Lecture 1: The Equilibrium Green Function Method

Mark Jarrell

April 27, 2011

Contents

1 Why Green functions?

We know the microscopic principles which govern the physics of the systems studied by condensed matter physicist, chemists and materials scientists. These systems include all metals, molecules, materials and possibly life itself. In principle all properties of these systems may be determined from the many-particle wave function

$$\Psi\left(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3 \cdots \mathbf{x}_N, t\right) \tag{1}$$

which is the solution to the Schrödinger equation

$$\left\{-\frac{\hbar^2}{2m}\sum_{j=1}^{N}\nabla_j^2 + \sum_{i<j} V(\mathbf{x}_i - \mathbf{x}_j) + \sum_j U(\mathbf{x}_j)\right\}\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{2}$$

where $V(\mathbf{x}_i - \mathbf{x}_j)$ is the Coulomb interaction. In addition, the effects of external fields may be incorporated into the kinetic energy and the external potential U, and we also need to incorporate spin, the parity of the wave function etc. Together, with this formula, these form a rather complete description of the microscopic behavior of materials.

Unfortunately, this does not help us to solve the many-body problem, e.g., composed of a complex molecule and the 10^{21} or so electrons in the leads. The problem is that the complexity of these systems grows exponentially, so that significant approximations are required even to treat the isolated molecule. The problem is even more daunting for non-equilibrium situations or in complex materials where many-body phenomena emerge. The amount of storage required to solve for the wave function grows exponentially with the number of interacting particles.

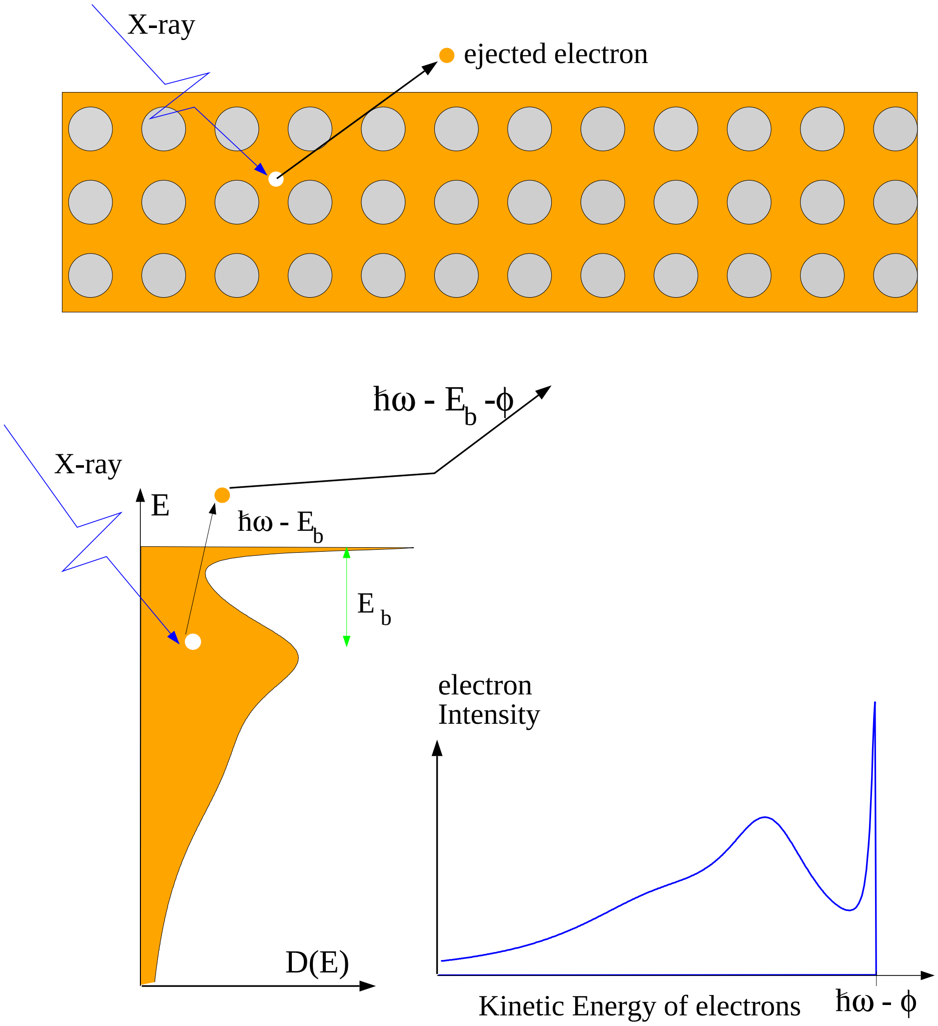

Figure 1: Photoemission measures the single-particle Green function.

On the other hand, experiments tend to measure the elementary excitations of these systems. A good example is photoemission, in which an incident photon causes an electron to be ejected from the system. It measures the angle-resolved density of electronic states, and to a good approximation (in which certain matrix elements are ignored) it is proportional to the imaginary part of the single-particle retarded Green function $G^r(\mathbf{k},\omega)$.

$$I(\mathbf{k},\omega) \propto -\mathrm{Im}G^r(\mathbf{k},\omega) \tag{3}$$

where $G^r(\mathbf{k},\omega)$ is the Fourier transform of

$$G^r(t-t') = -i\theta(t-t')\left\langle\left\{C_k(t), C_k^\dagger(t')\right\}\right\rangle \tag{4}$$

Other examples, include the bulk magnetic susceptibility

$$\chi(T) = \sum_i \int_0^\beta d\tau \, \langle \mathcal{T} S_z(\mathbf{x}_i,\tau) S_z(0,0)\rangle \tag{5}$$

which here we have related to the Matsubara time two-particle spin-spin Green function, inelastic neutron scattering which is described by a two-particle (density-density) phonon Green function, or linear transport which may be described by a two-particle current-current electronic Green function.

Within the Green function approach, it is also formally easy to isolate and treat only the correlated part of the problem, and to integrate out the non-interacting degrees of freedom (they can be folded in to the initial green function of a perturbative or even many non-perturbative approach).

2 Different types of Green functions

There are in fact (at least) two other types of Green functions in addition to the retarded and Matsubara Green functions used in Eqs. 4

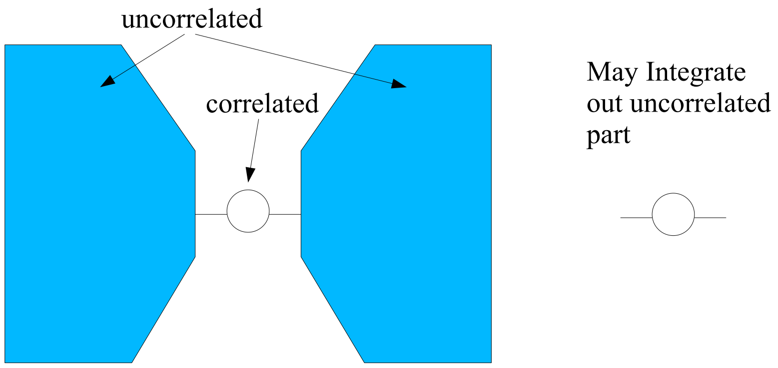

Figure 2: Non-interacting degrees of freedom may be integrated out of the problem within the Green function approach.

and 5. These include the advanced Green function G^a and the time ordered (sometimes called causal) Green function G^c. Later, when we discuss non-equilibrium Green function formalism, we will introduce two additional Green functions.

2.1 Retarded, advanced, time ordered and Matsubara Green functions

For two operators, $\mathcal{A}$ and $\mathcal{B}$, the different Green functions may be defined as

$$G^r(t,t') = -\frac{i}{\hbar}\Theta(t-t')\left\langle[\mathcal{A}(t),\mathcal{B}(t')]_\epsilon\right\rangle \tag{6}$$

$$G^a(t,t') = +\frac{i}{\hbar}\Theta(t'-t)\left\langle[\mathcal{A}(t),\mathcal{B}(t')]_\epsilon\right\rangle \tag{7}$$

$$\begin{aligned} G^c(t,t') &= -\frac{i}{\hbar}\left\langle\mathcal{T}\mathcal{A}(t)\mathcal{B}(t')\right\rangle \qquad (8) \\ &= -\frac{i}{\hbar}\Theta(t-t')\left\langle\mathcal{A}(t)\mathcal{B}(t')\right\rangle + \frac{i\epsilon}{\hbar}\Theta(t'-t)\left\langle\mathcal{B}(t')\mathcal{A}(t)\right\rangle \end{aligned}$$

and

$$\begin{aligned} G^m(\tau,\tau') &= -\frac{1}{\hbar}\left\langle \mathcal{T}\mathcal{A}(-i\tau)\mathcal{B}(-i\tau')\right\rangle \qquad (9) \\ &= -\frac{1}{\hbar}\Theta(\tau-\tau')\left\langle \mathcal{A}(-i\tau)\mathcal{B}(-i\tau')\right\rangle + \frac{\epsilon}{\hbar}\Theta(\tau'-\tau)\left\langle \mathcal{B}(-i\tau')\mathcal{A}(-i\tau)\right\rangle \end{aligned}$$

where $\mathcal{T}$ denotes time ordering so that the later operators move left, and each exchange of Fermionic operators is accompanied by a minus sign. The symbol $\epsilon = +1$ for Fermionic operators and $\epsilon = -1$ for Bosonic operators; likewise $[\cdots]_\epsilon$ is meant to denote a (anti)commutator for (Fermions)Bosons. Note that each Green function has units of inverse $\hbar$ in addition to the units of $\mathcal{A}$ times $\mathcal{B}$. In subsequent sections, we will choose units so that $\hbar = 1$. The time dependence of the operators is determined by the time-independent Hamiltonian H of the system:

$$O(t) = O_H(t) = e^{iHt}Oe^{-iHt} \qquad (10)$$

The bracket denotes a thermal average with the statistical operator $\rho = e^{-\beta H}/Z$. In order to describe a grand-canonical ensemble we have to replace H by $H - \mu N$. This can be accomplished by counting all single-particle energies from the chemical potential μ. We will do that also for the Hamiltonian describing the time dependence.

So what do all of these Green functions mean? In fact, two of the four, G^c and G^a, have no physical meaning at all. As we will see in the section 2.5, G^r has significant physical meaning, as it describes the linear response of the system to an external field (i.e. voltage), and G^m only has physical meaning in the zero τ or zero frequency limits where, as we will show in Sec. 2.2, G^m and G^r are equivalent. In fact, G^c, G^a and G^m are introduced only for calculational convenience. Fortunately, if we find an analytic form for any one of G^c, G^a and G^m, we generally can calculate the others, including G^r.

2.2 The relation between the Green functions

To establish a relationship between these different Green functions, we insert the identity $\sum_n |n><n|$ where $<n|$ are the eigenstates of the full Hamiltonian H. Each of the Green functions defined above is going to contain terms like

$$\langle \mathcal{A}(t)\mathcal{B}(t')\rangle = \frac{1}{Z}\sum_n <n|e^{-\beta H}e^{iHt}\mathcal{A}e^{-iHt}e^{iHt'}\mathcal{B}e^{-iHt'}|n> \tag{11}$$

After inserting an identity, we obtain, for e.g.,

$$G^r(\omega) = \frac{1}{Z}\int_{-\infty}^{\infty} dx \sum_{nm} \frac{e^{-\beta E_m} + \epsilon e^{-\beta E_n}}{\omega - x}\mathcal{A}_{mn}\mathcal{B}_{nm}\delta\left(x - E_n + E_m\right) \tag{12}$$

which we use to define the spectral function A so that

$$G^r(\omega) = \int_{-\infty}^{\infty} dx \frac{A(x)}{\omega + i\eta - x} \tag{13}$$

where $\eta = 0+$ is the positive infinitesimal. Similarly

$$G^a(\omega) = \int_{-\infty}^{\infty} dx \frac{A(x)}{\omega - i\eta - x} \tag{14}$$

so that G^r and G^a are Hermitian conjugates with $A(\omega) = -\frac{1}{\pi}\mathrm{Im}G^r(\omega)$.

Similarly, for the time-ordered Green functions, we may write

$$G^c(\omega) = \int_{-\infty}^{\infty} dx A(x)\left(\frac{P}{\omega - x} - i\pi\left[\frac{1 - \epsilon e^{-\beta x}}{1 + \epsilon e^{-\beta x}}\right]\delta(x - \omega)\right) \tag{15}$$

Finally, for the Matsubara Green function, we write

$$G^m(i\omega_n) = \int_{-\infty}^{\infty} dx \frac{A(x)}{i\omega_n - x} \tag{16}$$

where $\omega_n = 2n\pi T$ ($\omega_n = (2n+1)\pi T$) for Bosonic (Fermionic) G^m since it is a (anti)periodic function of τ as may be easily seen from its definition above.

Thus, if we know any one of G^c, G^a, G^m or G^r, we may calculate the spectral function $A(\omega)$, and from this we may calculate the remaining Green functions.

2.3 Schroedinger, Heisenberg and Interaction Representations

Three different representations of quantum mechanics are typically employed. For $H = H_0 + V$

Representation	States	Operators
Schrödinger	evolve rapidly (H) $i\frac{\partial}{\partial t}\vert\psi_S(t)\rangle = H\vert\psi_S(t) >$	constant
Heisenberg	constant	evolve rapidly (H) $-i\frac{\partial O_H(t)}{\partial t} = [H, O_H(t)]$
Interaction	evolve slowly (V) $i\frac{\partial}{\partial t}\vert\psi_I(t)\rangle = V_I(t)\vert\psi_I(t) >$	evolve rapidly (H_0) $-i\frac{\partial O_I(t)}{\partial t} = [H_0, O_I(t)]$

where

$$|\psi_I(t)\rangle = e^{iH_0 t}|\psi_S(t)\rangle \quad O_I(t) = e^{iH_0 t} O_S e^{-iH_0 t} \tag{17}$$

In both the equilibrium and non-equilibrium Green function approach, we will use the Interaction picture. The time independent solution to H_0 serves as a starting point and we treat the (possibly time dependent V) as a perturbation.

2.4 Time ordering and the S-matrix

Our strategy will be to evolve the system from a time when the perturbation $V = 0$ and we may solve the $H = H_0$ problem exactly, to the "present" when V is finite. We write

$$|\psi_I(t)\rangle = e^{iH_0 t}|\psi_S(t)\rangle = e^{iH_0 t}e^{-iHt}|\psi_S(t=-\infty)\rangle \tag{18}$$

Thus, the time evolution operator in the interaction picture, is

$$U(t) = e^{iH_0 t}e^{-iHt} \tag{19}$$

Note, this is **not** just e^{-iVt} since H_0 and H generally do not commute. To find the form of U, we evaluate

$$i\frac{\partial U}{\partial t} = V_I(t)U \text{ so that } U(t) = U(t_0) - i\int_{t_0}^{t} V_I(t')U(t')dt' \tag{20}$$

To simplify things, let's define the S-matrix $S(t,t') = U(t)U^\dagger(t')$, then

$$S(t,t_0) = 1 - i\int_{t_0}^{t} V_I(t')S(t',t_0)dt' \tag{21}$$

This equation may be solved by iteration.

$$S(t,t_0) = 1 - i\int_{t_0}^{t} V_I(t')dt' + \cdots + (-i)^n \int_{t_0}^{t} V_I(t_1)dt_1 \int_{t_0}^{t_1} V_I(t_2)dt_2 \cdots \int_{t_0}^{t_{n-1}} V_I(t_n)dt_n + \cdots \tag{22}$$

where $t > t_1 > t_2 \cdots t_n > t_0$ in the nth term. In order to write it in a simple analytic form, we divide the nth term in the series by $1/n!$, and consider all of the permutations of the times. Of course, this only make sense if we maintain the ordering of the times, to do this, we introduce the time ordering operator $\mathcal{T}$, then we may write

$$S(t, t_0) = \mathcal{T} \exp\left(-i \int_{t_0}^{t} V_I(t')dt'\right) \tag{23}$$

The S matrix serves as the starting point for Feynman-Dyson perturbation theory. We will see this in Sec.3.1.

2.5 Linear Response

However, the S matrix also can be used to illustrate the physical meaning of G^r. Suppose a system, described by the Hamiltonian H_0 is perturbed by an external field $f(t)$ which couples to the operator $\mathcal{A}$, so that $V(t) = -f(t)\mathcal{A}$. E.g., if $f(t) = B(t)$, a small magnetic field along z, then $\mathcal{A} = S_z$ the system spin operator along z. Let's also multiply the perturbation by $\exp(-\eta|t|)$ so that $H = H_0$ at $t = \pm\infty$. Then, in the Heisenberg representation,

$$\mathcal{A}_H(t) = S^\dagger(t, -\infty)\mathcal{A}_I(t)S(t, -\infty) \tag{24}$$

then, since V is small,

$$S(t, -\infty) = \mathcal{T} \exp\left(-i \int_{-\infty}^{t} V_I(t')dt'\right) \approx 1 - i \int_{-\infty}^{t} V_I(t')dt' \tag{25}$$

so that

$$\mathcal{A}_H(t) = \mathcal{A}_I(t) - i \int_{-\infty}^{t} dt' \left[\mathcal{A}_I(t), \mathcal{A}_I(t')\right] f(t') \tag{26}$$

If we assume $\langle \mathcal{A}_I(t) \rangle = 0$, then

$$\langle \mathcal{A}_H(t) \rangle = \int_{-\infty}^{\infty} dt' G^r(t-t') f(t') \tag{27}$$

where

$$G^r(t-t') = -i\Theta(t-t') \left\langle [\mathcal{A}(t), \mathcal{A}(t')] \right\rangle \tag{28}$$

I.e. $G^r(t-t')$ yields the linear response of the system to a small perturbation $V(t) = -f(t)\mathcal{A}$. Note that the assumption, $H = H_0$ at $t = \pm\infty$ requires that the perturbation turn on so slowly, that the system evolves while always remaining in thermodynamic equilibrium (since equilibrium statistics have been employed).

3 Perturbation Theory

We will employ this same idea (that the problem is unperturbed and hence solvable at times $t = \pm\infty$) to construct the diagrammatic perturbation theory of Bosonic and Fermionic systems. This idea is manifest in the theorem of Gell-Mann and Low.

3.1 The Gell-Mann–Low Theorem

Suppose we wish to evaluate the Green function

$$G(t_1, t_2, \ldots) = \langle \phi \left| \mathcal{T} \mathcal{A}(t_1) \mathcal{B}(t_2) \cdots \mathcal{R}(t_r) \right| \phi \rangle \tag{29}$$

where each of the operators and the states are in the Heisenberg representation, and $H(t) = H_0 + V(t)$ where H_0 is exactly solvable (bilinear in creation and destruction operators) and V is a small perturbation. In the present form, we cannot solve Eq.29, since we don't know the exact the Heisenberg states nor the operators, due to the perturbation V. We need to convert to the Interaction representation, using

$$\mathcal{A}_H(t) = U^\dagger(t)\mathcal{A}_I(t)U(t) \tag{30}$$

We assume, as above, that $|-\infty\rangle = |\phi\rangle$ since the perturbation is zero at $t = -\infty$. If we make these substitutions in Eq. 29, collect all the the U together (which is possible due to time ordering), then we get

$$G(t_1, t_2, \ldots) = \langle +\infty \,|\mathcal{T} S(\infty, -\infty)\mathcal{A}_I(t_1)\mathcal{B}_I(t_2)\cdots\mathcal{R}_I(t_r)| -\infty\rangle \tag{31}$$

If adiabadicity holds, then

$$\langle +\infty| = \frac{\langle +\infty|}{\langle +\infty\,||-\infty\rangle} \tag{32}$$

Using this, and the fact that $S(\infty, -\infty)\,|-\infty\rangle = |+\infty\rangle$, we may write

$$G(t_1, t_2, \ldots) = \frac{\langle -\infty\,|\mathcal{T} S(\infty, -\infty)\mathcal{A}_I(t_1)\mathcal{B}_I(t_2)\cdots\mathcal{R}_I(t_r)| -\infty\rangle}{\langle -\infty\,|\mathcal{T} S(\infty, -\infty)| -\infty\rangle} \tag{33}$$

This is *an extremely important result*, since this is something that can be evaluated quite easily. First, we expand $S(\infty, -\infty)$ in the numerator and denominator. Since each of the operators in S as well as those in the numerator are in the interaction representation (where the operators evolve with H_0) and the states $|-\infty\rangle$ are non-interacting, all of the expectation values involve only non-interacting states and operators which evolve with H_0. Since by construction, H_0 describes a solvable problem, each term in the terms in the expansion may be solved exactly.

3.2 Wick's Theorem

This may be done using Wick's theorem, provided that each of the operators $\mathcal{A}$, $\mathcal{B}, \cdots$ and V may be written as products of Fermionic or Bosonic creation and destruction operators, and that H_0 is bilinear in these operators. For example, when $V \propto S_z = \sum_i S_{zi}$ we can write $S_{zi} = \sum_\sigma \sigma C^\dagger_{i\sigma} C_{i\sigma}$. Then the terms generated in Eq. 33 by expanding the S-matrices, will contain terms like

$$\left\langle -\infty \left| \mathcal{T} C(x_1) C(x_2) \cdots C^\dagger(x'_1) C^\dagger(x'_2) \right| - \infty \right\rangle \tag{34}$$

Only terms with like numbers of creation and destruction operators are finite. The proof of Wicks's theorem is more complicated than can be presented here (it is done in several of the references provided on the web page). However, the result is quite intuitive, the term above may be written as a sum of products of single-particle Green functions representing different permutations of the operators. For Fermionic operators, each particle exchange is accompanied by a minus sign, so

$$-\left\langle -\infty \left| \mathcal{T} C(x_1) C \cdots C^\dagger(x'_1) C^\dagger(x'_2) \right| - \infty \right\rangle = \sum_P (-1)^P G(x_1, P(x'_1) G(x_2, P(x'_2)) \cdots \tag{35}$$

This is an intuitive result, since the Green function describes the evolution of the system. For example, if we have a system with N particles, then the evolution of the N-particle wave function is

$$\Psi(x'_1, x'_2, \cdots, x'_N) = \int dx G(x'_1, x'_2, \cdots, x'_N; x_1, x_2, \cdots, x_N) \Psi(x_1, x_2, \cdots, x_N) \tag{36}$$

As illustrated in the figure below, if these particle are non-interacting like ours, then each should evolve independently from the others allowing for particle exchange.

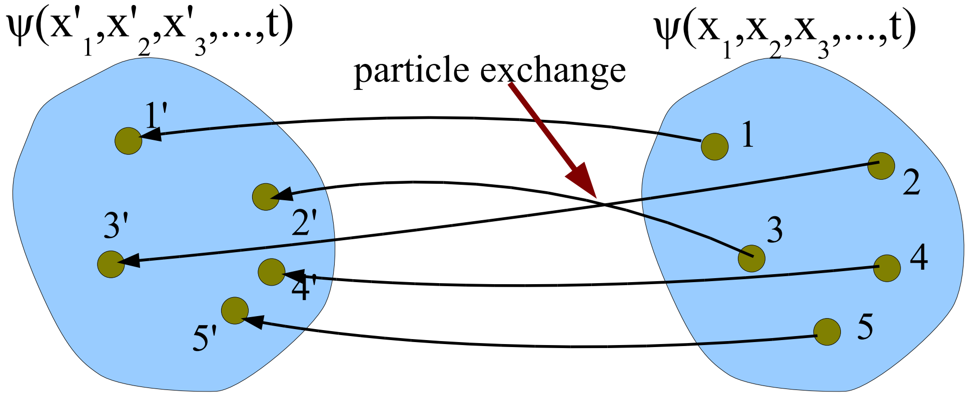

Figure 3: Illustration of evolution of identical non-interaction particles. Since they are identical, all particle exchanges must be considered.

We now have all of the elements necessary to write down a Feynman-Dyson perturbation theory. Each term in the expansion of Eq. 33 may be represented by a Feynman graph. Not all of the graphs will be connected; i.e it may be possible to split a graph into two parts. However, these disconnected parts will be canceled by the denominator of Eq. 33. Thus,

$$\begin{aligned} G(t_1, t_2, \ldots) &= \frac{\langle -\infty \,|\mathcal{T} S(\infty, -\infty)\mathcal{A}_I(t_1)\mathcal{B}_I(t_2)\cdots\mathcal{R}_I(t_r)| -\infty\rangle}{\langle -\infty \,|\mathcal{T} S(\infty, -\infty)| -\infty\rangle} \\ &= \langle -\infty \,|\mathcal{T} S(\infty, -\infty)\mathcal{A}_I(t_1)\mathcal{B}_I(t_2)\cdots\mathcal{R}_I(t_r)| -\infty\rangle_{\text{connected}} \end{aligned} \tag{37}$$

any correlation function (Fermionic or Bosonic) may be constructed by summing all connected graphs. There are also rules (called Feynman rules) for the signs and weighting of the different graphs (see the references on the course web page).

As an example, consider the case of free conduction electrons perturbed by a weak interaction V. If we want to calculate the ARPES spectra, then we need the single-particle Green function, so we let $\mathcal{A} = \psi(x) = \frac{1}{\sqrt{N}} \sum_k C_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}$ and $\mathcal{B} = \psi^\dagger(x)$ where $C_{\mathbf{k}}$ is the destruction operator for the free electron state with wavevector $\mathbf{k}$ we obtain after a Fourier transformation in space

$$G_0^{r,a}(k\omega) = \frac{1}{\omega \pm i\delta - \epsilon_k + \mu} \tag{38}$$

$$A_0(k, \omega) = 2\pi\delta(\omega - \epsilon_k + \mu) \tag{39}$$

as the single-particle Green and spectral function for the unperturbed problem. Here we see that $A_0(\mathbf{k}, \omega)$ contains information about the single-particle excitation spectrum, while the distribution function $f(\omega)$ which appears in the correlation functions describes the thermal occupation of such states.

Figure 4: Graphs for the single-particle Green function and interaction.

In order to solve for the dressed Green function, we need to sum the corresponding Feynman graphs. Typically straight directed lines are used to represent Fermionic single-particle green function and wavy lines to represent the interaction V as shown in Fig. 4.

The first few graphs for the Green function are also shown in Fig. 5.

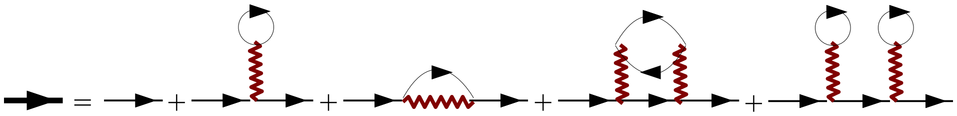

Figure 5: First few graphs for the electronic single-particle Green function.

The last two graphs on the right are second order in V, while the one furthest right is composed of repetitions or products of first order graphs. Such graphs may be generated by simple iteration. To see this, let's divide the graphs into those which cannot be split in two by cutting a singe Green function line (called irreducible graphs) and those which may be cut in two (called reducible). The rigthmost second order graph is reducible while the leftmost is irreducible. The reducible graphs may be generated by collecting all of the irreducible graphs together into the self energy Σ, shown in Fig. 6 (right) and calculating the Green function using the Dyson equation

$$G(\mathbf{k},\omega) = G_0(\mathbf{k},\omega) + G_0(\mathbf{k},\omega)\Sigma(\mathbf{k},\omega)G(\mathbf{k},\omega) \tag{40}$$

which is also illustrated in Fig. 6 (left).

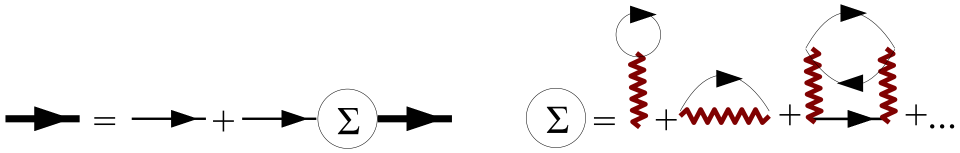

Figure 6: The Dyson equation, relating the full Green function, represented by the thick line, to the bare green function (the thin line) and the self energy Σ. Σ, shown on the right, contains only irreducible graphs.

Copies of these notes, supporting materials and links are available *at http://www.physics.uc.edu/∼jarrell/Green . Much of the material came from standard texts and on-line books like Coleman's, linked on the site.*