zone

A high energy cut-off momentum k_0' is chosen in such a way as to reproduce the bandwidth $(k' = k - k_F)$

$$v_F k_0' = 2t$$

With these simplifying assumptions Eq. (Δ) above reduces to

$$\frac{1}{U} = \frac{1}{2\pi v_F}\int_0^{k_0'}\frac{dk'}{\sqrt{k'^2+\frac{U^2\Omega^2}{v_F^2}}} = \frac{1}{2\pi v_F}\sinh^{-1}\left(\frac{|v_F k_0'|}{U\Omega}\right),$$

which is equivalent to

$$U\Omega = \Delta = \frac{|v_F k_0'|}{\sinh\left(\frac{2\pi|v_F|}{U}\right)} \simeq 4t\, e^{-\frac{2\pi t}{U}}$$

$U\Omega$ has the meaning of half the gap that opens at the boundary of the folded Brillouin zone. This gap is finite for any $U > 0$.

Despite being small, the gap is present even in the weak-coupling limit. As long as the gap spans the Fermi surface (NESTING, a situation that is characteristic of 1d systems, and rarely takes place in $d > 1$) it is possible to think of Wannier states of localized spins; their difference from localized spins in strong coupling is their much larger spatial extent (coherence length) ξ, which can be estimated as

$$\frac{\xi}{a} \sim \frac{W}{2U\Omega} .$$

Because the gap $2U\Omega$ is a very small fraction of the bandwidth W, the coherence length is quite large, e.g., $\xi \sim 1000\, a$. This resulting weak-coupling antiferromagnet is called a spin-density wave (SDW). — it is something like a Fermi fluid with a

a wave of spin-density superimposed on it.

The SDW's occur in 1d not only at half-filling but also at other filling fractions; the nesting then happens at different wave numbers than $\frac{\pi}{2a}$ and instead of a doubling of a unit cell the SDW can ~~be~~ even be found with wavelengths incommensurate with the original lattice period.

Since in higher dimensions ($d>1$) nesting occurs only in very special cases (e.g., a Hubbard model on a square lattice with nearest-neighbor hopping only) the SDW's are special to the one-dimensional systems.

In nature, they are typically realized as quasi-1d systems. There is, for instance, a large class of quasi-1d organic systems which are metallic at room temperature and undergo a transition to SDW at some lower temperature. An example is furnished by the so-called Bechgaard salts.