5. Response functions

5.1 Random Phase Approximation

The truncation of the equation of motion for the Greens function with the Hartree Fock mean field approximation transforms the Hamiltonian into an effective single particle operator; this too simple treatment of the influence of interactions leads to a lack of realism. A better approach than the truncation of the equation of motion hierarchy is the approximate evaluation also of the higher order equations of motion. This allows to better account for the interaction as the full Hamiltonian enters the equation of motion at each step.
The so called random phase approximation (RPA) involves replacement of operator products by averages as in the mean field approximation (neglect of the fluctuation of averages). For the single particle Greens function

$$G_{\vec{k}\sigma}(\omega) = \langle\langle c_{\vec{k}\sigma}; c^{\dagger}_{\vec{k}\sigma}\rangle\rangle \tag{5.1}$$

the result is again the Hartree-Fock result.
The magnetic susceptibility is an important quantity describing the response of a material to an external magnetic field $\vec{H}(t) = \vec{H}_0 e^{-(\omega+i\delta)t}$:

$$\langle M^{\alpha}\rangle(t) = \langle M^{\alpha}\rangle - \sum_{\beta}\int_{-\infty}^{\infty} dt' \langle\langle M^{\alpha}(t); M^{\beta}(t')\rangle\rangle H_0^{\beta} e^{-i(\omega+i\delta)t'} \tag{5.2}$$

with cartesian directions α, β. As the Greens function is homogeneous in time we have

$$\begin{aligned}\langle M^{\alpha}\rangle_{(t)} &= \langle M^{\alpha}\rangle - \sum_{\beta}\int_{-\infty}^{\infty} dt' \langle\langle M^{\alpha}; M^{\beta}(t'-t)\rangle\rangle H_0^{\beta} e^{-i(\omega+i\delta)(t'-t)} e^{-i(\omega+i\delta)t} \\ &= \langle M^{\alpha}\rangle - \sum_{\beta}\int_{-\infty}^{\infty} dt' \langle\langle M^{\alpha}; M^{\beta}(t')\rangle\rangle e^{-i(\omega+i\delta)t'} H^{\beta}(t)\end{aligned} \tag{5.3}$$

with a field independent part of the magnetization $\langle M^\alpha \rangle$ which is important for ferromagnetic systems and the second part describing the magnetization induced by an external magnetic field. This part is proportional to $H(t)$; the prefactor represents the magnetic susceptibility χ:

$$\langle M^\alpha \rangle(t) = \langle M^\alpha \rangle + \sum_\beta \chi^{\alpha\beta}(\omega) H^\beta(t) \tag{5.4}$$

Comparison yields

$$\chi^{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} dt\, e^{-i(\omega+i\delta)t} \langle\langle M^\alpha; M^\beta(t) \rangle\rangle \equiv -\langle\langle M^\alpha; M^\beta \rangle\rangle(\omega - i\delta) \tag{5.5}$$

Thus, $\chi^{\alpha\beta}(\omega)$ is given by the Fourier transform of the Greens function. We can now replace the magnetic moment operator $\vec{M}_i$ at site i by a spin operator $\vec{S}_i$ to obtain

$$\chi_{ij}^{\mu\nu}(\omega) = -\langle\langle M_i^\mu; M_j^\nu \rangle\rangle(\omega) = -g^2 \mu_B^2 \langle\langle S_i^\mu; S_j^\nu \rangle\rangle(\omega) \tag{5.6}$$

with gyromagnetic factor g and Bohr magneton μ_B. Of particular interest are the longitudinal susceptibility

$$\chi_{ij}^{zz}(\omega) = -g^2 \mu_B^2 \langle\langle S_i^z; S_j^z \rangle\rangle(\omega) \tag{5.7}$$

and the transversal susceptibility

$$\chi_{ij}^{+-}(\omega) = -g^2 \mu_B^2 \langle\langle S_i^+; S_j^- \rangle\rangle(\omega) \quad \text{where } S_i^\pm = S_i^x \pm i S_i^y \tag{5.8}$$

The operators S_i^z, S_i^+ and S_i^- can again be replaced by creation and annihilation operators:

$$S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}), \quad S_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}, \quad S_i^- = c_{i\downarrow}^\dagger c_{i\uparrow} \tag{5.9}$$

which leads to

$$\chi_{ij}^{zz}(\omega) = -\frac{1}{4} g^2 \mu_B^2 (2\delta_{\sigma\sigma'} - 1) \langle\langle n_{i\sigma}; n_{j\sigma'} \rangle\rangle(\omega) \tag{5.10}$$

and

$$\chi_{ij}^{+-}(\omega) = -g^2 \mu_B^2 \langle\langle c_{i\uparrow}^\dagger c_{i\downarrow}; c_{i\downarrow}^\dagger c_{i\uparrow} \rangle\rangle(\omega) \tag{5.11}$$

linking the susceptibilities to special two particle Greens functions. We will now apply the random phase approximation to the calculation of the transversal magnetic susceptibility within the Hubbard model; this approximation will be valid in the limit of weak interactions. In $\vec{k}$ space we have for the susceptibility

$$\chi^{+-}(\vec{q},\omega) = -g^2\mu_B^2 \sum_{\vec{k}\vec{k}'} \langle\langle c^\dagger_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow}; c^\dagger_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow}\rangle\rangle(\omega) \tag{5.12}$$

The equation of motion for this two-particle Greens function is

$$\begin{aligned}\omega\langle\langle c^\dagger_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow}; c^\dagger_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow}\rangle\rangle(\omega) &= \left(\langle n_{\vec{k}\uparrow}\rangle - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle\right)\delta_{\vec{k},\vec{k}+\vec{q}} + \\ &+ \left(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}\right)\langle\langle c^\dagger_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow}; c^\dagger_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow}\rangle\rangle(\omega) + \\ &+ \frac{U}{N}\sum_{\vec{k}_1,\vec{q}_1} \langle\langle (c^\dagger_{\vec{k}\uparrow} c^\dagger_{\vec{k}_1\uparrow} c_{\vec{k}_1-\vec{q}_1\uparrow} c_{\vec{k}+\vec{q}-\vec{q}_1\downarrow} - c^\dagger_{\vec{k}+\vec{q}_1\uparrow} c^\dagger_{\vec{k}_1\downarrow} c_{\vec{k}_1+\vec{q}_1\downarrow} c_{\vec{k}+\vec{q}\downarrow}); c^\dagger_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow}\rangle\rangle(\omega)\end{aligned} \tag{5.13}$$

According to the principles of the random phase approximation the excess operators in the higher order Greens functions are replaced by averages:

$$c^\dagger_{\vec{k}\uparrow} c^\dagger_{\vec{k}_1\uparrow} c_{\vec{k}_1-\vec{q}_1\uparrow} c_{\vec{k}+\vec{q}+\vec{q}_1\downarrow} \approx \langle n_{\vec{k}_1\uparrow}\rangle \delta_{\vec{q}_1,0} c^\dagger_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow} - \langle n_{\vec{k}\uparrow}\rangle \delta_{\vec{k}_1\vec{k}_1-\vec{q}_1} c^\dagger_{\vec{k}-\vec{q}_1\uparrow} c_{\vec{k}-\vec{q}-\vec{q}_1\downarrow} \tag{5.14}$$

Here, conservation of momentum and spin was used:

$$\langle c^\dagger_{\vec{k}\sigma} c_{\vec{k}'\sigma'}\rangle = \langle n_{\vec{k}\sigma}\rangle \delta_{\vec{k}\vec{k}'}\delta_{\sigma\sigma'} \tag{5.15}$$

Also

$$c_{\vec{k}+\vec{q}_1\uparrow} c_{\vec{k}_1\downarrow} c_{\vec{k}_1+\vec{q}_1\downarrow} c_{\vec{k}+\vec{q}\downarrow} \approx \langle n_{\vec{k}_1\downarrow}\rangle \delta_{\vec{q}_1,0} c^\dagger_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow} - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle \delta_{\vec{k}_1,\vec{k}+\vec{q}} c^\dagger_{\vec{k}+\vec{q}_1} c_{\vec{k}+\vec{q}+\vec{q}_1\downarrow} \tag{5.16}$$

This yields

$$\begin{aligned}\left(\omega - \omega^{\uparrow\downarrow}_{\vec{k}}(\vec{q})\right)\langle\langle c^\dagger_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow}; c^\dagger_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow}\rangle\rangle(\omega) &= \Big[\left(\langle n_{\vec{k}\uparrow}\rangle - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle\right) \\ &- \frac{U}{N}\sum_{\vec{k}''} \langle\langle c^\dagger_{\vec{k}''\uparrow} c_{\vec{k}''+\vec{q}\downarrow}; c^\dagger_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow}\rangle\rangle(\omega)\Big]\end{aligned} \tag{5.17}$$

with the Stoner single particle excitation spectrum

$$\omega^{\sigma\sigma'}_{\vec{k}}(\vec{q}) = \varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} + U(n_{-\sigma'} - n_{-\sigma}) \tag{5.18}$$

Now we divide Eq. (5.17) by ω and sum over $\vec{k}$:

$$\sum_{\vec{k}} \langle\langle c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow}; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) = \sum_{\vec{k}} \frac{\langle n_{\vec{k}\uparrow}\rangle - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle}{\omega - \omega^{\uparrow\downarrow}_{\vec{k}}(\vec{q})} \delta_{\vec{k}',\vec{k}+\vec{q}}$$
$$- \sum_{\vec{k}} \frac{\langle n_{\vec{k}\uparrow}\rangle - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle}{\omega - \omega^{\uparrow\downarrow}_{\vec{k}}(\vec{q})} \frac{U}{N} \sum_{\vec{k}''} \langle\langle c^{\dagger}_{\vec{k}''\uparrow} c_{\vec{k}''+\vec{q}\downarrow}; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) \quad (5.19)$$

After renaming summations indices this means

$$\sum_{\vec{k}} \langle\langle c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow}; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) = \frac{\sum_{\vec{k}} \frac{\langle n_{\vec{k}\uparrow}\rangle - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle}{\omega - \omega^{\uparrow\downarrow}_{\vec{k}}(\vec{q})} \delta_{\vec{k}',\vec{k}+\vec{q}}}{1 + \frac{U}{N} \sum_{\vec{k}''} \frac{\langle n_{\vec{k}''\uparrow}\rangle - \langle n_{\vec{k}''+\vec{q}\downarrow}\rangle}{\omega - \omega^{\uparrow\downarrow}_{\vec{k}''}(\vec{q})}} \quad (5.20)$$

with the susceptivility of the Stoner model

$$\chi^0(\vec{q}, \omega) = g^2 \mu_B^2 \sum_{\vec{k}} \frac{\langle n_{\vec{k}\uparrow}\rangle - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle}{\omega - \omega^{\uparrow\downarrow}_{\vec{k}}(\vec{q})} \quad (5.21)$$

This yields for the transverse susceptibility

$$\chi^{+-}(\vec{q}, \omega) = \frac{\chi^0(\vec{q}, \omega)}{1 - \frac{U}{N g^2 \mu_B^2} \chi^0(\vec{q}, \omega)} \quad (5.22)$$

The denominator in this RPA expression for the susceptibility can become small for certain $\vec{q}$ and ω values so that the susceptibility becomes big.