

3.2.3 Green's functions in many-body problems (at zero temperature)

Now we extend the Green's-function approach to many-body problems using the expansion (3.2.2) and the Wick theorem (see Section 3.1.5). In the expansion (3.2.2), we encounter products of creation and annihilation operators with the evolution operators $\exp(-itH_0)$ inserted between them. It will be therefore convenient to define the time-dependent operators

$$a(t) = e^{itH} a e^{-itH}, \quad a^+(t) = e^{itH} a^+ e^{-itH}, \quad (3.2.24)$$

where H may be either the full Hamiltonian or the quadratic Hamiltonian H_0 , depending on the situation.

Note that in the case of a *quadratic Hamiltonian*, $a(t)$ and $a^+(t)$ always remain linear combinations of the original creation and annihilation operators a and a^+ . Proof: they obey the linear equations of motion

$$\dot{a}(t) = i[H_0, a(t)] \quad (3.2.25)$$

[and similarly for $a^+(t)$], so if $a(t)$ is linear in a and a^+ at some moment t , it will remain linear at the “next” moment, too. From the linearity property, it follows that $a(t)$ and $a^+(t)$ obey the Wick theorem.

Now we are ready to introduce the time-dependent Green's functions $\langle a^+(t_1)a(t_2) \rangle$. More precisely, we introduce three different Green's functions:

- the *retarded* Green's function:

$$G^R(t_1 - t_2; x_1, x_2) = -i \langle \{a(t_1, x_1), a^+(t_2, x_2)\} \rangle \theta(t_1 - t_2); \quad (3.2.26)$$

- the *advanced* Green's function:

$$G^A(t_1 - t_2; x_1, x_2) = i \langle \{a(t_1, x_1), a^+(t_2, x_2)\} \rangle \theta(t_2 - t_1); \quad (3.2.27)$$

- the *causal* (or time-ordered) Green's function:

$$G^c(t_1 - t_2; x_1, x_2) = -iT \langle a(t_1, x_1) a^+(t_2, x_2) \rangle, \quad (3.2.28)$$

where T denotes time ordering:

$$T A(t_1) B(t_2) = \begin{cases} A(t_1) B(t_2) & \text{if } t_1 > t_2 \\ -B(t_2) A(t_1) & \text{if } t_2 > t_1 \end{cases} \quad (3.2.29)$$

(we assumed that the operators a and a^+ are fermionic; for bosonic operators, there is no sign change when permuting them).

The above Green's functions may be defined either for the quadratic part of the Hamiltonian H_0 (with the time evolution by H_0 and average taken over the ground state of H_0) or for the full Hamiltonian. As before, we will denote the Green's functions defined for the full Hamiltonian by tildes, while the Green's function for the quadratic part written without additional marks.

In the general case, we can establish the following relations between these Green's functions:

$$\tilde{G}_\omega^R(k) = [\tilde{G}_\omega^A(k)]^* \quad (3.2.30)$$

$$\tilde{G}_\omega^c(k) = \begin{cases} \tilde{G}_\omega^R(k), & \omega > 0 \\ \tilde{G}_\omega^A(k), & \omega < 0. \end{cases} \quad (3.2.31)$$

(here ω is measured from the chemical potential μ or, equivalently, μ is included in the Hamiltonian).

In the case of a quadratic Hamiltonian, more properties hold:

- In the definitions of G^R and G^A we may remove the averaging $\langle \dots \rangle$, since the anticommutators are just numbers, not operators. In other words, G^R and G^A do not depend on the many-particle state, but are single-particle properties.
- G^R coincides with the quantum-mechanical Green's function (as can be seen from considering its definition in the vacuum state).
- For the free-particle Hamiltonian, we can find

$$G^R(\omega, k) = \frac{1}{\omega - (\varepsilon_k - \mu) + i\delta} \quad (3.2.32)$$

$$G^A(\omega, k) = \frac{1}{\omega - (\varepsilon_k - \mu) - i\delta} \quad (3.2.33)$$

$$G^c(\omega, k) = \frac{1}{\omega - (\varepsilon_k - \mu) + i\delta \operatorname{sign} \omega} \quad (3.2.34)$$

In other words, in the ω - k representation, G^R , G^A , and G^c differ only by the regularization of the poles: G^R corresponds to all states empty, G^A to all states occupied, and G^c keeps track of the occupation number being 0 or 1.

The time-ordered Green's function G^c turns out to be useful for the diagrammatic technique, since the expansion (3.2.2) naturally produces time-ordered correlation functions. Note also that the Wick theorem can be reformulated for time-ordered products, since time ordering guarantees the same order of operators in the left and right-hand sides of (3.1.34). At the same time, the Green's function $\tilde{G}^c$ can be used to express single-particle average quantities. The poles of the Green's functions correspond to the spectrum of excitations (the poles above and below the real axis of ω correspond to hole and electron excitations, respectively).

3.2.4 Diagrammatic expansion of a single Green's function

Let us illustrate the diagrammatic approach with a perturbative expansion of a single Green's function. In other words, we would like to express the full Green's function $\tilde{G}^c$ in terms of the bare Green's function G^c and the interaction parameters. We assume that the Hamiltonian has the usual form

$$H = H_0 + V, \quad (3.2.35)$$

where the quadratic Hamiltonian H_0 is the free-fermion one (3.1.19) and the interaction V is a pairwise potential interaction (3.1.24).

The Green's function (3.2.28) involves interaction both in the time-evolution part between the moments t_1 and t_2 and in the ground state over which we average. To treat them on equal footing, we express the ground state as a result of an “adiabatic switching” of the interaction:

$$|\Psi_0\rangle = e^{-iH(0-t_{-\infty})}|\Psi_{\infty}\rangle, \quad (3.2.36)$$

where the perturbative expression is assumed to switch on adiabatically (or the time is assumed to have a small imaginary part), so that the ground state is selected after a sufficiently slow evolution. The starting time $t_{-\infty}$ will be taken to $-\infty$ at the end of the calculation. The starting state $|\Psi_{\infty}\rangle$ is the ground state of the unperturbed Hamiltonian H_0 . Then we can represent the Green's function (3.2.28) as (we put $t_1 > t_2$, to be specific):

$$\tilde{G}^c(t_1 - t_2; x_1, x_2) = -i \frac{\langle \Psi_{\infty} | e^{-iH(t_{\infty}-t_1)} a(x_1) e^{-iH(t_1-t_2)} a^+(x_2) e^{-iH(t_2-t_{-\infty})} | \Psi_{\infty} \rangle}{\langle \Psi_{\infty} | e^{-iH(t_{\infty}-t_{-\infty})} | \Psi_{\infty} \rangle}. \quad (3.2.37)$$

The evolution operators in both the numerator and the denominator can now be expanded in V by writing $H = H_0 + V$ and using the expansion (3.2.2). Then the result can be expressed in terms of products of the unperturbed Green's functions G^c by using the Wick theorem. Each of these terms can be represented as a diagram.

An important observation (which can be proven by a combinatoric counting): disconnected loops of the diagrams in the numerator are exactly canceled by the diagrams from the denominator! So the actual sum must include only connected diagrams.

3.2.5 Hartree–Fock as a renormalization of the Green's function

To the first order in V , the procedure described above produces two diagrams shown in Fig. 10. The integrals corresponding to these diagrams are:

$$\delta_1 \tilde{G}^c(t_1 - t_2; x_1, x_2) = \iiint dx dy dt V(x-y) n(y) G^c(t_1 - t; x_1, x) G^c(t - t_2; x, x_2), \quad (3.2.38)$$

where $n(y) = -iG^c(\Delta t = -0; y, y)$ is the average particle density at point y (in the uniform case, it is simply the average density n), and

$$\delta_2 \tilde{G}^c(t_1 - t_2; x_1, x_2) = i \iiint dx dy dt V(x - y) \times G^c(t_1 - t; x_1, x) G^c(\Delta t = -0; x, y) G^c(t - t_2; y, x_2). \quad (3.2.39)$$

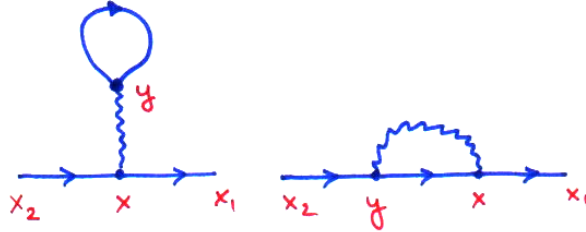


Figure 10: The two leading corrections to the Green's function due to interaction.

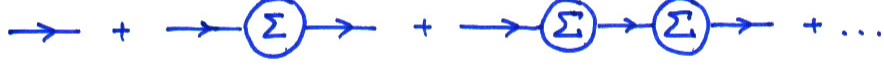


Figure 11: The geometric series (3.2.43). Σ denotes the “irreducible” part of the expansion.

We can also rewrite the same integrals in the frequency-momentum representation (in the translationally invariant case):

$$\delta_1 \tilde{G}_\omega^c(k) = V_{k=0} n [G_\omega^c(k)]^2, \quad (3.2.40)$$

$$\delta_2 \tilde{G}_\omega^c(k) = i \int \frac{d^3 k'}{(2\pi)^3} \left[\int \frac{d\omega}{2\pi} e^{i\omega 0} G_\omega^c(k') \right] V_{k-k'} [G_\omega^c(k)]^2. \quad (3.2.41)$$

The factor $e^{i\omega 0}$ indicates that we have to close the integration contour in the upper half plane:

$$G^c(\Delta t = -0; k') = \int \frac{d\omega}{2\pi} e^{i\omega 0} G_\omega^c(k') = i n_{k'} \quad (3.2.42)$$

is simply the occupation number at the momentum k .

Now we remark that these are in fact corrections to the *denominator* of the Green’s function. Indeed, if we know the irreducible *self-energy* part (i.e., the part which cannot be disconnected by breaking any single Green’s-function line), then we can sum the series [compare with (3.2.13)]:

$$\begin{aligned} G_\omega^c(k) + G_\omega^c(k) \Sigma_\omega(k) G_\omega^c(k) + G_\omega^c(k) \Sigma_\omega(k) G_\omega^c(k) \Sigma_\omega(k) G_\omega^c(k) + \dots \\ = \frac{1}{\omega - (\varepsilon_k - \mu + \Sigma_\omega(k)) + i\delta \text{sign } \omega} \end{aligned} \quad (3.2.43)$$

(see Fig. 11). In our case, this means that we can interpret the corrections (3.2.40) and (3.2.41) as corrections to the energy

$$\delta \varepsilon_k = \Sigma_\omega(k) = n V_{k=0} - \int \frac{d^3 k'}{(2\pi)^3} n_{k'} V_{k-k'}, \quad (3.2.44)$$

which reproduces our earlier result (3.1.45).

Moreover, if we assume that the chemical potential is controlled by the overall density of particles and is not renormalized by the interaction (which is the case in the metal), then our calculation amounts, in fact, to summing a large number of diagrams, which can be written in a recursive way in Fig. 12. Some diagrams are, however, not included (Fig. 13), in particular those responsible for screening.



Figure 12: The recursive equation for the Hartree–Fock sum.

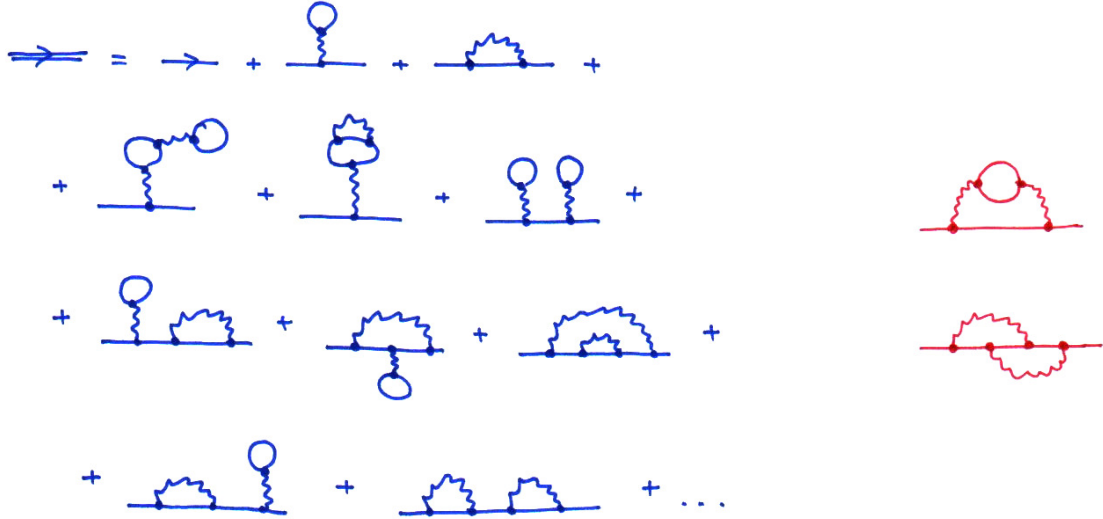


Figure 13: Left: the diagram included in the Hartree–Fock series recursively defined in Fig. 12. Right: two second-order diagrams not included in this series.

3.2.6 Hartree–Fock as a variational method

Ref: [AM] Chapter 17

The same Hartree–Fock approximation may also be understood as a variational procedure. Suppose that we look for a Slater-determinant state

$$\Psi = S_-(\varphi_1 \otimes \dots \otimes \varphi_N) \quad (3.2.45)$$

with the lowest variational energy. The variational parameters are the single-particle states $\varphi_1, \dots, \varphi_N$. These states are optimized to minimize the expectation value $\langle \Psi | H | \Psi \rangle$ of the Hamiltonian

$$H = \sum_{i=1}^N \left[-\frac{1}{2m} \nabla^2 + U(x_i) \right] + \frac{1}{2} \sum_{i \neq j} U(x_i - x_j) \quad (3.2.46)$$

under the normalization condition $\langle \Psi | \Psi \rangle = 1$. Without loss of generality, we may assume the single-particle states φ_i to be orthonormal, and then the normalization condition may be reduced to fixing the normalization of each of the single-particle states $\langle \varphi_i | \varphi_i \rangle = 1$. This would lead to introducing N Lagrange multipliers for each of these conditions.

The expectation value of the Hamiltonian may be shown to be given by

$$\begin{aligned} \langle \Psi | H | \Psi \rangle &= \sum_{i=1}^N \langle \varphi_i | -\frac{1}{2m} \nabla^2 + U | \varphi_i \rangle \\ &\quad + \frac{1}{2} \sum_{i,j} \iint dx dy |\varphi_i(x)|^2 |\varphi_j(x)|^2 U(x - y) \\ &\quad - \frac{1}{2} \sum_{i,j} \iint dx dy \varphi_i^*(x) \varphi_j(x) \varphi_j^*(y) \varphi_i(y) U(x - y), \end{aligned} \quad (3.2.47)$$

which is nothing else but the Wick theorem for the Slater-determinant state (3.2.45). Its variation leads to a set of nonlinear equations that need to be solved self-consistently:

$$\left(-\frac{1}{2m}\nabla^2 + U + \Sigma\right)\varphi_i = \varepsilon_i\varphi_i, \quad (3.2.48)$$

where

$$[\Sigma\varphi_i](x) = \int dy n(y) U(x-y) \varphi_i(x) - \sum_j \int dy \varphi_j(x) \varphi_j^*(y) \varphi_i(y) U(x-y) \quad (3.2.49)$$

and

$$n(y) = \sum_j |\varphi_j(y)|^2. \quad (3.2.50)$$

Note the resemblance of these formulas to the diagrammatic expression in Fig. 12 [eqs. (3.2.38) and (3.2.39)] for the self-energy Σ . In fact, this correspondence is exact, if we relate the Green's function to the single-particle states

$$G_\omega^c(x, y) = \sum_i \frac{\varphi_i(x) \varphi_i^*(y)}{\omega - (\varepsilon_i - \mu) + i\delta \operatorname{sign} \omega}, \quad (3.2.51)$$

where the sum is taken over all (empty and occupied) states. The equal-time Green's function is then

$$G^c(\Delta t = -0; x, y) = \sum_{i=1}^N \varphi_i(x) \varphi_i^*(y), \quad (3.2.52)$$

with the sum taken over the N occupied states. The Lagrange multipliers ε_i in the variational approach correspond to the single-particle energies in the Hartree-Fock approximation.

In other words, the variational procedure is exactly equivalent to the diagrammatic approximation described in the previous section.

The Hartree-Fock approximation may be used for calculating the electronic structure of solids and molecules. However, its mean-field nature (neglecting correlations between electrons of opposite spins) makes the results not very accurate, and other more efficient approximations (such as density-functional theory) are more commonly used.

Problem Set 7

Problem 7.1 Time-ordered Green's function.

(a) Using the results of Problem 6.1 for the single-particle Green's function, find the *time-ordered* Green's function $G_\omega^c(R)$ of a free Fermi gas in 3D. You may use the relations (3.2.30) and (3.2.31).

(b) By an explicit integration of $G_\omega^c(R)$, check that

$$G^c(t=0, R) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} G_\omega^c(R)$$

coincides with the Green's function (3.1.39).

Problem 7.2 RKKY interaction.

(a) RKKY (Ruderman–Kittel–Kasuya–Yosida) interaction is a mechanism of coupling of localized magnetic moments (nuclear magnetic moments or spins of localized electrons in inner shells) through conduction electrons. The physics of mechanism is as follows: If we have a localized magnetic moment $\mathbf{S}$, it couples locally to electrons via

$$H_{\text{int}} = \alpha \mathbf{S} a_\alpha^+(x) \sigma_{\alpha\beta} a_\beta(x).$$

Without loss of generality, assume that $\mathbf{S} \parallel \mathbf{z}$. Then it is equivalent to the potential $\pm\alpha S$ at the position x for up/down spins respectively. This potential leads to the modulation of density (the actual density, not the density of states!)

$$\delta n_\uparrow(y) = U(x-y) \alpha S, \quad \delta n_\downarrow(y) = -U(x-y) \alpha S$$

with some function $U(x-y)$. If there is another local spin at the position y , this modulation of electronic density leads to the interaction between the two magnetic moments given by

$$E_{\text{RKKY}} = 2\alpha^2 \mathbf{S}_1 \mathbf{S}_2 U(x-y).$$

Our goal is to calculate the function $U(x-y)$. It is a linear response of the density δn at the position y to the potential at the position x . Show that this response function is given by the same diagram in Fig. 9, with the only difference that now we integrate over the time difference at the positions x and y and use the time-ordered Green's function. In the frequency representation, it is given by

$$U(R) = \int \frac{d\omega}{2\pi} [G_\omega^c(R)]^2$$

(where, as usual, we denote $R = |x-y|$). Use what you know from Problems 6.1 and 7.1 to compute this function. You should get

$$U(R) = \frac{1}{16\pi^3} \frac{m}{R^4} [2k_F R \cos(2k_F R) - \sin(2k_F R)] . \quad (3.2.53)$$

If you are interested, you can take a look at the original paper M. A. Rudermann and C. Kittel, Phys. Rev. **96**, 99 (1954).

(b) In the experimental paper S. S. P. Parkin and D. Mauri Phys. Rev. B **44**, 7131 (1991), the authors observe RKKY-type oscillations in magnetic coupling of two $\text{Ni}_{80}\text{Co}_{20}$ layers through a thin layer of Ruthenium. They compare their results to the theoretical prediction $U(R) \propto R^{-p} \sin(2k_F R + \phi)$ with $p = 2$. Explain this power dependence on R .