

# Advanced Theory of Condensed Matter

## Assignment 2

This assignment has to be handed in at the start of the lecture of October 23.

### 3 Weak coupling: spin density waves

In exercises 1 and 2 we have discussed the strong coupling regime where interaction energies are much larger than the kinetic energies associated with the quantum-mechanical zero-point motion of the particle. For this reason, the latter could be taken into account perturbatively, giving rise to small corrections on the scale of the interaction energies.

A major achievement has been the discovery that the classical paradigm also applies to the opposite limit where the quantum kinetic energies dominate over the interaction energies: the “weak coupling limit”. The discovery of the microscopic theory of superconductivity by Bardeen, Cooper and Schrieffer (BCS) has played a key role in the development, and in hindsight one could claim that they really deserved their Nobel prize, because they showed how to construct the classical state from the microscopic quantum soup.

The reason to introduce weak-coupling theory in the context of magnetism is that anti-ferromagnets occur in nature both in their weak-coupling (“spin-density waves”) and strong-coupling versions (see exercise 2). In contrast, crystals only occur in the strong-coupling limit, and superconductors only in the weak-coupling limit.

Magnetism is the ideal playing ground to demonstrate the equivalence of the macroscopic physics in both limits: at long wavelength and small energies it is all the same. The difference is that in weak coupling, the classical features are only seen on scales much larger than the atomic scales.

In the weak-coupling limit, the kinetic energy dominates and the natural starting point is single-particle momentum space. In forming the classical condensates, one needs now coherent superpositions of single-particle momentum states in order to construct condensate wave functions.

These wave functions can be constructed but this is technically rather clumsy and a much more efficient approach exists: semi-classical mean-field theory or “Hartree–Fock approximation”. This exercise is meant to illustrate this approach in the context of spin condensates.

The starting point is again the single-band Hubbard model

$$\hat{\mathcal{H}} = t \sum_{\mathbf{r}\delta\sigma} c_{\mathbf{r},\sigma}^\dagger c_{\mathbf{r}+\delta,\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}. \quad (3.1)$$

The central step in mean-field theory is straightforward. The existence of Néel order is anticipated. Orienting the staggered order parameter along the  $z$ -axis, its presence implies that the operator  $S_{\mathbf{r}}^z$  acquires a finite expectation value (“vacuum amplitude”) on every site.

In terms of the fermion operators (recall the  $su(2)$ -algebra for  $S = \frac{1}{2}$  in terms of fermion operators (2.13)):

$$\langle S_{\mathbf{r}}^z \rangle = \frac{1}{2} (\langle n_{\mathbf{r}\uparrow} \rangle - \langle n_{\mathbf{r}\downarrow} \rangle) \neq 0. \quad (3.2)$$

- (a) Decompose  $n_{\mathbf{r}\sigma}$  into the scalar vacuum amplitude  $O_{\mathbf{r}\sigma} := \langle n_{\mathbf{r}\sigma} \rangle$  and fluctuations  $\delta O_{\mathbf{r}\sigma}$  around it:  $n_{\mathbf{r}\sigma} = O_{\mathbf{r}\sigma} + \delta O_{\mathbf{r}\sigma}$  to demonstrate that the “mean-field Hamiltonian” is given by

$$\hat{\mathcal{H}}^{\text{HF}} = t \sum_{\mathbf{r}\delta\sigma} c_{\mathbf{r},\sigma}^\dagger c_{\mathbf{r}+\delta,\sigma} + U \sum_{\mathbf{r}} (O_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} + O_{\mathbf{r}\downarrow} n_{\mathbf{r}\uparrow} - O_{\mathbf{r}\uparrow} O_{\mathbf{r}\downarrow}), \quad (3.3)$$

where in this classical limit the fluctuation term  $\delta O_{\mathbf{r}\uparrow} \delta O_{\mathbf{r}\downarrow}$  is neglected. As long as the order parameter exists, it should be possible to treat these fluctuations perturbatively.

- (b) Rewrite  $\hat{\mathcal{H}}^{\text{HF}}$  in a more transparent way by introducing scalars which refer directly to the local  $z$ -axis spin ( $\Omega_{\mathbf{r}}^z$ ) and charge density ( $2\bar{n}_{\mathbf{r}}$ ):

$$\Omega_{\mathbf{r}}^z := \frac{1}{2} (O_{\mathbf{r}\uparrow} - O_{\mathbf{r}\downarrow}) \quad (3.4)$$

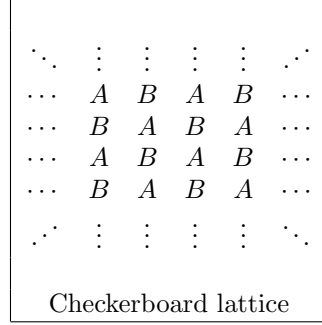
$$\bar{n}_{\mathbf{r}} := \frac{1}{2} (O_{\mathbf{r}\uparrow} + O_{\mathbf{r}\downarrow}) \quad (3.5)$$

Show that

$$\hat{\mathcal{H}}^{\text{HF}} = t \sum_{\mathbf{r}\delta\sigma} c_{\mathbf{r},\sigma}^\dagger c_{\mathbf{r}+\delta,\sigma} + U \sum_{\mathbf{r}} \left( \bar{n}_{\mathbf{r}} (n_{\mathbf{r}\uparrow} + n_{\mathbf{r}\downarrow}) - \Omega_{\mathbf{r}}^z (n_{\mathbf{r}\uparrow} - n_{\mathbf{r}\downarrow}) - \bar{n}_{\mathbf{r}}^2 + (\Omega_{\mathbf{r}}^z)^2 \right). \quad (3.6)$$

From now on, we restrict ourselves to the half-filled Hubbard model on a square lattice. In principle, one should allow for every possible field configuration. However, for an arbitrary configuration the single-particle problem becomes very complicated and this can only be handled numerically.

In fact, the half-filled case has been thoroughly investigated and it turns out that the ground state indeed corresponds to the Néel state, with a uniform charge density. Hence, we limit ourselves to the part of configuration space with  $\bar{n}_{\mathbf{r}} \equiv \bar{n}$  and  $\vec{\Omega}_{\mathbf{r}} \equiv (0, 0, \Omega)$  for  $\mathbf{r} \in A$  and  $\vec{\Omega}_{\mathbf{r}} \equiv (0, 0, -\Omega)$  for  $\mathbf{r} \in B$  ( $A$  and  $B$  denote the two sublattices of the checkerboard division of the square lattice):



$$\hat{\mathcal{H}}_{\text{Néel}}^{\text{HF}} = t \sum_{\mathbf{r}\delta\sigma} c_{\mathbf{r},\sigma}^\dagger c_{\mathbf{r}+\delta,\sigma} + U \sum_{\mathbf{r} \in A, B} \left( \bar{n} (n_{\mathbf{r}\uparrow} + n_{\mathbf{r}\downarrow}) \mp \Omega (n_{\mathbf{r}\uparrow} - n_{\mathbf{r}\downarrow}) - \bar{n}^2 + \Omega^2 \right). \quad (3.7)$$

- (c) Convince yourself that  $\hat{\mathcal{H}}_{\text{Néel}}^{\text{HF}}$  is nothing but a tight-binding problem on a square lattice with one orbital per site and staggered spin-dependent on-site energies  $\epsilon_{A\sigma} \neq \epsilon_{B\sigma}$ . Express  $\epsilon_{A\sigma}, \epsilon_{B\sigma}$  in terms of  $U, \bar{n}$  and  $\Omega$ .

Establish the Bravais lattice and the basis and deduce the shape of the Brillouin Zone (BZ).

Transform the Hamiltonian to  $\mathbf{k}$ -space, write it in matrix form (drop any constants):

$$\hat{\mathcal{H}} = \sum_{\mathbf{k} \in \text{BZ}} (c_{\mathbf{k}A\uparrow}^\dagger, c_{\mathbf{k}B\uparrow}^\dagger, c_{\mathbf{k}A\downarrow}^\dagger, c_{\mathbf{k}B\downarrow}^\dagger) M_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}A\uparrow} \\ c_{\mathbf{k}B\uparrow} \\ c_{\mathbf{k}A\downarrow} \\ c_{\mathbf{k}B\downarrow} \end{pmatrix}, \quad (3.8)$$

and diagonalize to demonstrate that we have two doubly degenerate bands with dispersion

$$\omega_{\mathbf{k}}^{\pm}(\bar{n}, \Omega) = U\bar{n} \pm \sqrt{U^2\Omega^2 + 4t^2(\cos k_x + \cos k_y)^2}. \quad (3.9)$$

For simplicity, we have set lattice constant to  $a = 1$ .

Sketch the bands along high-symmetry directions and the Fermi surface for half-filling for  $\Omega = 0$  and infinitesimal  $\Omega$ . Is the Fermi surface nested?

In the case  $\Omega = 0$ , one can also start with one site per unit cell. What is the relation of this single-band model to the band structure calculated for two sites per unit cell?

We still have to determine  $\bar{n}$  and  $\Omega$  by minimizing the classical energy

$$E(\bar{n}, \Omega) = \frac{\langle \hat{\mathcal{H}}_{\text{Néel}}^{\text{HF}} \rangle}{N}, \quad (3.10)$$

with respect to  $\bar{n}$  and  $\Omega$ .

- (d) Motivate that, at half-filling, this corresponds to the saddle-point equations:

$$\frac{\partial E(\bar{n}, \Omega)}{\partial \bar{n}} = -2\bar{n}U + \frac{1}{N} \sum_{\mathbf{k} \in \text{BZ}} \frac{\partial}{\partial \bar{n}} \omega_{\mathbf{k}}^{-}(\bar{n}, \Omega) = 0, \quad (3.11)$$

$$\frac{\partial E(\bar{n}, \Omega)}{\partial \Omega} = 2\Omega U + \frac{1}{N} \sum_{\mathbf{k} \in \text{BZ}} \frac{\partial}{\partial \Omega} \omega_{\mathbf{k}}^{-}(\bar{n}, \Omega) = 0, \quad (3.12)$$

and demonstrate that from eq. (3.11) we immediately obtain  $2\bar{n} = 1$ . Why is also this clear without doing any calculation?

Furthermore, show that the saddle-point equation (3.12) for the Néel order parameter  $\Omega$  can be explicitly written as

$$\frac{2}{\pi^2} \int_0^{\pi/2} dh_x \int_0^{\pi/2} dh_y \frac{1}{\sqrt{1 + \left(\frac{4t}{U\Omega} \cos h_x \cos h_y\right)^2}} = \Omega, \quad (3.13)$$

where the summation was replaced by an integration

$$\frac{1}{N} \sum_{\mathbf{k} \in \text{BZ}} \mapsto \frac{1}{V_{\text{BZ}}} \int_{\text{BZ}} d^2k \quad (\text{large } N)$$

with  $V_{\text{BZ}}$  the volume of the Brillouin zone, and we used the transformation  $h_x = \frac{1}{2}(k_x + k_y)$ ,  $h_y = \frac{1}{2}(k_x - k_y)$  ( $\frac{\pi}{4}$ -rotation and rescaling).

Let us first consider strong coupling:  $U \gg t$ . This is very important: there is no instance in the derivation of the saddle-point equation where we demanded anything from  $U/t$ . All we needed was the existence of a Néel state, and this is controlled by  $1/S$  and the dimensionality. It is quite often claimed that the above mean-field theory is only correct for small  $U/t$  (weak coupling), and this is a gross misunderstanding! It is controlled by ‘classicalness’. We will now

demonstrate that mean-field theory precisely reproduces the result of the exact strong-coupling expansion (see exercise 2), given that the spins in the result

$$\hat{\mathcal{H}} = J \sum_{\mathbf{r}\delta} (\vec{S}_{\mathbf{r}} \cdot \vec{S}_{\mathbf{r}+\delta} - \frac{1}{4}), \quad (3.14)$$

are taken to be classical.

- (e) First expand the saddle-point equation (3.13) for  $t/U \ll 1$  to demonstrate that

$$\Omega = \frac{1}{2} \left( 1 - 2 \left( \frac{t}{U\Omega} \right)^2 + \dots \right), \quad (3.15)$$

leading to  $\Omega = \frac{1}{2} - 2 \frac{t^2}{U^2} + \dots$

Expand the energy  $E(\bar{n} = \frac{1}{2}, \Omega) = U(\Omega^2 - \bar{n}^2) + \frac{1}{V_{\text{BZ}}} \int_{\mathbf{k} \in \text{BZ}} d^2k \omega_{\mathbf{k}}^-$  up to order  $t^2/U^2$  and show that at the saddle point we have  $E = -z \frac{t^2}{U}$  with  $z = 4$  the coordination number of the square lattice. Compare this with the classic limit of the exact strong-coupling expansion.

- (f) Let us now go back to the saddle-point equation (3.13) for the Néel order parameter. Substitute  $\cos h_y$  by the averaged value over  $[0; \frac{\pi}{2}]$  and linearize  $\cos h_x$  around the Fermi surface ( $h_x = \frac{\pi}{2}$ ). Calculate the integral and demonstrate that in the limit  $t/U \gg 1$  the order parameter  $\Omega$  is exponentially suppressed but finite.

The saddle-point equation (or gap equation) obtained in the previous question in the weak-coupling limit is quite general—we will see it again, for instance, in the form of the famous BCS-gap equation for superconductivity. It is crucial for the existence of a weak coupling instability that the system is characterized by nesting: the gap opens everywhere at the Fermi surface, because the Fermi surface lies exactly at the new zone boundary, associated with the symmetry breaking. Here however, the nesting is related to the simplicity of the model, i.e. nearest-neighbour hopping only.

- (g)<sup>(\*)</sup> Discuss qualitatively what changes if we include a small next-nearest-neighbour hopping  $t'$  and argue that we need a finite  $U$  in order for the spin-density wave to occur.