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# Advanced Theoretical Condensed Matter Physics — SS11

## Exercise 4

### 4.1. Ferromagnetic Instability and the Stoner Criterion

The Hubbard model is one of the most well-known model of physical systems available to condensed matter physicists. It has been used to describe strongly correlated electronic systems, the emergence of magnetism in lattice systems, transport of current etc. The Hubbard Hamiltonian is given in general by the following Hamiltonian:

$$\begin{aligned} H &= H_0 + H_1 \\ &= \sum_{\mathbf{p}\sigma} \epsilon_{\mathbf{p}} \hat{c}^\dagger_{\mathbf{p}\sigma} \hat{c}_{\mathbf{p}\sigma} + \frac{U}{N} \sum_{\mathbf{p}\mathbf{p}'\mathbf{q}} \hat{c}^\dagger_{\mathbf{p}+\mathbf{q}\uparrow} \hat{c}_{\mathbf{p}\uparrow} \hat{c}^\dagger_{\mathbf{p}'-\mathbf{q}\downarrow} \hat{c}_{\mathbf{p}'\downarrow} \end{aligned}$$

where the parameter $U$ is often used to denote the Coulomb interaction, although it could also have alternative meaning when considering magnetism, as we will see in the next exercise sheet. For the purpose of this sheet, it will be a constant parameter denoting the strength of the Coulomb interaction. The operators $\hat{c}^\dagger_{\mathbf{p}\sigma}$ and $\hat{c}_{\mathbf{p}\sigma}$ are fermionic creation and annihilation operators respectively.

In this exercise sheet we would like to calculate magnetic excitations of the Hubbard model. The relevant physical quantity is the *spin-spin* correlation function

$$\chi^{ij}(\mathbf{x}-\mathbf{x}', t-t') = \mathrm{i}\theta(t-t')\langle[\hat{s}^i(\mathbf{r}, t), \hat{s}^j(\mathbf{r}', t')]_-\rangle \qquad i, j = x, y, z$$

where the operators $\hat{s}^i$ are the usual 2nd-quantized spin operators

$$\hat{s}^i(\mathbf{x}, t) = \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} \sum_{\mathbf{p}} \sum_{\alpha\beta} \hat{c}^\dagger_{\mathbf{p}+\mathbf{q}\alpha}(t) \sigma^i_{\alpha\beta} \hat{c}_{\mathbf{p}\beta}(t) \quad i = x, y, z$$

and $\sigma^i_{\alpha\beta}$ denotes an appropriate element of the Pauli matrices.

In this problem, we look specifically at the *transversal* spin correlation function, defined as

$$\chi^{-+}(\mathbf{x}-\mathbf{x}', t-t') = \mathrm{i}\theta(t-t')\langle[\hat{s}^-(\mathbf{r}, t), \hat{s}^+(\mathbf{r}', t')]_-\rangle \tag{1}$$

where $\hat{s}^\pm(\mathbf{r}, t)$ are the spin *raising* and *lowering* operators.

a) Show that using the definitions of the raising / lowering operators and finally translational invariance that (1) can be rewritten as

$$\chi^{-+}(\mathbf{x}, t) = \sum_{\mathbf{p}\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} \chi^{-+}(\mathbf{p}, \mathbf{q}, t) \tag{2}$$

where $\chi^{-+}(\mathbf{p}, \mathbf{q}, t) = \mathrm{i}\theta(t)\langle[\hat{c}^\dagger_{\mathbf{p}+\mathbf{q}\downarrow}(t)\hat{c}_{\mathbf{p}\uparrow}(t), \hat{s}^+(0,0)\ ]\rangle$ , $\hat{s}^+(0,0) = \sum_{\mathbf{p}'\mathbf{q}'} \hat{c}^\dagger_{\mathbf{p}'+\mathbf{q}'\uparrow}(0)\hat{c}_{\mathbf{p}'\downarrow}(0)$.

b) Due to convenience we usually derive an expression for the spin susceptibility starting with $\chi^{-+}(\mathbf{p},\mathbf{q},t)$. We will use the equation of motion method and (2).

i) Show that

$$[\hat{c}^\dagger_{\mathbf{p}+\mathbf{q}\downarrow}\hat{c}_{\mathbf{p}\uparrow}, H] = -(\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}})\hat{c}^\dagger_{\mathbf{p}+\mathbf{q}\downarrow}\hat{c}_{\mathbf{p}\uparrow} + \frac{U}{N}\sum_{\mathbf{p}'\mathbf{q}'}(\hat{c}^\dagger_{\mathbf{p}+\mathbf{q}\downarrow}\hat{c}_{\mathbf{p}-\mathbf{q}'\uparrow}\hat{c}^\dagger_{\mathbf{p}'-\mathbf{q}'\downarrow}\hat{c}_{\mathbf{p}'\downarrow} - \hat{c}^\dagger_{\mathbf{p}'+\mathbf{q}'\uparrow}\hat{c}_{\mathbf{p}'\uparrow}\hat{c}^\dagger_{\mathbf{p}+\mathbf{q}-\mathbf{q}'\downarrow}\hat{c}_{\mathbf{p}\uparrow}) \quad (3)$$

ii) The generalized Hartree-Fock approximation now consists of replacing, in the products of four operators on the right-hand side of (3), all *possible* pairs of the type $\hat{c}^\dagger\hat{c}$ by their expectation values and paying regard to sign changes due to commutation of the operators. Specifically, write

$$\left\langle \hat{c}^\dagger_{\mathbf{p}\alpha}\hat{c}_{\mathbf{p}'\beta}\right\rangle = \delta_{\mathbf{p}\mathbf{p}'}\delta_{\alpha\beta}f_{\mathbf{p}\alpha}$$

Show that the second term in (3) is now

$$\frac{U}{N}\sum_{\mathbf{p}'}(f_{\mathbf{p}\uparrow} - f_{\mathbf{p}+\mathbf{q}\downarrow})\hat{c}^\dagger_{\mathbf{p}+\mathbf{p}'+\mathbf{q}\downarrow}\hat{c}_{\mathbf{p}+\mathbf{p}'\uparrow} + (f_{\mathbf{p}'\downarrow} - f_{\mathbf{p}'\uparrow})\hat{c}^\dagger_{\mathbf{p}+\mathbf{q}\downarrow}\hat{c}_{\mathbf{p}\uparrow}$$

and therefore derive the equation of motion for $\chi^{-+}(\mathbf{p},\mathbf{q},t)$

$$\left\{i\frac{\partial}{\partial t} + (\tilde{\epsilon}_{\mathbf{p}+\mathbf{q}\uparrow} - \tilde{\epsilon}_{\mathbf{p}\downarrow})\right\}\chi^{-+}(\mathbf{p},\mathbf{q},t) = -\delta(t)(f_{\mathbf{p}+\mathbf{q}\downarrow} - f_{\mathbf{p}\uparrow}) - (f_{\mathbf{p}+\mathbf{q}\downarrow} - f_{\mathbf{p}\uparrow})\frac{U}{N}\sum_{\mathbf{p}'}\chi^{-+}(\mathbf{p}',\mathbf{q},t) \quad (4)$$

What are the expressions $\tilde{\epsilon}_{\mathbf{p}+\mathbf{q}\uparrow}$ and $\tilde{\epsilon}_{\mathbf{p}\downarrow}$?

iii) Write (4) in $(\mathbf{p},\mathbf{q},\omega)$ representation and solve for $\chi^{-+}(\mathbf{p},\mathbf{q},\omega)$. You should obtain an equation of the form

$$\chi^{-+}(\mathbf{q},\omega) = \frac{\Gamma^{-+}(\mathbf{q},\omega)}{1 - U\Gamma^{-+}(\mathbf{q},\omega)} \quad (5)$$

with $\chi(\mathbf{q}) = \sum_{\mathbf{p}}\chi(\mathbf{p},\mathbf{q})$. What is the explicit form of $\Gamma^{-+}(\mathbf{q},\omega)$?

c) We now derive the Stoner criterion. We first set $f_{\mathbf{p}\uparrow} = f_{\mathbf{p}\downarrow} = f_{\mathbf{p}}$, $\tilde{\epsilon}_{\mathbf{p}\uparrow} = \tilde{\epsilon}_{\mathbf{p}\downarrow} = \epsilon_{\mathbf{p}}$, and $\Gamma^{-+}(\mathbf{q},\omega) = \Gamma(\mathbf{q},\omega)$ which places us in the paramagnetic regime, where the populations of the "up" and "down" spin states are equal. Particularly important if one is searching for the point where a fundamental change in the ground state happens is the quantity $\Gamma(\mathbf{q},\omega = 0)$.

i) In (5) identify the point where you expect a fundemental change in the property of the system to occur.

ii) We now want to look at the *static* correlation function $\Gamma(\mathbf{q},0)$ at long length scales, i.e., for $\mathbf{q} \to 0$. Expand both the numerator and denominator of $\Gamma(\mathbf{q},0)$ up to first order in $\mathbf{q}$, and using the fact that at zero temperature, $\partial f/\partial\epsilon = -\delta(\epsilon - \epsilon_f)$ to derive the *Stoner criterion*

$$U\mathcal{N}(\epsilon_f) = 1 \quad (6)$$

Physically speaking, an instability at $\mathbf{q} = 0$ corresponds to the tendency for the system to acquire spontaneously a uniform, or ferromagnetic, spin density.