Chapter 9

Equation of motion theory

In the previous chapters we saw how various physical observables can be expressed in terms of retarded Green's functions and correlation functions. In many cases we need to calculate the time-dependence of these functions. There are several ways of attacking this problem, one of which is the equation of motion technique. The basic idea of this method is to generate a series of coupled differential equations by differentiating the correlation function at hand a number of times. If these equations close the problem is in principle solvable, and if not, one needs to invoke physical arguments to truncate the set of equations in a reasonable fashion. For example one can neglect certain correlations. We shall study examples of both situations in this chapter.

9.1   The single-particle Green's function

Let us consider the retarded Green's function G^R for either fermions or bosons, Eq. (8.28)

$$G^R(\mathbf{r}t, \mathbf{r}'t') = -i\theta\left(t - t'\right) \langle [\Psi(\mathbf{r}t), \Psi^\dagger(\mathbf{r}'t')]_{B,F}\rangle. \tag{9.1}$$

We find the equation of motion for G^R as the derivative with respect to the first time argument

$$\begin{aligned}
i\partial_t G^R(\mathbf{r}t, \mathbf{r}'t') &= (-i)\left(i\partial_t\theta(t-t')\right)\langle[\Psi(\mathbf{r}t), \Psi^\dagger(\mathbf{r}'t')]_{B,F}\rangle \\
&\quad + (-i)\,\theta(t-t')\langle[i\partial_t\Psi(\mathbf{r}t), \Psi^\dagger(\mathbf{r}'t')]_{B,F}\rangle, \\
&= \delta(t-t')\delta(\mathbf{r}-\mathbf{r}') + \\
&\quad + (-i)\,\theta(t-t')\langle[i\partial_t\Psi(\mathbf{r}t), \Psi^\dagger(\mathbf{r}'t')]_{B,F}\rangle.
\end{aligned} \tag{9.2}$$

Here we used that the derivative of a step function is a delta function and the commutation relations for field operators at equal times $\left[\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')\right]_{B,F} = \delta(\mathbf{r} - \mathbf{r}')$. Next, let us study the time-derivative of the annihilation operator (throughout this chapter we assume that H is time independent)

$$i\partial_t\Psi(\mathbf{r}t) = -\left[H, \Psi(\mathbf{r})\right](t) = -[H_0, \Psi(\mathbf{r})](t) - [V_{\text{int}}, \Psi(\mathbf{r})](t), \tag{9.3}$$

where the interaction part of the Hamiltonian includes all the interactions in the given problem, while H_0 describes the quadratic part of the Hamiltonian, for example the kinetic energy. If H_0 is the usual kinetic energy Hamiltonian of free particles, we have

$$-[H_0, \Psi(\mathbf{r})] = \frac{1}{2m} \int d\mathbf{r} \left[\Psi^\dagger(\mathbf{r}')\nabla^2_{\mathbf{r}'}\Psi(\mathbf{r}'), \Psi(\mathbf{r}) \right]$$

$$= -\frac{1}{2m}\nabla^2_{\mathbf{r}}\Psi(\mathbf{r}). \tag{9.4}$$

In this case the equation of motion becomes

$$\left(i\partial_t + \frac{1}{2m}\nabla^2_{\mathbf{r}} \right) G^R(\mathbf{r}t, \mathbf{r}'t') = \delta(t - t')\delta(\mathbf{r} - \mathbf{r}') + D^R(\mathbf{r}t, \mathbf{r}'t'), \tag{9.5a}$$

$$D^R(\mathbf{r}t, \mathbf{r}'t') = -i\theta(t - t') \left\langle \left[-[V_{\text{int}}, \Psi(\mathbf{r})](t), \Psi^\dagger(\mathbf{r}'t') \right]_{B,F} \right\rangle. \tag{9.5b}$$

The function D^R thus equals the corrections to the free particle Green's function. After evaluating $[V_{\text{int}}, \Psi(\mathbf{r})]$ we can, as in Sec. 5.5, continue the generation of differential equations. It is now evident why the many-body functions, G^R, are called Green's functions. The equation in (9.5a) has the structure of the classical Green's function we saw in Sec. 8.1, where the Green's function of a differential operator, L, was defined as $LG =$ delta function.

Often it is convenient to work in some other basis, say $\{\nu\}$. The Hamiltonian is again written as $H = H_0 + V_{\text{int}}$, where the quadratic part of the Hamiltonian is

$$H_0 = \sum_{\nu\nu'} t_{\nu'\nu}a^\dagger_{\nu'}a_\nu. \tag{9.6}$$

The differential equation for the Green's function in this basis

$$G^R(\nu t, \nu't') = -i\theta(t - t')\langle[a_\nu(t), a^\dagger_{\nu'}(t')]_{B,F}\rangle \tag{9.7}$$

is found in exactly the same way as above. By differentiation the commutator with H_0 is generated

$$-[H_0, a_\nu] = \sum_{\nu''} t_{\nu\nu''}a_{\nu''}, \tag{9.8}$$

and hence

$$\sum_{\nu''} \left(i\delta_{\nu\nu''}\partial_t - t_{\nu\nu''} \right) G^R(\nu''t, \nu't') = \delta(t - t')\delta_{\nu\nu'} + D^R(\nu t, \nu't'), \tag{9.9a}$$

$$D^R(\nu t, \nu't') = -i\theta(t - t') \left\langle \left[-[V_{\text{int}}, a_\nu](t), a^\dagger_{\nu'}(t') \right]_{B,F} \right\rangle. \tag{9.9b}$$

In this course we will mainly deal with problems where the Hamiltonian does not depend explicitly on time (linear response was an exception, but even there the time dependent problem was transformed into a correlation function of a time independent problem). Therefore the Green's function can only depend on the time difference $t - t'$ and in this case

it is always useful to work with the Fourier transforms. Recalling that when performing the Fourier transformation of the derivative it becomes $\partial_t \to -i\omega$, and that the Fourier transform of a delta function is unity, $\delta(t) \to 1$. We can write the equation of motion in frequency domain

$$\sum_{\nu''} \left[\delta_{\nu\nu''}(\omega + i\eta) - t_{\nu\nu''} \right] G^R(\nu''\nu'; \omega) = \delta_{\nu\nu'} + D^R(\nu, \nu'; \omega), \tag{9.10a}$$

$$D^R(\nu, \nu'; \omega) = -i \int_{-\infty}^{\infty} dt e^{i(\omega + i\eta)(t-t')} \theta(t - t') \left\langle \left[-[V_{\text{int}}, a_\nu](t), a_{\nu'}^\dagger(t') \right]_{B,F} \right\rangle. \tag{9.10b}$$

Here it is important to remember that the frequency of the retarded functions must carry a small positive imaginary part, η, to ensure proper convergence.

9.1.1   Non-interacting particles

For non-interacting particles, which means that the Hamiltonian is bilinear in annihilation or creation operators, we can in fact solve for the Green's function[1]. In this case we have

$$\sum_{\nu''} \left(\delta_{\nu\nu''}(\omega + i\eta) - t_{\nu\nu''} \right) G_0^R(\nu''\nu'; \omega) = \delta_{\nu\nu'} \tag{9.11}$$

where the subindex 0 on G_0^R indicates that it is the Green's function corresponding to a non-interacting Hamiltonian. As in Sec. 8.1 we define the inverse Green's function as

$$\left(G_0^R \right)^{-1} (\nu\nu'; \omega) = \delta_{\nu\nu'}(\omega + i\eta) - t_{\nu\nu'} \equiv \left(\mathbf{G}_0^R \right)_{\nu\nu'}^{-1} \tag{9.12}$$

and in matrix notation Eq. (9.11) becomes

$$\left(\mathbf{G}_0^R \right)^{-1} \mathbf{G}_0^R = \mathbf{1}. \tag{9.13}$$

Therefore, in order to find the Green's function all we need to do is to invert the matrix $\left(\mathbf{G}_0^R \right)_{\nu\nu'}^{-1}$. For a diagonal basis, i.e. $t_{\nu\nu'} = \delta_{\nu\nu'}\varepsilon_\nu$, the solution is

$$\left(\mathbf{G}_0^R \right)_{\nu\nu'} = G_0^R(\nu, \omega) \delta_{\nu\nu'} = \frac{1}{\omega - \varepsilon_\nu + i\eta} \delta_{\nu\nu'}, \tag{9.14}$$

which of course agrees with the result found in Eq. (8.4).

9.2   Single level coupled to continuum

To illustrate how the equation of motion theory can be used to determine the Green's function, we now take a model which we will use several times in the book, namely

$$H = H_0 + H_{\text{hyb}} + H_l, \tag{9.15}$$

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[1]Here we only consider terms of the form $c^\dagger c$ but also anomalous terms like cc could be included. In Chap. 4 we saw that such a term is indeed relevant for superconductors. For the Green's function in a superconductor we should therefore solve the linear problem in a way similar to the Bogoliubov transformation introduced in Chap.Chap. 4. We return to this in Chap. 18.

where H_0 describes a non-interacting electron gas

$$H_0 = \sum_\nu \xi_\nu c_\nu^\dagger c_\nu, \tag{9.16}$$

and H_l is the Hamiltonian of a single localized level

$$H_l = \xi_0 c_l^\dagger c_l, \tag{9.17}$$

and where finally H_{hyb} describes the hybridization or tunneling between the localized level and the continuum of states

$$H_{\text{hyb}} = \sum_\nu (t_\nu^* c_\nu^\dagger c_l + t_\nu c_l^\dagger c_\nu). \tag{9.18}$$

We are interested in finding the diagonal Green's function for the local state. In order to do that in turns out that we need the following two Green's functions

$$G^R(l, l, t - t') = -i\theta(t - t')\langle [c_l(t), c_l^\dagger(t')] \rangle \tag{9.19a}$$

$$G^R(\nu, l, t - t') = -i\theta(t - t')\langle [c_\nu(t), c_l^\dagger(t')] \rangle. \tag{9.19b}$$

The equations of motion are now found by letting ν and ν'' in Eq. (9.11) run over both the continuum states ν and the localized state l, and we obtain the coupled equations

$$(\omega + i\eta - \xi_l)\, G^R(l, l, \omega) - \sum_\nu t_\nu G^R(\nu, l, \omega) = 1, \tag{9.20}$$

$$(\omega + i\eta - \xi_\nu)\, G^R(\nu, l, \omega) - t_\nu^* G^R(l, l, \omega) = 0. \tag{9.21}$$

It is now a simple matter to solve the last equation and insert it into the first. We obtain

$$G^R(l, l, \omega) = \frac{1}{\omega - \xi - \Sigma^R(\omega)}, \tag{9.22}$$

where

$$\Sigma^R(\omega) = \sum_\nu \frac{|t_\nu|^2}{\omega - \xi_\nu + i\eta}. \tag{9.23}$$

The function $\Sigma^R(\omega)$ is our first encounter with the concept known as "self-energy". The self-energy changes the pole of $G^R(l, l)$ and furthermore gives some broadening to the spectral function. In the time domain the imaginary part translates into a life-time. It arises because the coupling to the continuum states introduces off-diagonal terms in the Hamiltonian, so that it is no longer diagonal in the l-operator. The true diagonal modes are instead superpositions of ν- and l-states.
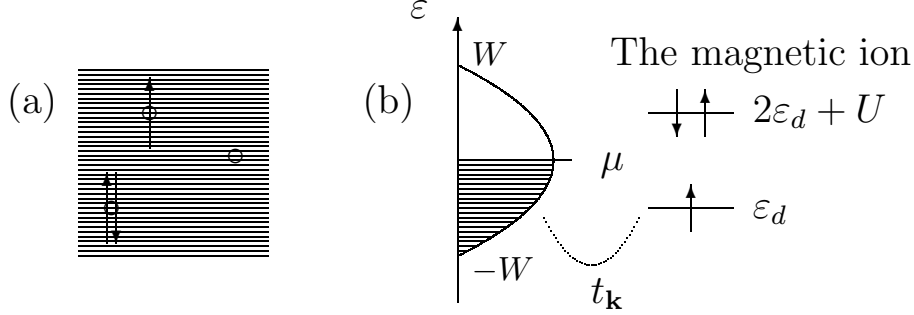
Figure 9.1: The Anderson model describing magnetic impurities embedded in a homogeneous host metal. The electrons in the conduction band of the non-magnetic host metal, indicated by the dashed areas, couple to the level of the magnetic impurity ion. The bare onsite energy of the state on the magnetic ion is ϵ_d. But the energy of electrons residing on the impurity ion also depends on whether it is doubly occupied or not, therefore the state with two electrons residing on the ion has energy $2\epsilon_d + U$, as seen in (b).

9.3 Anderson's model for magnetic impurities

In order to exemplify the usefulness of the equation of motion technique, we proceed by solving a famous model for the appearance of a magnetic moment of impurities of certain magnetic ions embedded in a non-magnetic host metal. The host metal, e.g. Nb or Mo, has a conduction band, which can be described by an effective non-interacting model

$$H_c = \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} - \mu) \, c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}. \tag{9.24}$$

For the impurity ion we assume that it has only one spin-degenerate state in the active shell, which is typically the d shell. In addition to the bare energy cost for an electron to reside in the d-state, there is an interaction energy that depends on the state being doubly occupied or not. The impurity ion Hamiltonian is thus modelled as

$$H_d + H_U = \sum_{\sigma} (\varepsilon_d - \mu) \, c_{d\sigma}^{\dagger} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}. \tag{9.25}$$

where $n_{d\sigma} = c_{d\sigma}^{\dagger} c_{d\sigma}$ is the number operator for d-electrons. The crucial input is here the correlation between electrons on the impurity ion, because the interaction in the narrower d-shell of a magnetic ion is particular strong and this is in fact the reason for the magnetism. The states forming the conduction band are primarily s-states that are more extended in space, and hence interactions are less important for those.

The electrons occupying the conduction band couple to the outer-most electrons of the magnetic impurity ions, e.g. the d-shell of a Fe ion. The coupling occurs because the d-orbital and the conduction band states overlap spatially and also lie close in energy, giving rise to a "hybridization" between the two. The overlapping orbitals leads to a

non-diagonal matrix element of the Hamiltonian

$$H_{\text{hyb}} = \sum_{\mathbf{k}\sigma} t_{\mathbf{k}} c_{d\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} t_{\mathbf{k}}^{*} c_{\mathbf{k}\sigma}^{\dagger} c_{d\sigma}. \tag{9.26}$$

The bare d-electron energy, ε_d, is below the chemical potential and from the kinetic energy point of view, it is favorable to fill the orbital by two electrons. However, this costs potential energy, U, and it is not possible if $2\varepsilon_d + U > 2\mu$. Furthermore, the system gains further kinetic energy by the hybridization, which on the other hand is complicated by the fact that the hopping in and out of the impurity orbital with, say, spin up electrons depends on the occupation of spin down electrons. The hybridization therefore seems to randomize the spin on the magnetic ion. The sum of these three energy contributions

$$H = H_c + H_d + H_U + H_{\text{hyb}} \tag{9.27}$$

is known as the Anderson model. See Fig. 9.1 for an illustration. Although the Anderson model looks simple, its full solution is very complicated and in fact the model has a very rich phase diagram. The Anderson model has been used to describe numerous effects in the physics of strongly correlated electron systems.[2]

It turns 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 (thus gaining maximum hybridization energy). The physical question we try to answer here is: Under which circumstances is the material magnetic?

9.3.1   The equation of motion for the Anderson model

The magnetization in the z-direction is given by the expectation value of the difference $n_\uparrow - n_\downarrow$ between spin up and down occupancy. The occupation of a quantum state was found in Eq. (8.10) in terms of the spectral function. For the d-electron occupation we therefore have

$$\langle n_{d\sigma} \rangle = \int \frac{d\omega}{2\pi} n_F(\omega) A(d\sigma, \omega), \tag{9.28}$$

where $A(d\sigma, \omega)$ is the spectral function, which follows from the retarded Green's function, G^R, see Eq. (8.51). All we need to find is then

$$G^R(d\sigma; t - t') = -i\theta\left(t - t'\right)\left\langle \{c_{d\sigma}\left(t\right), c_{d\sigma}^{\dagger}\left(t'\right)\} \right\rangle. \tag{9.29}$$

Let us write the equation of motion of this function using Eq. (9.10). Due to the hybridization term the Hamiltonian is not diagonal in the d-operators and the equations of motion will involve another Green's function, namely

$$G^R(\mathbf{k}\sigma, d\sigma, t - t') = -i\theta\left(t - t'\right)\left\langle \{c_{\mathbf{k}\sigma}\left(t\right), c_{d\sigma}^{\dagger}\left(t'\right)\} \right\rangle. \tag{9.30}$$

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[2]The model in fact has a known exact solution, but the solution fills an entire book, and it is hard to extract useful physical information from this solution.

The equations of motion are thus found by letting ν'' in Eq. (9.10) run over both d and k and we obtain the coupled equations

$$\left(\omega + i\eta - \varepsilon_d + \mu\right) G^R(d\sigma, \omega) - \sum_{\mathbf{k}} t_{\mathbf{k}} G^R(\mathbf{k}\sigma, d\sigma, \omega) = 1 + U D^R(d\sigma, \omega), \qquad (9.31)$$

$$\left(\omega + i\eta - \varepsilon_{\mathbf{k}} + \mu\right) G^R(\mathbf{k}\sigma, d\sigma, \omega) - t_{\mathbf{k}}^* G^R(d\sigma, \omega) = 0, \qquad (9.32)$$

where

$$D^R(d\sigma, \omega) = -i \int_{-\infty}^{\infty} dt e^{i(\omega + i\eta)(t-t')} \theta\left(t - t'\right) \left\langle \left\{ -[n_{d\uparrow} n_{d\downarrow}, c_{d\sigma}](t), c_{d\sigma}^\dagger(t') \right\} \right\rangle. \qquad (9.33)$$

The commutator in this expression is for $\sigma = \uparrow$

$$[n_{d\uparrow} n_{d\downarrow}, c_{d\uparrow}] = n_{d\downarrow}[n_{d\uparrow}, c_{d\uparrow}] = -n_{d\downarrow} c_{d\uparrow}, \qquad (9.34)$$

and likewise we find the commutator for spin down by interchanging up and down. We thus face the following more complicated Green's function

$$D^R(d\uparrow, t - t') = -i\theta\left(t - t'\right) \langle\{n_{d\downarrow}(t) c_{d\uparrow}(t), c_{d\uparrow}^\dagger(t')\}\rangle. \qquad (9.35)$$

9.3.2 Mean-field approximation for the Anderson model

Differentiating the function in Eq. (9.35) with respect to time would generate yet another function $\langle\{[H, n_{d\downarrow}(t) d_{\uparrow}(t)], d_{\sigma}^\dagger(t')\}\rangle$ to be determined, and the set of equations does not close. However a mean-field approximation still grasps the important physics that the spin-up electron population depends on the spin-down population, therefore we replace the interaction part H_U by its mean-field version

$$H_U^{MF} = U \langle n_{d\uparrow}\rangle n_{d\downarrow} + U \langle n_{d\downarrow}\rangle n_{d\uparrow} - U \langle n_{d\uparrow}\rangle \langle n_{d\downarrow}\rangle. \qquad (9.36)$$

With this truncation, the function D^R becomes

$$D^R(d\uparrow, t - t') = -i\theta(t - t') \langle n_{d\downarrow}\rangle \langle\{c_{d\uparrow}(t), c_{d\uparrow}^\dagger(t')\}\rangle = \langle n_{d\downarrow}\rangle G^R\left(d\uparrow, t - t'\right). \qquad (9.37)$$

In other words, since the mean-field approximation makes the Hamiltonian quadratic we can include $U \langle n_{d\downarrow}(t)\rangle$ to the energy of the spin-up d-electrons in our equation of motion. Inserting (9.37) in Eq. (9.31), and solving Eq. (9.32) for $G^R(d\uparrow, \omega)$ gives

$$\left(\omega + i\eta - \varepsilon_d + \mu - U \langle n_{d\downarrow}\rangle\right) G^R(d\uparrow, \omega) - \sum_{\mathbf{k}} \frac{|t_{\mathbf{k}}|^2}{\omega - \varepsilon_{\mathbf{k}} + \mu + i\eta} G^R(d\uparrow, \omega) = 1, \qquad (9.38)$$

and likewise for the spin-down Green's function. The final answer is

$$G^R(d\uparrow, \omega) = \frac{1}{\omega - \varepsilon_d + \mu - U \langle n_{d\downarrow}\rangle - \Sigma^R(\omega)}, \qquad (9.39a)$$

$$\Sigma^R(\omega) = \sum_{\mathbf{k}} \frac{|t_{\mathbf{k}}|^2}{\omega - \varepsilon_{\mathbf{k}} + \mu + i\eta}. \qquad (9.39b)$$

The function $\Sigma^R(\omega)$ is recognized as the self-energy in Eq. (9.23). As mentioned, the self-energy changes the pole and broadens G^R. The "bare" d-electron energy, ε_d, is thus seen to be renormalized by two effects: first the energy is shifted by $U\langle n_{d\downarrow}\rangle$ due to the interaction with the averaged density of electrons having opposite spin, and secondly, the coupling to the conduction band electrons gives through $\Sigma(\omega)$ an energy shift and most importantly an imaginary part.

9.3.3 Solving the Anderson model and comparison with experiments

Assuming that the coupling $t_{\mathbf{k}}$ only depends on the length of $\mathbf{k}$ and thus on ε, the self-energy Σ is

$$\Sigma^R(\omega) = \int d\varepsilon\, d(\varepsilon) \frac{|t(\varepsilon)|^2}{\omega - \varepsilon + \mu + i\eta} = \mathcal{P}\int d\varepsilon\, d(\varepsilon) \frac{|t(\varepsilon)|^2}{\omega - \varepsilon + \mu} - i\pi d(\omega+\mu)|t(\omega+\mu)|^2. \quad (9.40)$$

The density of states $d(\varepsilon)$ and the coupling matrix element $t(\varepsilon)$ depend on the details of the material, but fortunately it is not important for the present considerations. Let us assume that the product $d(\varepsilon)|t(\varepsilon)|^2$ is constant within the band limits, $-W < \varepsilon < W$, and define the important parameter Γ by

$$2\pi d(\varepsilon)|t(\varepsilon)|^2 = \Gamma\theta(W - |\varepsilon|). \quad (9.41)$$

This approximation is good if the width of the Green's function (which we shall see shortly is given by Γ) turns out to be small compared to the scale on which $d(\varepsilon)|t(\varepsilon)|^2$ typically changes. Since in practice $\Gamma \ll \varepsilon_F$, the approximation is indeed valid. For $\omega+\mu \in [-W, W]$ we get

$$\Sigma^R(\omega) \approx \frac{\Gamma}{\pi}\int_{-W}^{W} \frac{d\varepsilon}{\omega - \varepsilon + \mu} - i\Gamma/2$$

$$= -\frac{\Gamma}{\pi}\ln\left|\frac{W + \omega + \mu}{W - \omega - \mu}\right| - i\Gamma/2, \quad -W < \omega + \mu < W. \quad (9.42)$$

The real part gives a shift of energy and since it is a slowly varying function, we simply include it as a shift of ε_d and define the new onsite energy $\tilde{\varepsilon} = \varepsilon_d + \operatorname{Re}\Sigma^R$.

The spectral function hence becomes

$$A(d\uparrow, \omega) = -2\operatorname{Im}G^R(d\uparrow, \omega)$$

$$= \frac{\Gamma}{(\omega - \tilde{\varepsilon} + \mu - U\langle n_{d\downarrow}\rangle)^2 + (\Gamma/2)^2}, \quad (9.43)$$

where Γ is the width of the spectral function. Note that the spectral function derived here is an example of the Lorentzian form discussed in Sec. 8.3.5.

Now the self-consistent mean-field equation for $\langle n_{d\uparrow}\rangle$ follows as

$$\langle n_{d\uparrow}\rangle = \int \frac{d\omega}{2\pi} n_F(\omega) A(d\uparrow, \omega)$$

$$= \int \frac{d\omega}{2\pi} n_F(\omega) \frac{\Gamma}{(\omega - \tilde{\varepsilon} + \mu - U\langle n_{d\downarrow}\rangle)^2 + (\Gamma/2)^2}. \quad (9.44)$$
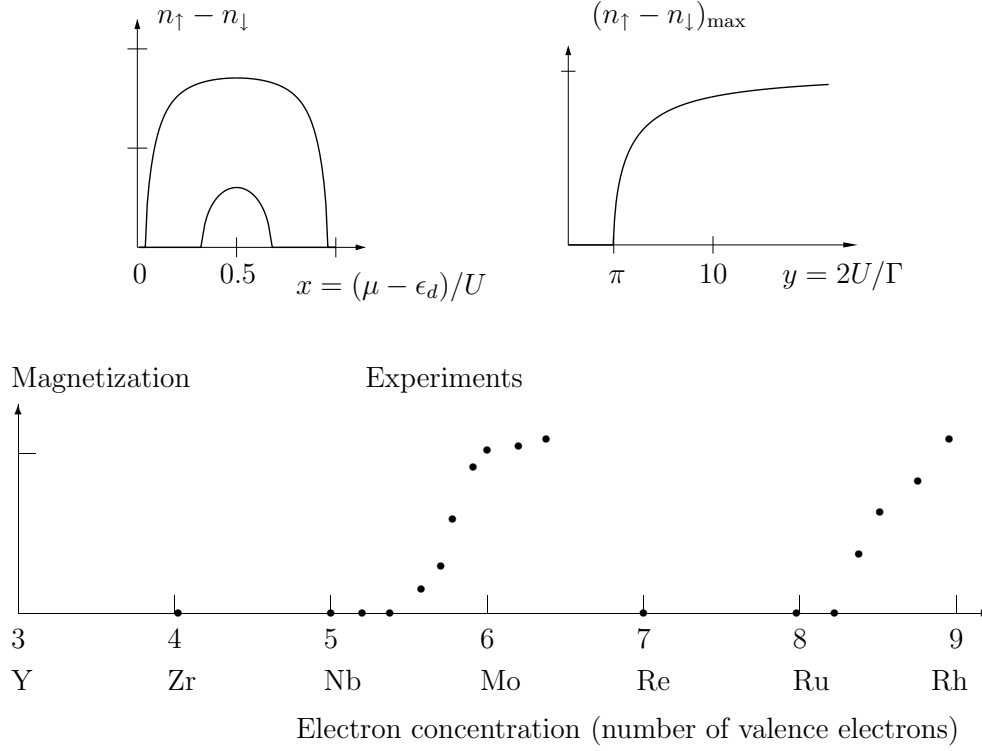
Figure 9.2: The upper part shows the mean field solution of the Anderson model with the left panel being magnetization as a function of electron density n_{el}, i.e. the chemical potential, for two different Γ-values, while the right panel is the maximum magnetization as function of the correlation energy. We see that there is a critical density and a critical U/Γ where the magnetization sets in. The latter means that too strong hybridization destroys the magnetization. The bottom panel shows experimental results (Clogston et al. (1962)) for the magnetic moment of Fe embedded in transition metals. The electron concentration and hence μ is varied by changing the alloy. For $4 < n_{el} < 8$ the magnetization curve is seen to be quite similar to the prediction of the model. For $n_{el} > 8$ the effect of having more than two d-orbitals in the Fe-atoms becomes important and the simple model is no longer adequate.

If we neglect the finite bandwidth, which is justified because $\Gamma \ll W$, and if we furthermore consider low temperatures, $T = 0$, we get

$$
\begin{aligned}
\langle n_{d\uparrow} \rangle &\approx \int_{-\infty}^{0} \frac{d\omega}{2\pi} \frac{\Gamma}{\left(\omega - \tilde{\varepsilon} + \mu - U \langle n_{d\downarrow} \rangle\right)^2 + (\Gamma/2)^2}, \\
&= \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left(\frac{\tilde{\varepsilon} - \mu + U \langle n_{d\downarrow} \rangle}{\Gamma/2} \right).
\end{aligned}
\tag{9.45}
$$

We obtain the two coupled equations

$$
\cot\left(\pi n_{\uparrow}\right) = y(n_{\downarrow} - x), \qquad x = -\left(\tilde{\varepsilon} - \mu\right)/U,
\tag{9.46a}
$$

$$
\cot\left(\pi n_{\downarrow}\right) = y(n_{\uparrow} - x), \qquad y = 2U/\Gamma.
\tag{9.46b}
$$

The solution of these equation gives the occupation of the d-orbital and in particular tells us whether there is a finite magnetization, i.e. whether there exists a solution $n_{\downarrow} \neq n_{\uparrow}$, different from the trivial solution $n_{\downarrow} = n_{\uparrow}$.[3] In Fig. 9.2 solutions of these equations are shown together with experimental data. As is evident there, the model describes the observed behavior, at least qualitatively.

9.4   The two-particle correlation function

The two particle correlation functions, such as the density-density correlation, was in Chap. 6 shown to give the linear response properties. Also for this quantity one can generate a set of equation of motions, and as for the single particle Green's function they are not solvable in general. But even so they may provide a good starting point for various approximation schemes.

Consider for example the retarded charge-charge correlation function

$$
\chi^{R}(\mathbf{r}t, \mathbf{r}'t') = -i\theta\left(t - t'\right) \langle [\rho(\mathbf{r}t), \rho(\mathbf{r}'t')] \rangle.
\tag{9.47}
$$

In Chap. 6 it was shown that this function is related to the dielectric response function and therefore tells about the screening properties of the material.

9.4.1   The Random Phase Approximation (RPA)

A commonly used approximation scheme for correlation functions is the so-called Random Phase Approximation (RPA). For the case of the electron gas, which is one of our main topics in this course, RPA is exact in some limits, but also in general gives a decent description of the interacting electron gas. In Chap.12 RPA is derived using Feynman diagrams, but here we derive it using the equation of motion technique. The two derivations give complementary insight into the physical content of the approximation.

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[3]We should also convince ourselves that the magnetic solution has lower energy, which it in fact does have.

We will for simplicity work with the translation-invariant electron gas with the Hamiltonian given by the usual kinetic energy plus interaction energy (here we disregard the spin degree of freedom because it is not important)

$$H = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{kk'q} \neq \mathbf{0}} V(q) c_{\mathbf{k+q}}^{\dagger} c_{\mathbf{k'-q}}^{\dagger} c_{\mathbf{k'}} c_{\mathbf{k}} = H_0 + V_{\text{int}}. \tag{9.48}$$

Furthermore, the $\mathbf{q} = \mathbf{0}$ component is cancelled by the positively charged background.

The charge-charge correlation function is

$$\chi^R(\mathbf{q}, t - t') = -i\theta\left(t - t'\right) \frac{1}{\mathcal{V}} \left\langle \left[\rho\left(\mathbf{q},t\right), \rho\left(-\mathbf{q},t'\right)\right] \right\rangle, \quad \rho\left(\mathbf{q}\right) = \sum_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q}}. \tag{9.49}$$

However, it turns out to be better to work with the function

$$\chi^R(\mathbf{kq}, t - t') = -i\theta\left(t - t'\right) \langle [(c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q}})\left(t\right), \rho\left(-\mathbf{q},t'\right)] \rangle, \tag{9.50}$$

from which we can easily obtain $\chi(\mathbf{q})$ by summing over $\mathbf{k}$, $\chi^R(\mathbf{q}) = \sum_{\mathbf{k}} \chi^R(\mathbf{kq})$. Let us find the equation of motion

$$i\partial_t \chi^R(\mathbf{kq}, t - t') = \delta(t - t') \langle [(c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q}})(t), \rho(-\mathbf{q},t')] \rangle$$
$$- i\theta(t - t') \langle [-[H, c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q}}]\left(t\right), \rho(-\mathbf{q}, t')] \rangle, \tag{9.51}$$

and for this purpose we need the following commutators

$$\left[c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q}}, \rho\left(-\mathbf{q}\right)\right] = \sum \left[c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q}}, c_{\mathbf{k'}}^{\dagger} c_{\mathbf{k'-q}}\right] = c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} - c_{\mathbf{k+q}}^{\dagger} c_{\mathbf{k+q}}, \tag{9.52}$$

$$[H_0, c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q}}] = (\xi_{\mathbf{k}} - \xi_{\mathbf{k+q}}) c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q}}, \tag{9.53}$$

$$[V_{\text{int}}, c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q}}] = -\frac{1}{2} \sum_{\mathbf{k'q'}} V(q') \left\{ c_{\mathbf{k+q'}}^{\dagger} c_{\mathbf{k'-q'}}^{\dagger} c_{\mathbf{k'}} c_{\mathbf{k+q}} + c_{\mathbf{k'+q'}}^{\dagger} c_{\mathbf{k-q'}}^{\dagger} c_{\mathbf{k+q}} c_{\mathbf{k'}} \right.$$
$$\left. - c_{\mathbf{k'+q'}}^{\dagger} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q+q'}} c_{\mathbf{k'}} - c_{\mathbf{k}}^{\dagger} c_{\mathbf{k'-q}}^{\dagger} c_{\mathbf{k'}} c_{\mathbf{k+q-q'}} \right\}. \tag{9.54}$$

When this is inserted into Eq. (9.51) a new 6-particle Green's function is generated. Furthermore for each level of the equation of motion a Green's function with two more electron operators pops up. At this stage we truncate this series by the random phase approximation which says that the right hand side of (9.54) is replaced by a mean-field expression where pairs of operators are replaced by their average values. Using the recipe from Chap. 4, we get

$$[V_{\text{int}}, c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q}}] \approx -\frac{1}{2} \sum_{\mathbf{k'q'} \neq \mathbf{0}} V(q') \left\{ c_{\mathbf{k+q'}}^{\dagger} c_{\mathbf{k+q}} \left\langle c_{\mathbf{k'-q'}}^{\dagger} c_{\mathbf{k'}} \right\rangle + \left\langle c_{\mathbf{k+q'}}^{\dagger} c_{\mathbf{k+q}} \right\rangle c_{\mathbf{k'-q'}}^{\dagger} c_{\mathbf{k'}} \right.$$
$$+ \left\langle c_{\mathbf{k-q'}}^{\dagger} c_{\mathbf{k+q}} \right\rangle c_{\mathbf{k'+q'}}^{\dagger} c_{\mathbf{k'}} + c_{\mathbf{k-q'}}^{\dagger} c_{\mathbf{k+q}} \left\langle c_{\mathbf{k'+q'}}^{\dagger} c_{\mathbf{k'}} \right\rangle$$
$$- c_{\mathbf{k'+q'}}^{\dagger} c_{\mathbf{k'}} \left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q+q'}} \right\rangle - \left\langle c_{\mathbf{k'+q'}}^{\dagger} c_{\mathbf{k'}} \right\rangle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q+q'}}$$
$$- c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q-q'}} \left\langle c_{\mathbf{k'-q}}^{\dagger} c_{\mathbf{k'}} \right\rangle - \left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k+q-q'}} \right\rangle c_{\mathbf{k'-q}}^{\dagger} c_{\mathbf{k'}} + \text{const.} \right\}$$
$$= V(q) \left(\langle n_{\mathbf{k+q}} \rangle - \langle n_{\mathbf{k}} \rangle \right) \sum_{\mathbf{k'}} c_{\mathbf{k'-q'}}^{\dagger} c_{\mathbf{k'}}, \tag{9.55}$$

where we used that $\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}'} \rangle = \langle n_{\mathbf{k}} \rangle \delta_{\mathbf{k},\mathbf{k}'}$. Note that the exchange pairings which we included in the Hartree-Fock approximation is not included here.

Collecting everything and going to the frequency domain the equation of motion becomes,

$$\left(\omega + i\eta + \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}} \right) \chi^{R}(\mathbf{k}\mathbf{q}, \omega) = -\left(\langle n_{\mathbf{k}+\mathbf{q}} \rangle - \langle n_{\mathbf{k}} \rangle \right) \left(1 - V(q) \sum_{\mathbf{k}'} \chi^{R}(\mathbf{k}'\mathbf{q}, \omega) \right),$$
(9.56)

which, when summed over $\mathbf{k}$, allows us to find an equation for $\chi^{R}(\mathbf{q}, \omega)$

$$\chi^{R}(\mathbf{q}, \omega) = -\frac{1}{\mathcal{V}} \sum_{\mathbf{k}} \chi^{R}(\mathbf{k}\mathbf{q}, \omega) = \frac{1}{\mathcal{V}} \sum \frac{\langle n_{\mathbf{k}+\mathbf{q}} \rangle - \langle n_{\mathbf{k}} \rangle}{\omega + \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}} + i\eta} \left(1 + V(q) \chi^{R}(\mathbf{q}, \omega) \right), \quad (9.57)$$

and hence

$$\chi^{R,\mathrm{RPA}}(\mathbf{q}, \omega) = \frac{\chi_{0}^{R}(\mathbf{q}, \omega)}{1 - V(q)\chi_{0}^{R}(\mathbf{q}, \omega)}.$$
(9.58)

This is the RPA result of the polarizability function. The free particle polarizability $\chi_{0}^{R}(\mathbf{q}, \omega)$ was derived in Sec. 8.5. The RPA dielectric function becomes

$$\varepsilon^{\mathrm{RPA}}(\mathbf{q}, \omega) = \left[1 + V(q)\chi^{R}(\mathbf{q}, \omega) \right]^{-1} = 1 - V(q) \chi_{0}^{R}(\mathbf{q}, \omega).$$
(9.59)

Replacing the expectation values, $n_{\mathbf{k}}$, by the Fermi-Dirac distribution function, we recognize the Lindhard function studied in Sec. 8.5. There we studied a non-interacting electron gas and found that $\chi^{R}(\mathbf{q}, \omega)$ indeed was equal to the numerator in (9.58) and the two results therefore agree nicely.

In Sec. 8.5 we also analyzed the excitation of the non-interacting electrons gas and the analysis there is basically still correct. The excitations which were shown in Sec. 8.5 to be related to the imaginary part of $\chi^{R}(\mathbf{q}, \omega)$ and therefore the structure of the electron-hole excitations of the non-interacting gas (depicted in Fig. 8.3) is preserved here, but of course the strength is modified by the real part of the denominator of (9.58).

However, the interactions add other fundamental excitations, namely collective modes, and in the case of a charge liquid these modes are the plasmon modes. The additional modes are given by the part where the imaginary part of $\chi_{0}^{R}(\mathbf{q}, \omega)$ is zero because then there is a possibility of a pole in the polarizability. If we set $\mathrm{Im}\,\chi_{0}^{R}(\mathbf{q}, \omega) = -i\delta$, we have

$$-\mathrm{Im}\,\chi^{R}(\mathbf{q}, \omega) = \frac{\delta}{\left[1 - V(q)\,\mathrm{Re}\,\chi_{0}^{R}(\mathbf{q}, \omega) \right]^{2} + \delta^{2}} = \pi\delta \left(1 - V(q)\,\mathrm{Re}\,\chi_{0}^{R}(\mathbf{q}, \omega) \right). \quad (9.60)$$

This means that there is a well-defined mode when $1 - V(q)\,\mathrm{Re}\,\chi_{0}^{R}(\mathbf{q}, \omega) = 0$ and this is the plasma oscillation mode, also called a plasmon. The plasmon is studied in detail in Chap. 12, here we just mention that the condition for the mode turns out to be $\omega \propto \sqrt{\omega_{\mathrm{pl}}^{2} + \mathrm{const.}\ q^{2}}$.

9.5   Summary and outlook

In this chapter we have seen a method to deal with the dynamical aspects of interacting many-body systems, namely the equation of motion method applied to the Green's functions. The set of differential equation is not soluble in general, and in fact only a very small set of Hamiltonians describing interacting systems can be solved exactly. Therefore approximations are necessary and we saw particular examples of this, namely the mean-field solution of a magnetic impurity embedded in a metallic host, and the RPA approximation for the charge auto correlation function.

In the following chapter we use the equation of motion to derive the Green's functions in the imaginary time formalism and to derive the famous Wick's theorem. Wick's theorem will then pave the way for introducing the Feynman diagrams.