7. Response functions

7.1 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.[1]

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

$$G_{\vec{k}\sigma}(\omega) = \langle\langle c_{\vec{k}\sigma}; c^\dagger_{\vec{k}\sigma} \rangle\rangle \tag{7.1}$$

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 $\vec{H}(t) = \vec{H}_0 e^{-(\omega+i\delta)t}$:

$$\langle M^\alpha \rangle(t) = \langle M^\alpha \rangle - \sum_\beta \int_{-\infty}^{\infty} dt' \langle\langle M^\alpha(t); M^\beta(t') \rangle\rangle H_0^\beta e^{-i(\omega+i\delta)t'} \tag{7.2}$$

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

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

[1]This chapter is based on K. Elk, W. Gasser, *“Die Methode der Greenschen Funktionen in der Festkörperphysik”*, Akademie-Verlag Berlin 1979, and W. Nolting, *“Grundkurs Theoretische Physik 7, Viel-Teilchen-Theorie”*, Springer 2009.

$$(7.3)$$

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:

$$\langle M^\alpha \rangle(t) = \langle M^\alpha \rangle + \sum_\beta \chi^{\alpha\beta}(\omega) H^\beta(t) \tag{7.4}$$

Comparison yields

$$\chi^{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} dt\, e^{-i(\omega+i\delta)t} \langle\langle M^\alpha; M^\beta(t) \rangle\rangle \equiv -\langle\langle M^\alpha; M^\beta \rangle\rangle(\omega - i\delta) \tag{7.5}$$

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

$$\chi^{\mu\nu}_{ij}(\omega) = -\langle\langle M^\mu_i; M^\nu_j \rangle\rangle(\omega) = -g^2 \mu_B^2 \langle\langle S^\mu_i; S^\nu_j \rangle\rangle(\omega) \tag{7.6}$$

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

$$\chi^{zz}_{ij}(\omega) = -g^2 \mu_B^2 \langle\langle S^z_i; S^z_j \rangle\rangle(\omega) \tag{7.7}$$

and the transversal susceptibility

$$\chi^{+-}_{ij}(\omega) = -g^2 \mu_B^2 \langle\langle S^+_i; S^-_j \rangle\rangle(\omega) \quad \text{where } S^\pm_i = S^x_i \pm i S^y_i \tag{7.8}$$

The operators S^z_i, S^+_i and S^-_i can again be replaced by creation and annihilation operators:

$$S^z_i = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}), \quad S^+_i = c^\dagger_{i\uparrow} c_{i\downarrow}, \quad S^-_i = c^\dagger_{i\downarrow} c_{i\uparrow} \tag{7.9}$$

which leads to

$$\chi^{zz}_{ij}(\omega) = -\frac{1}{4} g^2 \mu_B^2 (2\delta_{\sigma\sigma'} - 1) \langle\langle n_{i\sigma}; n_{j\sigma'} \rangle\rangle(\omega) \tag{7.10}$$

and

$$\chi^{+-}_{ij}(\omega) = -g^2 \mu_B^2 \langle\langle c^\dagger_{i\uparrow} c_{i\downarrow}; c^\dagger_{i\downarrow} c_{i\uparrow} \rangle\rangle(\omega) \tag{7.11}$$

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

$$H = \sum_{\vec{k}\sigma} (\varepsilon_{\vec{k}} - \mu) c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma} + \frac{U}{N} \sum_{\vec{k}\vec{k}_1\vec{q}} c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}-\vec{q}\uparrow} c^{\dagger}_{\vec{k}_1\downarrow} c_{\vec{k}_1+\vec{q}\downarrow} ; \tag{7.12}$$

the random phase approximation will be valid in the limit of weak interactions. In $\vec{k}$ space we have for the susceptibility

$$\chi^{+-}(\vec{q}, \omega) = -g^2 \mu_B^2 \sum_{\vec{k}\vec{k}'} \langle\langle c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow} ; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) \tag{7.13}$$

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

$$\begin{aligned} \omega \langle\langle c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow} ; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) &= \left(\langle n_{\vec{k}\uparrow} \rangle - \langle n_{\vec{k}+\vec{q}\downarrow} \rangle \right) \delta_{\vec{k}', \vec{k}+\vec{q}} + \\ &+ \left(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} \right) \langle\langle c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow} ; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) + \\ &+ \frac{U}{N} \sum_{\vec{k}_1, \vec{q}_1} \langle\langle (c^{\dagger}_{\vec{k}\uparrow} c^{\dagger}_{\vec{k}_1\uparrow} c_{\vec{k}_1-\vec{q}_1\uparrow} c_{\vec{k}+\vec{q}-\vec{q}_1\downarrow} - c^{\dagger}_{\vec{k}+\vec{q}_1\uparrow} c^{\dagger}_{\vec{k}_1\downarrow} c_{\vec{k}_1+\vec{q}_1\downarrow} c_{\vec{k}+\vec{q}\downarrow}) ; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) \end{aligned} \tag{7.14}$$

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

$$c^{\dagger}_{\vec{k}\uparrow} c^{\dagger}_{\vec{k}_1\uparrow} c_{\vec{k}_1-\vec{q}_1\uparrow} c_{\vec{k}+\vec{q}+\vec{q}_1\downarrow} \approx \langle n_{\vec{k}_1\uparrow} \rangle \delta_{\vec{q}_1,0} c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow} - \langle n_{\vec{k}\uparrow} \rangle \delta_{\vec{k}\vec{k}_1-\vec{q}_1} c^{\dagger}_{\vec{k}-\vec{q}_1\uparrow} c_{\vec{k}-\vec{q}-\vec{q}_1\downarrow} \tag{7.15}$$

Here, conservation of momentum and spin was used:

$$\langle c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}'\sigma'} \rangle = \langle n_{\vec{k}\sigma} \rangle \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'} \tag{7.16}$$

Also

$$c^{\dagger}_{\vec{k}+\vec{q}_1\uparrow} c^{\dagger}_{\vec{k}_1\downarrow} c_{\vec{k}_1+\vec{q}_1\downarrow} c_{\vec{k}+\vec{q}\downarrow} \approx \langle n_{\vec{k}_1\downarrow} \rangle \delta_{\vec{q}_1,0} c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow} - \langle n_{\vec{k}+\vec{q}\downarrow} \rangle \delta_{\vec{k}_1, \vec{k}+\vec{q}} c^{\dagger}_{\vec{k}+\vec{q}_1\uparrow} c_{\vec{k}+\vec{q}+\vec{q}_1\downarrow} \tag{7.17}$$

This yields

$$\begin{aligned} \left(\omega - \omega^{\uparrow\downarrow}_{\vec{k}}(\vec{q}) \right) \langle\langle c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow} ; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) &= \left(\langle n_{\vec{k}\uparrow} \rangle - \langle n_{\vec{k}+\vec{q}\downarrow} \rangle \right) \\ &\left[\delta_{\vec{k}', \vec{k}+\vec{q}} - \frac{U}{N} \sum_{\vec{k}''} \langle\langle c^{\dagger}_{\vec{k}''\uparrow} c_{\vec{k}''+\vec{q}\downarrow} ; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) \right] \end{aligned} \tag{7.18}$$

with the Stoner single particle excitation spectrum

$$\omega_{\vec{k}}^{\sigma\sigma'}(\vec{q}) = \varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} + U(n_{-\sigma'} - n_{-\sigma}) \tag{7.19}$$

Now we divide Eq. (7.18) by $\left(\omega - \omega_{\vec{k}}^{\uparrow\downarrow}(\vec{q})\right)$ and sum over $\vec{k}$:

$$\begin{aligned}\sum_{\vec{k}} \langle\langle c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow}; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) &= \sum_{\vec{k}} \frac{\langle n_{\vec{k}\uparrow}\rangle - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle}{\omega - \omega_{\vec{k}}^{\uparrow\downarrow}(\vec{q})} \delta_{\vec{k}',\vec{k}+\vec{q}} \\ &- \sum_{\vec{k}} \frac{\langle n_{\vec{k}\uparrow}\rangle - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle}{\omega - \omega_{\vec{k}}^{\uparrow\downarrow}(\vec{q})} \frac{U}{N} \sum_{\vec{k}''} \langle\langle c^{\dagger}_{\vec{k}''\uparrow} c_{\vec{k}''+\vec{q}\downarrow}; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega)\end{aligned} \tag{7.20}$$

After renaming summation indices this means

$$\sum_{\vec{k}} \langle\langle c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow}; c^{\dagger}_{\vec{k}'\downarrow} c_{\vec{k}'-\vec{q}\uparrow} \rangle\rangle(\omega) = \frac{\displaystyle\sum_{\vec{k}} \frac{\langle n_{\vec{k}\uparrow}\rangle - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle}{\omega - \omega_{\vec{k}}^{\uparrow\downarrow}(\vec{q})} \delta_{\vec{k}',\vec{k}+\vec{q}}}{\displaystyle 1 + \frac{U}{N} \sum_{\vec{k}''} \frac{\langle n_{\vec{k}''\uparrow}\rangle - \langle n_{\vec{k}''+\vec{q}\downarrow}\rangle}{\omega - \omega_{\vec{k}''}^{\uparrow\downarrow}(\vec{q})}} \tag{7.21}$$

with the susceptivility of the Stoner model

$$\chi^0(\vec{q}, \omega) = g^2 \mu_B^2 \sum_{\vec{k}} \frac{\langle n_{\vec{k}\uparrow}\rangle - \langle n_{\vec{k}+\vec{q}\downarrow}\rangle}{\omega - \omega_{\vec{k}}^{\uparrow\downarrow}(\vec{q})} \tag{7.22}$$

This yields for the transverse susceptibility

$$\chi^{+-}(\vec{q}, \omega) = \frac{\chi^0(\vec{q}, \omega)}{1 - \frac{U}{N g^2 \mu_B^2} \chi^0(\vec{q}, \omega)} \tag{7.23}$$

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.

Noninteracting susceptibility

The spin susceptibility[2] χ_1 can be expressed[3] in terms of the Matsubara spin-spin correlation function

$$(\chi_1)_t^s = \frac{1}{3} \int_0^{\beta} d\tau e^{i\omega\tau} \left\langle T_\tau \vec{S}_s(q, \tau) \vec{S}_t(-q, 0) \right\rangle$$

[2]This part was worked out by Michaela Altmeyer; thank you!

[3]S. Graser, T.A. Maier, P.J. Hirschfeld, D.J. Scalapino, New J. Phys. **11**, 025016 (2009).

with the Matsubara frequency ω, the imaginary time τ and the spin operators for the different orbitals s

$$\vec{S}_s(q) = \frac{1}{2} \sum_{k,\alpha\beta} d^{\dagger}_{s\alpha}(k+q) \vec{\sigma}_{\alpha\beta} d_{s\beta}(k), \tag{7.24}$$

where α and β are spin indices. The charge susceptibility χ_0 can be calculated in a very similar manner,

$$(\chi_0)^s_t = \int_0^{\beta} d\tau e^{i\omega\tau} \langle T_\tau n_s(q,t) n_t(-q,0) \rangle \tag{7.25}$$

with

$$n_s(q) = \frac{1}{N} \sum_{k,\alpha\beta} d^{\dagger}_{s\alpha}(k+q) d_{s\beta}(k) \delta_{\alpha,\beta}. \tag{7.26}$$

In the noninteracting case ($\sum_{i=1}^{3} \mathrm{Tr}(\sigma_i^2) = 6$), both are equivalent and can be written in a more general way as

$$\chi^{pq}_{st}(q, i\omega) = \frac{1}{N^2} \int_0^{\beta} d\tau e^{i\omega\tau} \sum_{kk'} \sum_{\alpha\beta} \big\langle T_\tau d^{\dagger}_{p\alpha}(k,\tau) d_{q\alpha}(k+q,\tau) \times \\ \times d^{\dagger}_{s\beta}(k',0) d_{t\beta}(k'-q,0) \big\rangle. \tag{7.27}$$

The imaginary-time ordered expectation value can be evaluated by means of Wick's theorem.

$$\chi^{pq}_{st}(q, i\omega) = -\frac{1}{N^2} \int_0^{\beta} d\tau e^{i\omega\tau} \sum_{kk'} \sum_{\alpha\beta} G^{pt}_{\alpha}(k+q,\tau) G^{sq}_{\alpha}(k,-\tau) \delta_{\alpha,\beta} \delta_{k',k+q} \\ + \frac{1}{N^2} \int_0^{\beta} d\tau e^{i\omega\tau} \sum_{kk'} \sum_{\alpha\beta} G^{pq}_{\alpha}(k,\tau) G^{st}_{\beta}(k,0) \delta_{q,0}. \tag{7.28}$$

The second term leads to an unphysical delta function $\delta_{q,0}$ and will therefore be neglected in the following considerations, while the first term can be further analyzed by writing the imaginary time Green's functions as Fourier transforms of Matsubara Green's functions (the summation over the spin index α leads to a factor of 2),

$$G^{pt}(k,\tau) = \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n\tau} G^{pt}(k, i\omega_n). \tag{7.29}$$

Insertion into equation (7.28) yields

$$\chi_{st}^{pq}(q, i\omega) = -\frac{1}{N}\int_0^\beta d\tau e^{i\omega\tau}\sum_k \frac{2}{\beta^2}\sum_{\omega_n,\omega_m} e^{-i\omega_n\tau}G^{pt}(k+q, i\omega_n)e^{i\omega_m\tau}G^{sq}(k, i\omega_m), \tag{7.30}$$

so that we can now perform the integration over imaginary time.

$$\chi_{st}^{pq}(q, i\omega) = -\frac{1}{N}\sum_k \frac{2}{\beta^2}\sum_{\omega_n,\omega_m} \frac{e^{i\beta(\omega-\omega_n+\omega_m)}-1}{i(\omega-\omega_n+\omega_m)}G^{pt}(k+q, i\omega_n)G^{sq}(k, i\omega_m). \tag{7.31}$$

Due to the fact that the frequencies are Fermionic Matsubara frequencies, the fraction is zero when $\omega \neq \omega_n + \omega_m$; however, when $\omega = \omega_n + \omega_m$ we have to consider the limit

$$\frac{e^{i\beta(\omega-\omega_n+\omega_m)}-1}{i(\omega-\omega_n+\omega_m)}\delta_{\omega_n,\omega+\omega_m} = \frac{1+i\beta(\omega-\omega_n+\omega_m)-1}{i(\omega-\omega_n+\omega_m)}\delta_{\omega_n,\omega+\omega_m} = \beta\delta_{\omega_n,\omega+\omega_m}, \tag{7.32}$$

so that

$$\begin{aligned}\chi_{st}^{pq}(q, i\omega) &= -\frac{2}{\beta N}\sum_k \sum_{\omega_n,\omega_m} G^{pt}(k+q, i\omega_n)G^{sq}(k, i\omega_m)\delta_{\omega_n,\omega+\omega_m}\\ &= -\frac{2}{\beta N}\sum_k \sum_{\omega_m} G^{pt}(k+q, i\omega+i\omega_m)G^{sq}(k, i\omega_m).\end{aligned} \tag{7.33}$$

Making use of the spectral representation of the Green's function

$$G^{pt}(k, i\omega_n) = \sum_\mu \frac{a_\mu^s(k)a_\mu^{p*}(k)}{i\omega_n - E_\mu(k)}, \tag{7.34}$$

where the E_μ denote the eigenvalues of the tight binding Hamiltonian and a_μ^s are the s components of the corresponding eigenvectors, this can be written as

$$\chi_{st}^{pq}(q, i\omega) = -\frac{2}{\beta N}\sum_k \sum_{\omega_m}\sum_{\mu\nu} \frac{a_\mu^s(k)a_\mu^{p*}(k)}{i\omega_m - E_\mu(k)}\frac{a_\nu^q(k+q)a_\nu^{t*}(k+q)}{i\omega + i\omega_m - E_\nu(k+q)}.$$

(7.35)

Evaluation of the sum over Matsubara frequencies leads to

$$\chi^{pq}_{st}(q, i\omega) = -\frac{2}{N}\sum_{k,\mu\nu}\frac{a^s_\mu(k)a^{p*}_\mu(k)a^q_\nu(k+q)a^{t*}_\nu(k+q)}{i\omega + E_\nu(k+q) - E_\mu(k)}\big[f(E_\nu(k+q)) - f(E_\mu(k))\big] \tag{7.36}$$

where N is the product of the number of considered k points and the number of bands in the model hamiltonian. The static homogeneous spin susceptibility can be calculated quite easily from

$$\begin{aligned}\chi_S(q) &= \frac{1}{2}\sum_{sp}(\chi_1)^{pp}_{ss}(q, \omega = 0)\\ &= -\frac{1}{N}\sum_{sp}\sum_{k,\mu\nu}\frac{a^s_\mu(k)a^{p*}_\mu(k)a^p_\nu(k+q)a^{s*}_\nu(k+q)}{E_\nu(k+q) - E_\mu(k)}\big[f(E_\nu(k+q)) - f(E_\mu(k))\big].\end{aligned} \tag{7.37}$$

The susceptibility (7.36) should be properly normalized, taking into account the number of possible spin orientations, the number of considered k points and the number of bands in the model Hamiltonian $(2 \cdot N_k \cdot n)$. The computational implementation needs an extra consideration. When the energies in the denominator are the same we have a unphysical singularity, which can be avoided using the rule of l'Hopital, so that

$$\begin{aligned}\chi_S(q) =& \frac{1}{2}\sum_{sp}(\chi_1)^{pp}_{ss}(q, \omega = 0)\\ =& \frac{\beta}{2N}\sum_{sp}\sum_{k,\mu\nu} a^s_\mu(k)a^{p*}_\mu(k)a^p_\nu(k+q)a^{s*}_\nu(k+q)\\ &\times\left[\frac{1}{e^{\beta(E_\nu(k+q)-\mu)} + e^{-\beta(E_\nu(k+q)-\mu)} + 2} + \frac{1}{e^{\beta(E_\mu(k)-\mu)} + e^{-\beta(E_\mu(k)-\mu)} + 2}\right].\end{aligned} \tag{7.38}$$

_R_andom _P_hase _A_pproximation (RPA) The random phase approximated susceptibilities can be obtained from a Dyson-type equation. The charge susceptibility can be calculated from

$$(\chi^{RPA}_0)^{pq}_{st} = \chi^{pq}_{st} - \sum_{uvwz}(\chi^{RPA}_0)^{pq}_{uv}(U^c)^{uv}_{wz}\chi^{wz}_{st}, \tag{7.39}$$

while the spin susceptibility has a plus sign instead,

$$(\chi_1^{\mathrm{RPA}})_{st}^{pq} = \chi_{st}^{pq} + \sum_{uvwz} (\chi_0^{\mathrm{RPA}})_{uv}^{pq} (U^s)_{wz}^{uv} \chi_{st}^{wz}. \tag{7.40}$$