# **TKM II:**

# Equation of motion technique - Anderson model and screening (RPA)

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# 1 Preliminaries: Bands etc

Let us consider the non-interacting Hamiltonian in second quantized form

$$H_0 = \int_{\mathcal{V}} d^3 r \sum_{\sigma} \hat{\psi}^{\dagger}_{\sigma}(\boldsymbol{r}) \left[ \frac{\boldsymbol{p}^2}{2m} - \mu + V(\boldsymbol{r}) \right] \hat{\psi}_{\sigma}(\boldsymbol{r}) \tag{1}$$

where  $V(\mathbf{r})$  is a periodic crystal potential. The eigenfunctions  $\phi_{n\mathbf{k}\sigma}(\mathbf{r}) = u_n(\mathbf{r})\chi_{\sigma}e^{i\mathbf{k}\cdot\mathbf{r}}$  of the single-particle Hamiltonian are characterized by **band index** n, **crystal momentum**  $\mathbf{k} \in 1$ st B.Z. and **spin index**  $\sigma$ . The energy spectrum is separated into bands  $\epsilon_{n\mathbf{k}}$ . If  $\epsilon_F = \mu(T = 0)$  crosses one of the bands the material is a **metal** and the band is referred to as **conduction band**. The bandwidth is defined as  $D_n = \max[\epsilon_{n\mathbf{k}}] - \min[\epsilon_{n\mathbf{k}}]$ . The field operator can be expanded in the complete set of eigenstates

$$\hat{\psi}_{\sigma}(\boldsymbol{r}) = \sum_{n\boldsymbol{k}} \phi_{n\boldsymbol{k}\sigma}(\boldsymbol{r}) \hat{c}_{n\boldsymbol{k}\sigma}$$
(2)

The Hamiltonian in this basis takes the form

$$H_0 = \sum_{n \boldsymbol{k}\sigma} \epsilon_{n \boldsymbol{k}\sigma} \hat{c}^{\dagger}_{n \boldsymbol{k}\sigma} \hat{c}_{n \boldsymbol{k}\sigma}$$
(3)

For metals it is common to restrict oneself to the conduction band and adopt an **effective mass** approximation

$$\begin{cases}
\phi_{n\boldsymbol{k}\sigma}(\boldsymbol{r}) \\
\boldsymbol{k} \in 1.B.Z. \\
m \\
\sum_{n\boldsymbol{k}\sigma} \epsilon_{n\boldsymbol{k}} \hat{c}^{\dagger}_{n\boldsymbol{k}\sigma} \hat{c}_{n\boldsymbol{k}\sigma}
\end{cases} \rightarrow \begin{cases}
\frac{1}{\sqrt{\mathcal{V}}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \chi_{\sigma} \\
\boldsymbol{k} \text{ unrestricted} \\
m^{*} \\
\sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{c}_{\boldsymbol{k}\sigma}
\end{cases} \tag{4}$$

We will, however, for the following discussion of the Anderson Model, assume that the spectrum has a certain bandwidth D.

The single particle Matsubara (thermal) Green's function is given by

$$G_{\sigma\sigma'}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau') = -\langle T_{\tau}\hat{\psi}_{\sigma}(\boldsymbol{r}, \tau)\hat{\psi}^{\dagger}_{\sigma'}(\boldsymbol{r}, \tau)\rangle$$
(5)

where

$$\hat{\psi}_{\sigma}(\boldsymbol{r},\tau) = e^{H_0\tau}\hat{\psi}_{\sigma}(\boldsymbol{r})e^{-H_0\tau}, \qquad \hat{\psi}_{\sigma}^{\dagger}(\boldsymbol{r},\tau) = e^{H_0\tau}\hat{\psi}_{\sigma}^{\dagger}(\boldsymbol{r})e^{-H_0\tau}$$
(6)

It is usually easier to work with the GF in momentum space

$$G_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'}(\tau,\tau') = -\langle T_{\tau}\hat{c}_{\boldsymbol{k}\sigma}(\tau)\hat{c}^{\dagger}_{\boldsymbol{k}'\sigma'}(\tau')\rangle \tag{7}$$

which is related to the GF in position space through

$$G_{\sigma\sigma'}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau') = -\frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}, \boldsymbol{k}'} \langle T_{\tau} \hat{c}_{\boldsymbol{k}\sigma}(\tau) \hat{c}^{\dagger}_{\boldsymbol{k}'\sigma'}(\tau') \rangle e^{i\boldsymbol{k}\cdot\boldsymbol{r}-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \chi_{\sigma} \chi^{\dagger}_{\sigma'}$$

$$= -\frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}, \boldsymbol{k}'} G_{\boldsymbol{k}\sigma, \boldsymbol{k}'\sigma'}(\tau, \tau') e^{i\boldsymbol{k}\cdot\boldsymbol{r}-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \chi_{\sigma} \chi^{\dagger}_{\sigma'}$$
(8)

If the system is invariant under spin-rotational symmetry, then the GF in Eq. (5) will be proportional to  $\delta_{\sigma\sigma'}$ , and if we have translational (periodic) invariance in space the GF's will only depend on the relative coordinate r - r'. Finally, if the Hamiltonian does not explicitly depend on imaginary time  $\tau$ , the GF will depend only on the relative coordinates  $\tau - \tau'$ . Thus under these conditions we may restrict ourselves to

$$G_{\boldsymbol{k},\sigma}(\tau) = -\langle T_{\tau} \hat{c}_{\boldsymbol{k}\sigma}(\tau) \hat{c}_{\boldsymbol{k}\sigma}^{\dagger}(0) \rangle \tag{9}$$

#### Single particle GF (Fermions)

The single particle Matsubara (thermal) Green's function is defined as

$$G_{\boldsymbol{k},\sigma}(\tau) = -\langle T_{\tau}\hat{c}_{\boldsymbol{k}\sigma}(\tau)\hat{c}_{\boldsymbol{k}\sigma}^{\dagger}(0)\rangle = -\left[\Theta(\tau)\langle\hat{c}_{\boldsymbol{k}\sigma}(\tau)\hat{c}_{\boldsymbol{k}\sigma}^{\dagger}(0)\rangle - \Theta(-\tau)\langle\hat{c}_{\boldsymbol{k}\sigma}^{\dagger}(0)\hat{c}_{\boldsymbol{k}\sigma}(\tau)\rangle\right]$$
(10)

with

$$\hat{c}_{\boldsymbol{k}}(\tau) = e^{\tau H} \hat{c}_{\boldsymbol{k}} e^{-\tau H}, \qquad \hat{c}_{\boldsymbol{k}}^{\dagger}(\tau) = e^{\tau H} \hat{c}_{\boldsymbol{k}}^{\dagger} e^{-\tau H}, \tag{11}$$

We note, in particular that

$$G_{\boldsymbol{k}\sigma}(0^-) = n_{\boldsymbol{k}\sigma} \tag{12}$$

The retarded and advanced GFs are obtained by analytical continuation of the Fourier-transform

$$G^{R}_{k\sigma}(\omega) = G_{k\sigma}(\omega + i\delta), \qquad G^{A}_{k\sigma}(\omega) = G_{k\sigma}(\omega - i\delta)$$
(13)

The (momentum- and spin resolved) spectral function is given by

$$A_{\boldsymbol{k}\sigma}(\omega) = i \left[ G^R_{\boldsymbol{k}\sigma}(\omega) - G^A_{\boldsymbol{k}\sigma}(\omega) \right] = -2 \mathrm{Im} G^R_{\boldsymbol{k}\sigma}(\omega)$$
(14)

For a non-interacting system,  $H = H_0 = \sum_{k} \xi_k \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma}$ , with  $\xi_k = (\epsilon_k - \mu)$ , we have

$$\hat{c}_{\boldsymbol{k}\sigma}(\tau) = e^{-\xi_{\boldsymbol{k}}\tau}\hat{c}_{\boldsymbol{k}\sigma}, \qquad \hat{c}^{\dagger}_{\boldsymbol{k}\sigma}(\tau) = e^{\xi_{\boldsymbol{k}}\tau}\hat{c}^{\dagger}_{\boldsymbol{k}\sigma}.$$
(15)

The Matsubara GF's can then be explicitly written as

$$G_{0,\boldsymbol{k}\sigma}(\tau) = -\left[\Theta(\tau)(1 - n_F(\epsilon_{\boldsymbol{k}})) - \Theta(-\tau)n_F(\epsilon_{\boldsymbol{k}})\right]e^{-\xi_{\boldsymbol{k}}\tau}$$
(16)

The unperturbed GF satisfies the equation of motion

$$(-\partial_{\tau} - \xi_{\mathbf{k}})G_{0,\mathbf{k}\sigma}(\tau) = \delta(\tau) \tag{17}$$

or in frequency domain

$$(i\omega_n - \xi_k)G_{0,k\sigma}(i\omega_n) = 1 \tag{18}$$

which yields

$$G_{0,\boldsymbol{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n - \xi_{\boldsymbol{k}}} \tag{19}$$

**Exercise:** Check that  $G_{0,\boldsymbol{k}\sigma}(\tau) = \frac{1}{\beta} \sum_{\omega_n} G_{0,\boldsymbol{k}\sigma}(i\omega_n) e^{-i\omega_n \tau}$ . The spectral density for the unperturbed system is given by

$$A_{0,\boldsymbol{k}\sigma}(\omega) = 2\pi\delta(\omega - \xi_{\boldsymbol{k}}) \tag{20}$$

# 2 Anderson's model for magnetic impurities

The Anderson model has been used to describe the appearance of a magnetic moment of impurities of certain magnetic ions embedded in a non-magnetic host metal. It has also been used in the description of coulomb blockade in quantum dots. It is a natural starting point to describe the Kondo effect in both metals and quantum dots.

The host metal is described as indicated above, i.e. by an effective mass Hamiltonian describing the conduction band. The impurity atoms are assumed to have only one spin-degenerate state in the active shell (usually the *d*-shell, hence the subsequent notation *d* for the impurity states). The system is described in the eigenbasis of the individual Hamiltonians of the metal and the impurity atoms,  $\phi_{k\sigma}(\mathbf{r})$  and  $\phi_{d\sigma}(\mathbf{r})$ , with corresponding energies and creation-/annihilation operators

$$\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu, \ \hat{c}_{\boldsymbol{k}\sigma}, \ \hat{c}_{\boldsymbol{k}\sigma}^{\dagger}, \qquad \xi_{d} = \epsilon_{d} - \mu, \ \hat{c}_{d\sigma}, \ \hat{c}_{d\sigma}^{\dagger}$$
(21)

Once the impurity atoms are embedded into the metal, the crystal- and impurity potentials are perturbed and the basis  $\phi_{k\sigma}$ ,  $\phi_{d\sigma}$  is no longer an eigen-basis of the full single particle Hamiltonian. Expanding the field-operators in this eigen-basis then does no longer lead to a diagonal form but will include overlaps between the states of the conduction band and the states of the impurities. These terms are usually called hopping terms and describe a probability amplitude of transitions from the impurity atoms to the conduction band and vice versa.

Furthermore, because of the highly localized wave functions at the impurity atom, the Coulomb interaction is much stronger between electrons occupying these states. Consequently, there is an additional energy cost associated with having both spin-degenerate impurity states occupied. This is modeled by a so-called on-site interaction with characteristic energy U.

The full Hamiltonian of this model is then given by

$$H = H_c + H_t + H_d + H_U \tag{22}$$

where

$$H_c = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{c}_{\boldsymbol{k}\sigma}, \qquad H_d = \sum_{\sigma} \xi_d \hat{c}^{\dagger}_{d\sigma} \hat{c}_{d\sigma}$$
(23)

describe the individual unperturbed Hamiltonians of the conduction band and the impurity atom and

$$H_t = \sum_{k\sigma} t_k \hat{c}^{\dagger}_{k\sigma} \hat{c}_{d\sigma} + \sum_{k\sigma} t^*_k \hat{c}^{\dagger}_{d\sigma} \hat{c}_{k\sigma}$$
(24)

describes the hopping between the two subsystems. Finally the last term

$$H_U = U\hat{n}_{\uparrow}\hat{n}_{\downarrow} \tag{25}$$

describes the on-site Coulomb interaction. The *d*-electron energy  $\epsilon_d$  is below the chemical potential (i.e.  $\xi_d < 0$ ) and from the kinetic energy point of view it is favorable to fill the orbital by two electrons. However, this costs potential energy U, which is not possible if  $2\epsilon_d + U > 2\mu$  (i.e. if  $2\xi_d + U > 0$ ). Single occupancy of the atom would appear to lead, quite naturally, to a magnetic moment (since only one of the spin-degenerate states must be occupied). On the other hand, the hopping between the impurity states and the conduction band implies that the direction of the spin may fluctuate strongly, and average out. The efficiency of such processes depends on the "strength" of the hopping. But strong hopping also increases the energy (the contribution  $H_t$  to the Hamiltonian) so there is a trade-off between on-site interaction and hopping.

It will turn out, that for certain values of the parameters it is energetically favorable for the system to have a magnetic moment (and thus minimizing the on-site interaction energy) while for other values there is no magnetic moment.

#### 2.1 Single level coupled to continuum

To get a better feel for the system let us first consider only the effect of the hopping between the impurity states and the conduction band states and, for the time being, neglect the on-site interaction.

$$H = H_c + H_t + H_d \tag{26}$$

The operators obey the equations of motion

$$\partial_{\tau} \hat{c}_{d\sigma}(\tau) = [H, \hat{c}_{d\sigma}(\tau)] = -\xi_d \hat{c}_{d\sigma}(\tau) - \sum_{\boldsymbol{k}} t_{\boldsymbol{k}}^* \hat{c}_{\boldsymbol{k}\sigma}$$

$$\partial_{\tau} \hat{c}_{\boldsymbol{k}\sigma}(\tau) = [H, \hat{c}_{\boldsymbol{k}\sigma}(\tau)] = -\xi_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}\sigma}(\tau) - t_{\boldsymbol{k}} \hat{c}_{d\sigma}$$
(27)

Analogous to the conduction band Green's functions, we define the GF of the impurity states

$$G_{d\sigma}(\tau) = -\langle T_{\tau} \hat{c}_{d\sigma}(\tau) \hat{c}^{\dagger}_{d\sigma'}(0) \rangle$$
(28)

This GF obeys the equation of motion

$$(-\partial_{\tau} - \xi_{d})G_{d\sigma}(\tau) = \delta(\tau - \tau') - \sum_{\boldsymbol{k}} t_{\boldsymbol{k}}^{*} \langle T_{\tau} \hat{c}_{\boldsymbol{k}\sigma}(\tau) \hat{c}_{d\sigma}^{\dagger}(0) \rangle$$
$$= \delta(\tau - \tau') + \sum_{\boldsymbol{k}} t_{\boldsymbol{k}}^{*} F_{\boldsymbol{k}\sigma}(\tau)$$
(29)

where we also defined

$$F_{\boldsymbol{k}\sigma}(\tau) = -\langle T_{\tau} \hat{c}_{\boldsymbol{k}\sigma}(\tau) \hat{c}_{d\sigma}^{\dagger}(0) \rangle.$$
(30)

This GF satisfies the equation of motion

$$(-\partial_{\tau} - \xi_{\mathbf{k}})F_{\mathbf{k}\sigma}(\tau) = t_{\mathbf{k}}G_{d\sigma}(\tau)$$
(31)

This gives us a system of coupled equations which in Fourier-space can be written

$$(i\omega_n - \xi_d)G_{d\sigma}(i\omega_n) = 1 + \sum_{\boldsymbol{k}} t_{\boldsymbol{k}}^* F_{\boldsymbol{k}\sigma}(i\omega_n)$$
  

$$(i\omega_n - \xi_{\boldsymbol{k}})F_{\boldsymbol{k}\sigma}(i\omega_n) = t_{\boldsymbol{k}}G_{d\sigma}(i\omega_n)$$
(32)

Using  $G_{0,\boldsymbol{k}\sigma}^{-1}(i\omega_n) = (i\omega_n - \xi_{\boldsymbol{k}})$  we can write the second equation in the form

$$F_{k\sigma}(i\omega_n) = G_{0,k\sigma}(i\omega_n) t_k G_{d\sigma}(i\omega_n)$$
(33)

Inserting into the first gets us

$$G_{d\sigma}(i\omega_n) = G_{0,d\sigma}(i\omega_n) + G_{0,d\sigma}(i\omega_n) \sum_{\boldsymbol{k}} t_{\boldsymbol{k}}^* G_{0,\boldsymbol{k}\sigma}(i\omega_n) t_{\boldsymbol{k}} G_{d\sigma}(i\omega_n)$$
(34)

If we define

$$\Sigma_{\sigma}(i\omega_n) = \sum_{\boldsymbol{k}} |t_{\boldsymbol{k}}|^2 G_{0,\boldsymbol{k}\sigma}(i\omega_n)$$
(35)

we have

$$G_{d\sigma}(i\omega_n) = G_{0,d\sigma}(i\omega_n) + G_{0,d\sigma}(i\omega_n)\Sigma_{\sigma}(i\omega_n)G_{d\sigma}(i\omega_n)$$
(36)

with the solution for  $G_{d\sigma}(i\omega_n)$ :

$$G_{d\sigma}(i\omega_n) = \frac{1}{G_{0,d\sigma}^{-1}(i\omega_n) + \Sigma_{\sigma}(i\omega_n)} = \frac{1}{i\omega_n - \xi_d + \Sigma_{\sigma}(i\omega_n)}$$
(37)

We have

$$\Sigma_{\sigma}(i\omega_n) = \sum_{\boldsymbol{k}} |t_{\boldsymbol{k}}|^2 G_{0,\boldsymbol{k}\sigma}(i\omega_n) = \sum_{\boldsymbol{k}} \frac{|t_{\boldsymbol{k}}|^2}{i\omega_n - \xi_{\boldsymbol{k}}}$$
(38)

Let us assume that  $t_{k}$  and  $\xi_{k}$  both only depend on k = |k| such that

$$\Sigma_{\sigma}(i\omega_n) = \sum_{\boldsymbol{k}} \frac{|t_{\boldsymbol{k}}|^2}{i\omega_n - \xi_{\boldsymbol{k}}} = \mathcal{V} \int \frac{d^3k}{(2\pi)^3} \frac{|t_{\boldsymbol{k}}|^2}{i\omega_n - \xi_{\boldsymbol{k}}} = \frac{\mathcal{V}}{2\pi^2} \int dk k^2 \frac{|t_{\boldsymbol{k}}|^2}{i\omega_n - \xi_{\boldsymbol{k}}}$$
$$= \int d\xi \; \frac{N(\xi)|t_{\boldsymbol{k}(\xi)}|^2}{i\omega_n - \xi}$$
$$= \int \frac{d\xi}{\pi} \; \frac{\Gamma(\xi)}{i\omega_n - \xi}$$
(39)

where  $\Gamma(\xi) = \pi N(\xi) |t_{k(\xi)}|^2$  is the hybridization energy and the density of states  $N(\xi)$  is defined such that

$$\frac{1}{\mathcal{V}}N(\xi) = \frac{1}{2\pi^2} \left(k^2 \frac{dk}{d\xi}\right)_{k=k(\xi)} = \nu(\xi) \tag{40}$$

**Note:** Here we distinguish between the density of states  $N(\xi)$  and the density of states per unit volume  $\nu(\xi)$  (compare dimensions).

To simplify matters, let us assume that the chemical potential lies in the middle of the gap and thus  $\xi \in [-D, D]$  where D is the bandwidth. We also assume that the hybridization energy is constant across the band  $\Gamma(\xi) = \Gamma$ . We then have

$$\Sigma(i\omega_n) = \frac{\Gamma}{\pi} \int_{-D}^{D} d\xi \frac{1}{i\omega_n - \xi} = \ln\left[\frac{i\omega_n + D}{i\omega_n - D}\right]$$
(41)

#### 2.1.1 Short on analytical continuation

Note  $\ln(z) = \ln(re^{i\varphi}) = \ln(r) + \ln e^{i\varphi} = \ln(r) + i\varphi$ , not periodic w.r.t.  $\varphi$  such that even though  $z = re^{i\varphi}$  and  $z' = re^{i\varphi+2\pi}$  represent the same complex number, the logarithm does not give the same result.  $\ln(z)$  is a multivalued function in the complex plane. To avoid this problem a **principal branch** is chosen as  $\varphi \in (-\pi, \pi)$  and a branch cut is introduced at  $\operatorname{Re} z \in (-\infty, 0)$ . The logarithm is discontinuous across this branch cut and the function is analytic everywhere else. For a complex number with an infinitesimally small imaginary part,  $z = x \pm i\delta$ ,  $\delta > 0$ , we have that the absolute value is  $r \approx |x|$  and that the phase is always either  $\varphi \approx \pm \pi \Theta(-x)$ 

$$\ln(x\pm i\delta) \approx \ln|x| + i\pi\Theta(-x) = \begin{cases} \ln|x|, & x > 0\\ \ln|x| \pm i\pi, & x < 0 \end{cases}$$
(42)



Figure 1: Left: Real part of  $\Sigma(z)$ . Right: Imaginary part of  $\Sigma(z)$ .

Thus we have

$$\Sigma(\omega \pm i\delta) = \frac{\Gamma}{\pi} \Big[ \ln(\omega \pm i\delta + D) - \ln(\omega \pm i\delta - D) \Big]$$
  
=  $\frac{\Gamma}{\pi} \Big[ \ln|\omega + D| - \ln|\omega - D| \pm i\pi\Theta(-\omega - D) \mp i\pi\Theta(-\omega + D) \Big]$  (43)  
=  $\frac{\Gamma}{\pi} \ln \left| \frac{\omega + D}{\omega - D} \right| \mp i\Gamma\Theta(D - |\omega|)$ 

We note that for  $\omega \ll D$  we have  $\ln |(\omega + D)/(\omega - D)| \approx |\omega/D| \approx 0$ Having  $G_{d\sigma}^{R}(\omega) = G_{d\sigma}(\omega + i\delta)$  we can write the spectral function

$$A_{d\sigma}(\omega) = -2\mathrm{Im}G^R(\omega) = \frac{\Gamma}{(\omega - \xi_d)^2 + \Gamma^2}$$
(44)



Figure 2: Effect of hybridization between d electron orbitals and conduction band.

## 2.2 Full Anderson Model

Let us now attack the full model

$$H = H_c + H_t + H_d + H_U \tag{45}$$

The equation of motion of the operators is given by

$$\partial_{\tau} \hat{c}_{d\sigma}(\tau) = -\xi_{d} \hat{c}_{d\sigma}(\tau) - \sum_{\mathbf{k}} t_{\mathbf{k}}^{*} \hat{c}_{\mathbf{k}\sigma} + [H_{U}, \hat{c}_{d\sigma}(t\tau)]$$

$$\partial_{\tau} \hat{c}_{\mathbf{k}\sigma}(\tau) = -\xi_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}(\tau) - t_{\mathbf{k}} \hat{c}_{d\sigma}$$
(46)

which is the same as before except for the extra term

$$[H_U, \hat{c}_{d\sigma}(\tau)] = U \left[ \hat{n}_{d\uparrow}(\tau) \hat{n}_{d\downarrow}(\tau), \hat{c}_{d\sigma}(\tau) \right]$$
  
=  $-U \hat{n}_{d,-\sigma}(\tau) \hat{c}_{d\sigma}(\tau)$  (47)

which follows from  $[\hat{n}_{d-\sigma}(\tau), \hat{c}_{d\sigma}(\tau)] = 0$  and  $[\hat{n}_{d\sigma}(\tau), \hat{c}_{d\sigma}(\tau)] = -\hat{c}_{d\sigma}(\tau)$ . We then have for the GFs

$$(-\partial_{\tau} - \xi_{d})G_{d\sigma}(\tau) = \delta(\tau) + \sum_{\mathbf{k}} t_{\mathbf{k}}^{*}F_{\mathbf{k}\sigma}(\tau) - U\langle T_{\tau}\hat{n}_{d,-\sigma}(\tau)\hat{c}_{d\sigma}(\tau)\hat{c}_{d\sigma}^{\dagger}(0)\rangle$$

$$(-\partial_{\tau} - \xi_{\mathbf{k}})F_{\mathbf{k}\sigma}(\tau) = t_{\mathbf{k}}G_{d\sigma}(\tau)$$

$$(48)$$

The last term of the top equation complicates the equation of motion as we need also the equation of motion of the two particle GF, which in turn depends on the three-particle GF etc. The straight forward route would be to perform perturbation theory. This, however, is only meaningful for weak interaction, and can not directly cover non-perturbative effects such as bound states and the appearance of local moments (which we are interested in here). Instead we make a so-called **mean-field approximation**:

$$\langle T_{\tau} \hat{n}_{d,-\sigma}(\tau) \hat{c}_{d\sigma}(\tau) \hat{c}_{d\sigma}^{\dagger}(0) \rangle = \langle \hat{c}_{d,-\sigma}^{\dagger}(\tau) \hat{c}_{d,-\sigma}(\tau) \hat{c}_{d\sigma}(\tau) \hat{c}_{d\sigma}^{\dagger}(0) \rangle$$

$$\approx \langle T_{\tau} \hat{c}_{d,-\sigma}^{\dagger}(\tau) \hat{c}_{d,-\sigma}(\tau) \rangle \langle T_{\tau} \hat{c}_{d\sigma}(\tau) \hat{c}_{d\sigma}^{\dagger}(0) \rangle$$

$$= -\langle \hat{n}_{d,-\sigma} \rangle G_{d\sigma}(\tau)$$

$$(49)$$

The equation of motion of the GFs are then in Fourier space given by (using from now on the notation  $n_{\sigma} = \langle \hat{n}_{d\sigma} \rangle$ )

$$(i\omega_n - \xi_d - Un_{-\sigma})G_{d\sigma}(i\omega_n) = 1 + \sum_{\boldsymbol{k}} t_{\boldsymbol{k}}^* F_{\boldsymbol{k}\sigma}(i\omega_n)$$

$$(i\omega_n - \xi_{\boldsymbol{k}})F_{\boldsymbol{k}\sigma}(i\omega_n) = t_{\boldsymbol{k}}G_{d\sigma}(i\omega_n)$$
(50)

Solving again for the second one and inserting into the first one we get

$$G_{d\sigma}(i\omega_n) = \frac{1}{i\omega_n - \xi_d - Un_{-\sigma} + \Sigma(i\omega_n)}$$
(51)

With the same approximations as in the previous section we find

$$A_{d\sigma}(\omega) = \frac{\Gamma}{(\omega - \xi_d - Un_{-\sigma})^2 + \Gamma^2}$$
(52)

#### 2.3 Self-consistency: Formation of local magnetic moment

Using the relationship (derived from the Lehmann-representation)

$$n_{\sigma} = \int \frac{d\omega}{2\pi} n_F(\omega) A(\omega) = \int \frac{d\omega}{2\pi} n_F(\omega) \frac{\Gamma}{(\omega - \xi_d - Un_{-\sigma})^2 + \Gamma^2}$$
(53)

we obtain a self-consistency equation. At T = 0, i.e.  $n_F(\omega) = \Theta(-\omega)$ , we get<sup>1</sup>

$$n_{\sigma} = \frac{1}{2} - \frac{1}{\pi} \arctan\left(\frac{\xi_d + Un_{-\sigma}}{\Gamma}\right)$$
(54)

or  $(using \cot(\frac{\pi}{2} - \arctan(x)) = x)$ 

$$\cot(\pi n_{\sigma}) = \frac{\xi_d + U n_{-\sigma}}{\Gamma}$$
(55)

Introducing the total occupation  $N = n_{\uparrow} + n_{\downarrow}$  and the magnetization  $M = n_{\uparrow} - n_{\downarrow}$  we may write this as

$$N = \frac{1}{\pi} \sum_{\sigma} \operatorname{arccot} \left( \frac{\xi_d + \frac{U}{2}(N - \sigma M)}{\Gamma} \right)$$
$$M = \frac{1}{\pi} \sum_{\sigma} \sigma \operatorname{arccot} \left( \frac{\xi_d + \frac{U}{2}(N - \sigma M)}{\Gamma} \right)$$
(56)

Note that there is always a solution with M = 0 since the second equation of (56) is trivially satisfied. The total occupation is then given by N = 2n where n is the occupation of one of the levels and given by (55) with index  $\sigma$  removed. It is useful to consider a special case where the states are half-filled on average. To find the condition for we set n = 1/2 and get the condition

Half-filling, 
$$(N = 1)$$
:  $\xi_d = -\frac{U}{2}$ , (for  $M = 0$ , i.e.  $n = n_\sigma = \frac{1}{2}$ ) (57)

The interesting thing about the Anderson model is, however, the existence of a solution with finite magnetization. To see that such a solution exists, let us try to find the condition for complete magnetization<sup>2</sup> M = 1 which implies also that N = M = 1. Effectively this means that only one state is occupied and the other is empty. Inserting this condition into (56) and adding/subtracting the two equations we get

$$\pi = \operatorname{arccot}\left(\frac{\xi_d}{\Gamma}\right), \qquad 0 = \operatorname{arccot}\left(\frac{\xi_d + U}{\Gamma}\right)$$
(58)

Using the half-filling condition from before  $\xi_d = -U/2$  the left and right equations become the same and lead to the condition

$$\frac{\xi_d}{\Gamma} = -\frac{U}{2\Gamma} = \cot(\pi) = -\infty \tag{59}$$

<sup>1</sup>Using the indefinite integral  $\int dx \frac{g}{(x-a)^2+g^2} = -\arctan\left(\frac{a-x}{g}\right)^2$ Note that  $M \in [-1, 1]$  since  $n_\sigma \in 0, 1$ 

This result should not be surprising since if the on-site interaction is infinitely strong (compared to hybridization) only one of the states should be occupied and processes where the electron occupying this state is exchanged with an electron from the conduction band are suppressed.

To find the critical values of the parameters for a finite magnetization we may linearize the left hand side of Eq. (56) by using  $\operatorname{arccot}(a+bx) = \operatorname{arccot}(a) - \frac{bx}{(1+a^2)} + \mathcal{O}(x^2)$  to obtain

$$N \approx \frac{2}{\pi} \operatorname{arccot}\left(\frac{\xi_d + \frac{U}{2}N}{\Gamma}\right)$$
$$M \approx \frac{1}{\pi} \frac{1}{1 + \left(\frac{\xi_d + \frac{U}{2}N}{\Gamma}\right)^2} \frac{U}{\Gamma}M$$
(60)

Thus, using again the half-filling condition  $\xi_d = -U/2$  we get N = 1 from the first equation while the second equation requires, for non-zero M, the following condition to be satisfied

$$\frac{U}{\Gamma} = \pi \tag{61}$$

which is the critical value for the ratio of interaction strength versus hybridization in order to form a local moment.



Figure 3: Top figures: Spectral density on x-axis, Energy on y-axis. Left:  $U = \Gamma = 0$ . Middle:  $U < \pi\Gamma$ . Right:  $U > \pi\Gamma$ . Bottom: Magnetic moment as a function of  $U/\Gamma$ .

# 3 Screening effects in metals

The electric potential  $\phi(\mathbf{r}, t)$  in a system can be separated into two parts, the externally applied potential  $\phi_{\text{ext}}(\mathbf{r}, t)$ , as well as an induced potential  $\phi_{\text{ind}}(\mathbf{r}, t)$ .

$$\phi(\mathbf{r},t) = \phi_{\text{ext}}(\mathbf{r},t) + \phi_{\text{ind}}(\mathbf{r},t)$$
(62)

In the absence of an externally applied electric potential a system at equilibrium has a vanishing  $electric potential^3$ 

$$\phi(\mathbf{r},t) = \phi_{\text{ind}}(\mathbf{r},t) = 0 \tag{63}$$

The induced electric potential is related to the induced charge through the **Poisson equation** 

$$\nabla^2 \phi_{\rm ind}(\boldsymbol{r},t) = -\frac{1}{\epsilon_0} \rho_{\rm ind}(\boldsymbol{r},t) \quad \Rightarrow \quad \phi(\boldsymbol{r},t) = \int d^3 r' V_c(\boldsymbol{r}-\boldsymbol{r}') \rho_{\rm ind}(\boldsymbol{r}',t) \tag{64}$$

where

$$V_c(\boldsymbol{r} - \boldsymbol{r}') = \frac{1}{4\pi\epsilon_0} \frac{1}{|\boldsymbol{r} - \boldsymbol{r}'|}$$
(65)

is the Coulomb interaction. At equilibrium the charge density from the electrons is cancelled (over macroscopic distances) by the charge density of the ions, i.e. at equilibrium we have **charge neutrality** and  $\rho_{ind}(\mathbf{r}, t) = 0$ . The induced charge  $\rho_{ind}$  is due to an induced displacement of the electron density  $\delta n(\mathbf{r}, t)$ . In the linear response regime, the induced charge density can be written as

$$\rho_{\rm ind}(\boldsymbol{r},t) = \int d^3 r' \int dt' \chi^R(\boldsymbol{r}t,\boldsymbol{r}'t')\phi_{\rm ext}(\boldsymbol{r}',t')$$
(66)

where  $\chi^R$  is known as the **polarizability function**.

#### 3.1 Dielectric response

The relationship between the external potential and the total potential defines the dielectric function  $\varepsilon$ 

$$\phi_{\text{ext}}(\boldsymbol{r},t) = \int d^3 r' \int dt' \varepsilon(\boldsymbol{r}t,\boldsymbol{r}'t')\phi(\boldsymbol{r}',t')$$
(67)

Usually it is more interesting/useful to talk about the inverse relationship

$$\phi(\mathbf{r},t) = \int d^3r' \int dt' \varepsilon^{-1}(\mathbf{r}t,\mathbf{r}'t')\phi_{\text{ext}}(\mathbf{r}',t')$$
(68)

Using the definitions from the previous section we can write this as

$$\varepsilon^{-1}(\boldsymbol{r}t,\boldsymbol{r}'t') = \delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t') + \int d^3r'' V_c(\boldsymbol{r}-\boldsymbol{r}')\chi^R(\boldsymbol{r}'t',\boldsymbol{r}''t'')$$
(69)

<sup>&</sup>lt;sup>3</sup>In principle it only needs to be constant, but such a potential is not observable since the electro-magnetic field depends on the gradient and time derivative of the potential - Gauge invariance

## Translational invariance

For a translationally invariant system the polarizability depends only on the relative coordinates  $\chi^R(\mathbf{r}t, \mathbf{r}'t') = \chi^R(\mathbf{r} - \mathbf{r}'; t - t')$  and therefore so does the dielectric function (and its inverse). It then makes sense to talk about the Fourier transformed quantities which are related through

$$\phi(\mathbf{k},\omega) = \epsilon^{-1}(\mathbf{k},\omega)\phi_{\text{ext}}(\mathbf{k},\omega)$$
(70)

with the dielectric function being related to the polarizability

C

$$\varepsilon^{-1}(\boldsymbol{k},\omega) = 1 + V_c(\boldsymbol{k})\chi^R(\boldsymbol{k},\omega)$$
(71)

Using  $E_{\text{ext}}(\mathbf{k},\omega) = -i\mathbf{k}\phi_{\text{ext}}(\mathbf{k},\omega)$  together with the continuity equation  $-i\omega\rho(\mathbf{k},\omega) + i\mathbf{k} \cdot \mathbf{j}(\mathbf{k},\omega) = 0$  we can obtain a relationship to the conductivity defined through

$$\boldsymbol{j}(\boldsymbol{k},\omega) = \sigma(\boldsymbol{k},\omega)\boldsymbol{E}_{\text{ext}}(\boldsymbol{k},\omega) \Rightarrow \epsilon^{-1}(\boldsymbol{k},\omega) = 1 - i\frac{k^2}{\omega}\sigma(\boldsymbol{k},\omega)$$
(72)

or

$$\sigma(\boldsymbol{k},\omega) = \frac{i\omega}{k^2} V_c(\boldsymbol{k}) \chi^R(\boldsymbol{k},\omega)$$
(73)

In a quantum mechanical system the coupling to the electric potential is described by adding a perturbation

$$H_{\text{ext}} = \int d^3 r \hat{\rho}(\boldsymbol{r}, t) \phi_{\text{ext}}(\boldsymbol{r}, t) = e \int d^3 r \; \hat{\psi}^{\dagger}(\boldsymbol{r}, t) \psi(\boldsymbol{r}, t) \phi_{\text{ext}}(\boldsymbol{r}, t)$$
(74)

to the Hamiltonian. **Note:** in this section we shall neglect spin, which only leads to a factor of two in the end-result. The linear response is then written as

$$\rho(\boldsymbol{r},t) = -i \int d^3 \boldsymbol{r}' \int dt' \Theta(t-t') \langle [\hat{\rho}(\boldsymbol{r},t), \hat{\rho}(\boldsymbol{r}',t')] \rangle \phi_{\text{ext}}(\boldsymbol{r}'t')$$
(75)

which identifies the polarizability function

$$\chi^{R}(\boldsymbol{r}t,\boldsymbol{r}'t') = -i\Theta(t-t')\langle [\hat{\rho}(\boldsymbol{r},t),\hat{\rho}(\boldsymbol{r}',t')]\rangle$$
(76)

In the basis of  $\phi_{k}(\mathbf{r}) = \frac{1}{\sqrt{\nu}} e^{i\mathbf{k}\cdot\mathbf{r}}$  the density can be written as

$$\hat{\rho}(\boldsymbol{r},t) = \frac{e}{\mathcal{V}} \sum_{\boldsymbol{k}\boldsymbol{k}'} \hat{c}^{\dagger}_{\boldsymbol{k}}(t) \hat{c}_{\boldsymbol{k}'}(t) e^{-i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} = \frac{e}{\mathcal{V}} \sum_{\boldsymbol{k}\boldsymbol{q}} \hat{c}^{\dagger}_{\boldsymbol{k}}(t) \hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(t) e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}$$
(77)

and we have

$$\chi^{R}(\boldsymbol{r}t,\boldsymbol{r}'t') = -i\Theta(t-t')\frac{e^{2}}{\mathcal{V}^{2}}\sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}\boldsymbol{q}'}\langle [\hat{c}_{\boldsymbol{k}}^{\dagger}(t)\hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(t),\hat{c}_{\boldsymbol{k}'}^{\dagger}(t')\hat{c}_{\boldsymbol{k}'+\boldsymbol{q}'}(t')]\rangle e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}e^{-i\boldsymbol{q}'\cdot\boldsymbol{r}'}$$
(78)

For a translationally invariant system the response function should only depend on the relative coordinate r - r', which means that q' = -q. Introducing the notation

$$\hat{\rho}_{\boldsymbol{q}}(t) = e \sum_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k}}(t) \hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(t)$$
(79)

we have

$$\chi^{R}(\boldsymbol{r}-\boldsymbol{r}';t) = -i\Theta(t)\frac{1}{\mathcal{V}^{2}}\sum_{\boldsymbol{q}} \langle [\hat{\rho}_{\boldsymbol{q}}(t), \hat{\rho}_{-\boldsymbol{q}}(0)] \rangle e^{-i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}$$
(80)

or in momentum space

$$\chi^{R}(\boldsymbol{q};t) = -i\Theta(t)\frac{1}{\mathcal{V}}\langle [\hat{\rho}_{\boldsymbol{q}}(t), \hat{\rho}_{-\boldsymbol{q}}(0)]\rangle$$
(81)

In the following sections we shall try to evaluate this response function by first deriving the Fourier transform of the corresponding imaginary time GF

$$\chi(\boldsymbol{q}, i\omega_n) = \int_0^\beta d\tau \chi(\boldsymbol{k}, \tau) e^{i\omega_n \tau}, \qquad \chi(\boldsymbol{k}, \tau) = -\frac{1}{\mathcal{V}} \langle T_\tau \hat{\rho}_{\boldsymbol{q}}(\tau) \hat{\rho}_{-\boldsymbol{q}}(0) \rangle$$
(82)

and then performing an analytical continuation to obtain the retarded GF  $\chi^R(\mathbf{k}, \omega)$ , i.e. the polarizability function.

### 3.2 Non-interacting case

We start by investigating the non-interacting case where the unperturbed Hamiltonian is given by

$$H_0 = \sum_{k} \xi_k \hat{c}_k^{\dagger} \hat{c}_k \tag{83}$$

and the equation of motion of the operators is

$$\partial_{\tau} \hat{c}_{\boldsymbol{k}}(\tau) = [H, \hat{c}_{\boldsymbol{k}}] = -\xi_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}}(\tau)$$

$$\partial_{\tau} \hat{c}_{\boldsymbol{k}}^{\dagger}(\tau) = [H, \hat{c}_{\boldsymbol{k}}^{\dagger}] = \xi_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}}(\tau)$$
(84)

It is useful to rewrite the two-particle GF as (the index 0 denotes non-interacting)

$$\chi_0(\boldsymbol{q},\tau) = \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}} \chi_0(\boldsymbol{k},\boldsymbol{q},\tau), \qquad (85)$$

where (from now on setting e = 1 for notational brevity)

$$\chi_0(\boldsymbol{k}, \boldsymbol{q}; \tau) = -\langle T_\tau \hat{c}^{\dagger}_{\boldsymbol{k}}(\tau) \hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(\tau) \hat{\rho}_{-\boldsymbol{q}}(0) \rangle \tag{86}$$

It is then useful to investigate the time derivative

$$\partial_{\tau} \left( \hat{c}_{\boldsymbol{k}}^{\dagger}(\tau) \hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(\tau) \right) = \left[ H_0, \hat{c}_{\boldsymbol{k}}^{\dagger}(\tau) \hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(\tau) \right] = -(\xi_{\boldsymbol{k}+\boldsymbol{q}} - \xi_{\boldsymbol{k}}) \hat{c}_{\boldsymbol{k}}^{\dagger}(\tau) \hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(\tau) \tag{87}$$

The equation of motion of the two-particle GF is then given by (remember to take into account the discontinuity due to the time ordering)

$$\left(-\partial_{\tau} - (\xi_{\boldsymbol{k}+\boldsymbol{q}} - \xi_{\boldsymbol{k}})\right)\chi(\boldsymbol{k}, \boldsymbol{q}; \tau) = \delta(\tau)\langle [\hat{c}_{\boldsymbol{k}}^{\dagger}\hat{c}_{\boldsymbol{k}+\boldsymbol{q}}, \hat{\rho}_{-\boldsymbol{q}}]\rangle$$
(88)

The commutator on the right hand side is

$$\langle [\hat{c}_{\boldsymbol{k}}^{\dagger}\hat{c}_{\boldsymbol{k}+\boldsymbol{q}},\hat{\rho}_{-\boldsymbol{q}}]\rangle = \langle \hat{c}_{\boldsymbol{k}}^{\dagger}\hat{c}_{\boldsymbol{k}}\rangle - \langle \hat{c}_{\boldsymbol{k}+\boldsymbol{q}}^{\dagger}\hat{c}_{\boldsymbol{k}+\boldsymbol{q}}\rangle = n_F(\xi_{\boldsymbol{k}}) - n_F(\xi_{\boldsymbol{k}+\boldsymbol{q}})$$
(89)

In Fourier space the equation of motion then becomes

$$\left(i\omega_n - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}})\right)\chi_0(\mathbf{k}, \mathbf{q}; i\omega_n) = n_F(\xi_{\mathbf{k}}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})$$
(90)

 $\operatorname{or}$ 

$$\chi_0(\mathbf{k}, \mathbf{q}; i\omega_n) = \frac{n_F(\xi_k) - n_F(\xi_{k+q})}{i\omega_n - (\xi_{k+q} - \xi_k)}$$
(91)

The polarizability function is then given by

$$\chi_0^R(\boldsymbol{q},\omega) = \chi_0(\boldsymbol{q},\omega+i\delta) = \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}} \frac{n_F(\boldsymbol{\xi}_{\boldsymbol{k}}) - n_F(\boldsymbol{\xi}_{\boldsymbol{k}+\boldsymbol{q}})}{\omega+i\delta - (\boldsymbol{\xi}_{\boldsymbol{k}+\boldsymbol{q}} - \boldsymbol{\xi}_{\boldsymbol{k}})}$$
(92)

The right hand side of this equation is known as the Lindhard function.

# 3.3 Lindhard function

The Lindhard function can be evaluated exactly but for most purposes it is sufficient to consider the low wave-length approximation  $\xi_{k+q} \approx \xi_k + q \cdot v_k$  with  $v_k = \partial_k \xi_k$ , which leads to

$$\chi_0^R(\boldsymbol{q},\omega) = \int \frac{d^3k}{(2\pi)^3} \frac{n_F(\boldsymbol{\xi}_{\boldsymbol{k}}) - n_F(\boldsymbol{\xi}_{\boldsymbol{k}+\boldsymbol{q}})}{\omega + i\delta - (\boldsymbol{\xi}_{\boldsymbol{k}+\boldsymbol{q}} - \boldsymbol{\xi}_{\boldsymbol{k}})}$$

$$\approx \int \frac{d^3k}{(2\pi)^3} \frac{\boldsymbol{q} \cdot \boldsymbol{v}_{\boldsymbol{k}}}{\omega + i\delta - \boldsymbol{q} \cdot \boldsymbol{v}_{\boldsymbol{k}}} \left(-\frac{dn_F}{d\epsilon}\right)$$
(93)

The imaginary part of the response is given by

$$\operatorname{Im}\chi_{0}^{R}(\boldsymbol{q},\omega) = \int \frac{d^{3}k}{(2\pi)^{3}} \boldsymbol{q} \cdot \boldsymbol{v_{k}} \pi \delta(\omega - \boldsymbol{q} \cdot \boldsymbol{v_{k}}) \frac{dn_{F}}{d\epsilon}$$

$$\approx -\omega \frac{k_{F}^{2}}{4\pi v_{F}} \int_{-1}^{1} d(\cos\theta) \delta(\omega - qv_{F}\cos\theta)$$

$$= -\frac{\omega}{v_{F}q} \frac{k_{F}^{2}}{4\pi v_{F}} \Theta(|\omega| - v_{F}q)$$

$$= -\pi \nu(0) \frac{\omega}{2v_{F}q} \Theta(|\omega| - v_{F}q)$$
(94)

We may use the Kramers-Kronig relation to obtain the real part

$$\operatorname{Re}\chi_{0}^{R}(\boldsymbol{q},\omega) = -\nu(0)\left[1 - \frac{\omega}{2v_{F}q}\ln\left|\frac{\omega + v_{F}q}{\omega - v_{F}q}\right|\right]$$
(95)

with  $\nu(0) = k_F m / 2\pi^2$ .



Figure 4: Absorbtion (imaginary part of  $\chi_0^R(\boldsymbol{q},\omega)$ ) at T=0 derived from full Lindhard-function. Dashed line indicating  $\omega = qv_F$ .

## 3.3.1 Limits

- For  $\omega = 0$  (static polarizability compressibility) we get  $\text{Im}\chi_0^R(\boldsymbol{q},0) = 0$  and  $\chi_0^R(\boldsymbol{q},0) = \text{Re}\chi_0^R(\boldsymbol{q},0) = -\nu(0)$ .
- For small  $v_F q/\omega$  the imaginary part of the polarizability goes to zero and for the real part we get to second order (using  $\ln(\frac{1+x}{1-x}) = 2x + 2x^3/3 + \mathcal{O}(x^4)$ )

$$\chi_0^R(\boldsymbol{q},\omega) = \operatorname{Re}\chi_0^R(\boldsymbol{q},\omega) \approx -\nu(0)\left(1 - 1 - \frac{1}{3}\left(\frac{v_F q}{\omega}\right)^2\right) = \frac{\nu(0)}{3}\left(\frac{v_F q}{\omega}\right)^2 = \frac{\bar{n}}{m}\frac{q^2}{\omega^2}$$
(96)

where we used the mean electron density  $\bar{n} = \int \frac{d^3k}{(2\pi)^3} n_F(\xi_k) = \frac{1}{(2\pi)^3} \frac{4\pi k_F^3}{3} = \frac{1}{2\pi^2} \frac{k_F^3}{3} = \frac{\nu(0)}{3} m v_F^2$ . This result could have been obtained more directly by expanding the integrand to first non-vanishing order in  $\boldsymbol{q}$  to get

$$\chi_0^R(\boldsymbol{q},\omega) \approx \int \frac{d^3k}{(2\pi)^3} \frac{(\boldsymbol{q}\cdot\boldsymbol{v}_k)^2}{\omega^2} \left(-\frac{dn_F}{d\epsilon}\right) = \frac{\bar{n}}{m} \frac{q^2}{\omega^2}$$
(97)

Note: First order expansion in q cancels for isotropic medium.

#### 3.4 Interacting system - RPA approximation

In this section we extend our analysis to the case of interacting electrons by adding the interaction Hamiltonian

$$H_{\rm int} = \frac{1}{2} \int d^3 r d^3 r' \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}') V_c(\boldsymbol{r} - \boldsymbol{r}') \hat{\psi}(\boldsymbol{r}') \hat{\psi}(\boldsymbol{r})$$
(98)

where  $V_c(\boldsymbol{r} - \boldsymbol{r}')$  is again the Coulomb interaction vertex. In momentum space the Hamiltonian takes the form

$$H_{\rm int} = \frac{1}{2\mathcal{V}} \sum_{\boldsymbol{k}\boldsymbol{k}', \boldsymbol{q}\neq 0} V_c(\boldsymbol{q}) \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}} \hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q}} \hat{c}_{\boldsymbol{k}'} \hat{c}_{\boldsymbol{k}}$$
(99)

The equation of motion of the operator  $\hat{c}^{\dagger}_{k}(\tau)\hat{c}_{k+q}(\tau)$  is then given by

$$\partial_{\tau} \left( \hat{c}_{\boldsymbol{k}}^{\dagger}(\tau) \hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(\tau) \right) = \left[ H_0, \hat{c}_{\boldsymbol{k}}^{\dagger}(\tau) \hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(\tau) \right] + \left[ H_{\text{int}}, \hat{c}_{\boldsymbol{k}}^{\dagger}(\tau) \hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(\tau) \right]$$
(100)

The first term is the same as before, while the last term is

$$[H_{\text{int}}, \hat{c}^{\dagger}_{\boldsymbol{k}}(\tau)\hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(\tau)] = -\frac{1}{2\mathcal{V}}\sum_{\boldsymbol{k}', \boldsymbol{q}'\neq 0} V(\boldsymbol{q}) \left\{ \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}'}\hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q}}\hat{c}_{\boldsymbol{k}'}\hat{c}_{\boldsymbol{k}+\boldsymbol{q}} + \hat{c}^{\dagger}_{\boldsymbol{k}'+\boldsymbol{q}'}\hat{c}^{\dagger}_{\boldsymbol{k}-\boldsymbol{q}'}\hat{c}_{\boldsymbol{k}-\boldsymbol{q}}\hat{c}_{\boldsymbol{k}'} - \hat{c}^{\dagger}_{\boldsymbol{k}'}\hat{c}^{\dagger}_{\boldsymbol{k}-\boldsymbol{q}'}\hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q}'}\hat{c}_{\boldsymbol{k}'}\hat{c}_{\boldsymbol{k}+\boldsymbol{q}-\boldsymbol{q}'} \right\}$$
(101)

We now apply what is known as the **Random Phase Approximation**, consisting in replacing pairs of operators by their expectation values. In essence this is also a type of mean-field approximation. The procedure requires us to take all the pairings between annihilation- and creation operators. For instance we get for the first term

$$\hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}'}\hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q}}\hat{c}_{\boldsymbol{k}'}\hat{c}_{\boldsymbol{k}+\boldsymbol{q}} \approx \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}'}\hat{c}_{\boldsymbol{k}+\boldsymbol{q}}\langle\hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q}}\hat{c}_{\boldsymbol{k}'}\rangle + \langle\hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}'}\hat{c}_{\boldsymbol{k}+\boldsymbol{q}}\rangle\hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q}}\hat{c}_{\boldsymbol{k}'}$$

$$= \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}'}\hat{c}_{\boldsymbol{k}+\boldsymbol{q}}n_F(\xi_{\boldsymbol{k}'})\delta_{\boldsymbol{q},0} + n_F(\xi_{\boldsymbol{k}})\delta_{\boldsymbol{q},\boldsymbol{q}'}\hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q}}\hat{c}_{\boldsymbol{k}'}$$
(102)

Doing this for all terms and summing over q' leads to

$$[H_{\rm int}, \hat{c}_{\boldsymbol{k}}^{\dagger}(\tau)\hat{c}_{\boldsymbol{k}+\boldsymbol{q}}(\tau)] = -V_c(\boldsymbol{q})\Big(n_F(\xi_{\boldsymbol{k}+\boldsymbol{q}}) - n_F(\xi_{\boldsymbol{k}})\Big)\frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}'}\hat{c}_{\boldsymbol{k}'-\boldsymbol{q}}^{\dagger}\hat{c}_{\boldsymbol{k}'}$$
(103)

Collecting everything we then get

$$\left(-\partial_{\tau} - (\xi_{\boldsymbol{k}+\boldsymbol{q}} - \xi_{\boldsymbol{k}})\right)\chi(\boldsymbol{k},\boldsymbol{q};\tau) = \left(n_{F}(\xi_{\boldsymbol{k}}) - n_{F}(\xi_{\boldsymbol{k}+\boldsymbol{q}})\right)\left(1 + V(\boldsymbol{q})\frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}'}\chi(\boldsymbol{k}',\boldsymbol{q};\tau)\right)$$
(104)

which in Fourier space becomes

$$\left(i\omega_n - (\xi_{\boldsymbol{k}+\boldsymbol{q}} - \xi_{\boldsymbol{k}})\right)\chi(\boldsymbol{k}, \boldsymbol{q}; i\omega_n) = \left(n_F(\xi_{\boldsymbol{k}}) - n_F(\xi_{\boldsymbol{k}+\boldsymbol{q}})\right)\left(1 + V_c(\boldsymbol{q})\frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}'}\chi(\boldsymbol{k}', \boldsymbol{q}; i\omega_n)\right) \quad (105)$$

Using the previous result for the non-interacting response  $\chi_0(\mathbf{k}, \mathbf{q}; i\omega_n)$  we can write

$$\chi(\boldsymbol{k},\boldsymbol{q};i\omega_n) = \chi_0(\boldsymbol{k},\boldsymbol{q};i\omega_n) \left(1 + V_c(\boldsymbol{q})\frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}'}\chi(\boldsymbol{k}',\boldsymbol{q};i\omega_n)\right)$$
(106)

Summing over  $\boldsymbol{k}$  we get

$$\chi(\boldsymbol{q}, i\omega_n) = \chi_0(\boldsymbol{q}, i\omega_n) \Big( 1 + V_c(\boldsymbol{q}) \chi(\boldsymbol{q}; i\omega_n) \Big)$$
(107)

Solving for  $\chi(\boldsymbol{q}, i\omega_n)$  yields

$$\chi(\boldsymbol{q}, i\omega_n) = \frac{\chi_0(\boldsymbol{q}, i\omega_n)}{1 - V_c(\boldsymbol{q})\chi_0(\boldsymbol{q}, i\omega_n)}$$
(108)

Since we have the analytical continuation of  $\chi^R_0({m q},\omega)$  we can insert this into the expression for

$$\chi^{R}(\boldsymbol{q},\omega) = \frac{\chi_{0}^{R}(\boldsymbol{q},\omega)}{1 - V_{c}(\boldsymbol{q})\chi_{0}^{R}(\boldsymbol{q},\omega)}$$
(109)

### 3.5 Plasma oscillations

Inserting the expression for the polarizability in the RPA approximation into the definition of the dielectric function we have

$$\varepsilon^{-1}(\boldsymbol{k},\omega) = 1 + \frac{V_c(\boldsymbol{k},\omega)}{1 - V_c(\boldsymbol{k})\chi_0^R(\boldsymbol{k},\omega)}\chi_0^R(\boldsymbol{k},\omega) = \frac{1}{1 - V_c(\boldsymbol{k})\chi_0^R(\boldsymbol{k},\omega)}$$
(110)

or inversely

$$\varepsilon(\boldsymbol{k},\omega) = 1 - V_c(\boldsymbol{k})\chi_0^R(\boldsymbol{k},\omega).$$
(111)

Thus we can write the polarizability as

$$\chi^{R}(\boldsymbol{k},\omega) = \frac{\chi^{R}_{0}(\boldsymbol{k},\omega)}{\varepsilon(\boldsymbol{k},\omega)}$$
(112)

which can be interpreted as a screened response to the external potential (with the inverse of the dielectric function representing the screening).

For very small  $\mathbf{k}$  we have  $\chi_0^R(\mathbf{k},\omega) = \frac{\bar{n}}{\bar{m}}\frac{\mathbf{k}^2}{\omega^2}$ . Then there exists a zero of the dielectric function at  $\omega = \omega_p = \sqrt{\frac{e^2\bar{n}}{\epsilon_0 m}}$ . This zero indicates a resonance associated with plasma oscillations.

## 3.6 Screened potential

Alternatively, we can write

$$\varepsilon^{-1}(\boldsymbol{k},\omega) = 1 + \frac{V_c(\boldsymbol{k},\omega)}{1 - V_c(\boldsymbol{k})\chi_0^R(\boldsymbol{k},\omega)}\chi_0^R(\boldsymbol{k},\omega) = 1 + \tilde{V}_c(\boldsymbol{k})\chi_0^R(\boldsymbol{k},\omega)$$
(113)

where

$$ilde{V}_c(m{k},\omega) = rac{V_c(m{k})}{1 - V_c(m{k})\chi_0^R(m{k},\omega)} = rac{V_c(m{k})}{arepsilon(m{k},\omega)}$$

represents a screened Coulomb interaction. For  $\omega = 0$  we have  $\chi_0^R(\mathbf{k}, 0) = -\nu(0)$ , and thus

$$\tilde{V}_{c}(\boldsymbol{k},0) = \frac{V_{c}(\boldsymbol{k})}{1 + \nu(0)V_{c}(\boldsymbol{k})} = \frac{1}{\epsilon_{0}|\boldsymbol{k}|^{2}\left(1 + \frac{\nu(0)}{\epsilon_{0}|\boldsymbol{k}|^{2}}\right)} = \frac{1}{\epsilon_{0}\left(|\boldsymbol{k}|^{2} + \kappa^{2}\right)}$$
(114)

where  $\kappa = \sqrt{\epsilon_0^{-1}\nu(0)}$  is the Thomas-Fermi screening length. The Fourier transform of this interaction gives a short range interaction

$$\tilde{V}_c(\boldsymbol{r} - \boldsymbol{r}') = \frac{e^{-\kappa|\boldsymbol{r} - \boldsymbol{r}'|}}{4\pi\epsilon_0|\boldsymbol{r} - \boldsymbol{r}'|}$$
(115)



Figure 5: Absorbtion as calculated by imaginary part of  $\chi_0^R(\boldsymbol{q},\omega)$  at T = 0 together with the plasma mode  $\omega(\boldsymbol{q}) = \omega_p + \frac{3}{10} \frac{v_F}{\omega_p} q^2$ .

# 4 Diagrammatic representation of the mean-field approximations

### 4.1 Anderson model without on-site interaction

Recall that the GF equation for the Anderson Model in the absence of on-site interaction can be written as

$$G_{d\sigma}(i\omega_n) = G_{0,d\sigma}(i\omega_n) + G_{0,d\sigma}(i\omega_n) \left(\sum_{\boldsymbol{k}} t_{\boldsymbol{k}}^* G_{0,\boldsymbol{k}\sigma}(i\omega_n) t_{\boldsymbol{k}}\right) G_{d\sigma}(i\omega_n)$$
(116)

This may be expressed diagrammatically by introducing the following representations of the propagators

$$G_{d\sigma} = - - , \quad G_{0,d\sigma} = - - , \quad G_{0,k\sigma} = \cdots$$
 (117)

and the vertices

$$t_{k}^{*} = -- \star \cdots, \quad t_{k} = \cdots \star -$$
(118)

It is then easy to see that the diagrammatic representation of the Anderson model without on-site interaction is given by

By inserting this equation into itself we can generate an infinite series of diagrams. Needless to say, it is a big advantage to sum up these diagrams up by defining

$$\Sigma = \star \cdots \blacktriangleright \star = \sum_{k} t_{k}^{*} G_{0,k\sigma} t_{k}$$
(120)

which justifies the use of the term "self-energy" for this object.

#### 4.2 Anderson model with on-site interaction

When we include on-site interaction in the Anderson model we also need to include the corresponding diagrams. To identify which diagrams are kept within the approximations used in this text, let us first look at the case when the hopping is absent,  $t_{\mathbf{k}} = 0$ . The equation of motion can then be written on the form

$$G_{d\sigma}(i\omega_n) = G_{0,d\sigma}(i\omega_n) + G_{0,d\sigma}(i\omega_n) \left[Un_{\sigma}\right] G_{d\sigma}(i\omega_n)$$
(121)

Here  $n_{\sigma} = G_{d\sigma}(\tau = 0^{-}) = \frac{1}{\beta} \sum_{\omega_n} G_{d\sigma}(i\omega_n) e^{-i\omega_n 0^{-}}$ . Using the diagrammatical representation of the vertex

$$U = \tag{122}$$

The term  $Un_{d\sigma}$  can then be represented by a **tadpole** diagram

$$Un_{d\sigma} = \tag{123}$$

and the equation of motion for the Greens function is given by

$$= + +$$

If we include also hopping we may write

$$G_{d\sigma}(i\omega_n) = G_{0,d\sigma}(i\omega_n) + G_{0,d\sigma}(i\omega_n) \left[ Un_{\sigma} + \sum_{\boldsymbol{k}} t_{\boldsymbol{k}}^* G_{0,\boldsymbol{k}\sigma}(i\omega_n) t_{\boldsymbol{k}} \right] G_{d\sigma}(i\omega_n)$$

or

where



Note that since the tadpole diagram contains the full propagator the self-energy has to be evaluated self-consistently together with the Dyson equation.

## 4.3 RPA

We write the unperturbed polarizability  $\chi_0$ 

$$\chi_0 = \tag{127}$$

while we write the full response function as

$$\chi = \tag{128}$$

Using the equation of motion for the polarizability

$$\chi(\boldsymbol{q}, i\omega_n) = \chi_0(\boldsymbol{q}, i\omega_n) + \chi_0(\boldsymbol{q}, i\omega_n) V_c(\boldsymbol{q}) \chi(\boldsymbol{q}; i\omega_n)$$
(129)

which we can represent diagrammatically as

$$(130)$$

If we use diagrammatic representation

$$\tilde{V}_c =$$
 ,  $V_c =$  (131)

for the screened- and unscreened Coulomb potential and rewrite the equation for the screened potential as

$$V_c(\boldsymbol{q},\omega) = V_c(\boldsymbol{q}) + V_c(\boldsymbol{q})\chi_0(\boldsymbol{q},\omega)V_c(\boldsymbol{q},\omega),$$

which we can represent as

$$\begin{array}{c} \\ \end{array} = \\ \end{array} + \\ \end{array} + \\ \end{array} + \\ \end{array} + \\ \end{array}$$