Quantum Many Body Theory

Victor Gurarie

Week 5

5 Green's functions of many body systems

When working with many body systems, it is often not convenient to work at a given fixed number of particles. Instead, the chemical potential is fixed, and the "grand canonical" Hamiltonian takes the form

$$\hat{H}_{\mathrm{GC}} = \hat{H} - \mu \sum_k \hat{a}_k^\dagger \hat{a}_k. \tag{5.1}$$

5.1 Heisenberg representation of the operators

In quantum mechanics one can assume that wave functions depend on time, while operators are time independent. Alternatively, one can assume that wave functions do not depend on time and it is operators which depend on time.

The evolution operator (Green's function in time domain) can be used to evolve the wave function in time

$$\Psi(t) = e^{-i\hat{H}t}\Psi. \tag{5.2}$$

The averages of an operator $\hat{A}$ at a time t can be computed using

$$\langle \Psi^* | \, e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t} \, | \Psi \rangle \, . \tag{5.3}$$

We call

$$\hat{A}(t) = e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t} \tag{5.4}$$

an operator in the Heisenberg (time dependent) representation.

It follows that the time derivative of $\hat{A}(t)$ is

$$\frac{\partial \hat{A}}{\partial t} = i[\hat{H}, \hat{A}], \tag{5.5}$$

where the brackets [] stand for the commutator.

Example: suppose we work with the free particle Hamiltonian

$$\hat{H} = \sum_k \frac{k^2}{2m} \hat{a}_k^\dagger \hat{a}_k. \tag{5.6}$$

Then

$$\frac{\partial \hat{a}_k}{\partial t} = -i \frac{k^2}{2m} \hat{a}_k. \tag{5.7}$$

Thus

$$\hat{a}(t) = e^{-i\frac{k^2}{2m}t} \hat{a}(0), \ \hat{a}^\dagger(t) = e^{i\frac{k^2}{2m}t} \hat{a}^\dagger(0) \tag{5.8}$$

Another example. In the coordinate representation the free particle Hamiltonian looks like

$$\hat{H}_0 = \frac{1}{2m}\int dx\; \frac{\partial\hat{\psi}^\dagger}{\partial x}\frac{\partial\hat{\psi}}{\partial x}. \tag{5.9}$$

The field operator $\hat{\psi}(x)$ depends on time in a simple way

$$\frac{\partial\hat{\psi}}{\partial t} = i[\hat{H}_0, \hat{\psi}] = \frac{i}{2m}\frac{\partial^2\hat{\psi}}{dx^2}. \tag{5.10}$$

This looks just like the Schrd̈oinger equation. But it is not. This is an equation for an operator, not the wave function. Moreover, suppose the particles now interact

$$\hat{H} = \frac{1}{2m}\int dx\; \frac{\partial\hat{\psi}^\dagger}{\partial x}\frac{\partial\hat{\psi}}{\partial x} + \frac{1}{2}\int dxdy\; \hat{\psi}^\dagger(y)\hat{\psi}^\dagger(x)U(|x-y|)\hat{\psi}(x)\psi(y). \tag{5.11}$$

The the equation becomes

$$\frac{\partial\hat{\psi}}{\partial t} = i[\hat{H}, \hat{\psi}] = i\left[\frac{1}{2m}\frac{\partial^2\hat{\psi}}{dx^2} - \int dy\; \hat{\psi}^\dagger(y)U(|x-y|)\hat{\psi}(x)\hat{\psi}(y)\right]. \tag{5.12}$$

This is a nonlinear operator equation, which in general is not possible to solve.

An important observation:

$$[\hat{\psi}(x,t), \hat{\psi}^\dagger(y,t)] = \delta(x-y). \tag{5.13}$$

However, if the two operators above where at different times, this would not be correct any more.

5.2 Retarded many body Green's functions

To construct the many body Green's functions, we will, from now on, work exclusively with the "grand canonical" Hamiltonian (5.1). A notation $\hat{H}$ will imply the grand canonical Hamiltonian.

The retarded many body Green's function is defined as follows

$$G^R(x_f, x_i; t_f, t_i) = -i\left\langle \hat{\psi}(x_f,t_f)\hat{\psi}^\dagger(x_i,t_i) - \hat{\psi}^\dagger(x_i,t_i)\hat{\psi}(x_f,t_f)\right\rangle \theta(t_f - t_i). \tag{5.14}$$

Here θ represents the usual θ-function, or $\theta(x) = 1$ is $x > 0$ and $\theta(x) = 0$ if $x < 0$. Brackets $<$ and $>$ represent averaging over the ground state wave function of the system we are studying. This is a natural definition which generalizes the corresponding definition for a one particle system.

Indeed, first of all $G^R = 0$ if $t_f < t_i$. Second,

$$\begin{aligned} \lim_{t_f \to t_i + 0} -i \left\langle \hat{\psi}(x_f, t_f)\hat{\psi}^\dagger(x_i, t_i) - \hat{\psi}^\dagger(x_i, t_i)\hat{\psi}(x_f, t_f) \right\rangle &= \\ -i \left\langle \hat{\psi}(x_f, t_f)\hat{\psi}^\dagger(x_i, t_f) - \hat{\psi}^\dagger(x_i, t_f)\hat{\psi}(x_f, t_f) \right\rangle &= -i\delta(x_f - x_i). \end{aligned} \tag{5.15}$$

Finally, for a system governed by a free Hamiltonian (5.9), (5.10) holds and as a result,

$$i \frac{\partial G^R}{\partial t_f} = \hat{H}_0 G^R. \tag{5.16}$$

Thus this proves that G^R coincides with the Green's function of a single particle defined earlier.

However, if the system is interacting, (5.10) gets replaced by (5.12) and the Green's function no longer satisfies any equation. Thus the definition (5.14) is a natural, yet nontrivial, generalization of the single particle Green's function. The advanced Green's function is defined accordingly,

$$G^A(x_f, x_i; t_f, t_i) = i \left\langle \hat{\psi}(x_f, t_f)\hat{\psi}^\dagger(x_i, t_i) - \hat{\psi}^\dagger(x_i, t_i)\hat{\psi}(x_f, t_f) \right\rangle \theta(t_i - t_f). \tag{5.17}$$

5.3 Time ordered Green's function

Feynman realized that in the many body settings the Green's function which is easiest to calculate is not retarded or advanced, but rather time ordered. It is defined as follows

$$G(x_f, x_i; t_f, t_i) = -i \left\langle T\hat{\psi}(x_f, t_f)\hat{\psi}^\dagger(x_i, t_i) \right\rangle. \tag{5.18}$$

Here the symbol T stands for "time order". It is defined like this

$$T\hat{\psi}(x_f, t_f)\hat{\psi}^\dagger(x_i, t_i) = \hat{\psi}(x_f, t_f)\hat{\psi}^\dagger(x_i, t_i) \text{ if } t_f > t_i, \tag{5.19}$$

$$T\hat{\psi}(x_f, t_f)\hat{\psi}^\dagger(x_i, t_i) = \hat{\psi}^\dagger(x_i, t_i)\hat{\psi}(x_f, t_f) \text{ if } t_i > t_f. \tag{5.20}$$

Note that in vacuum, where the brackets mean a state devoid of any particles, this Green's function coincides with the retarded Green's function. That because it is impossible to annihilate a particle first and create it later, as (5.20) attempts to do.

A very useful decomposition of the time ordered Green's function exists (similar to the expression of the single body Green's function in terms of the eigenstates of the Hamiltonian). To derive it, we rely on the following expression valid in any translationally invariant system.

$$\hat{\psi}(x, t) = e^{i\hat{H}t - i\hat{P}x}\hat{\psi}(0, 0)e^{-i\hat{H}t + i\hat{P}x}. \tag{5.21}$$

$\hat{P}$ is the operator of the overall momentum of all the particles. An arbitrary state is characterized by the energy E_n and the momentum P_n. Then, for $t_f > t_i$, we can write

$$G(x,t) = -i \sum_n \langle 0| \hat{\psi} |n\rangle \langle n| \hat{\psi}^\dagger |0\rangle \, e^{-i(\epsilon_n^+ - \mu)t + iP_n x}, \;\; t > 0 \tag{5.22}$$

where $t = t_f - t_i$, $x = x_f - x_i$. Here we introduced the following notation

$$\epsilon_n^+ = E_n(N+1) - E_0(N). \tag{5.23}$$

This is the energy difference between the ground state with N particles and the excited state with $N+1$ particles. Notice that

$$\epsilon_n^+ \approx E_n(N+1) - E_0(N+1) + \frac{dE_0}{dN} = E_n(N+1) - E_0(N+1) + \mu, \tag{5.24}$$

thus

$$\epsilon_n^+ - \mu > 0. \tag{5.25}$$

For $t < 0$, we write

$$G(x,t) = -i \sum_n \langle 0| \hat{\psi}^\dagger |n\rangle \langle n| \hat{\psi} |0\rangle \, e^{-i(\epsilon_n^- - \mu)t - iP_n x}, \;\; t < 0. \tag{5.26}$$

Here

$$\epsilon_n^- = E_0(N) - E_n(N-1) = E_0(N-1) - E_n(N-1) + \mu < \mu. \tag{5.27}$$

A Fourier transform with resect to t gives

$$G(x,E) = \sum_n \left[\frac{\left|\langle n| \hat{\psi}^\dagger |0\rangle\right|^2 e^{iP_n x}}{E + i0 - (\epsilon_n^+ - \mu)} - \frac{\left|\langle 0| \hat{\psi}^\dagger |n\rangle\right|^2 e^{-iP_n x}}{E - i0 - (\epsilon_n^- - \mu)} \right]. \tag{5.28}$$

Although this decomposition makes it appear as if the Green's functions have poles if E approaches $\epsilon_n^+ - \mu$ or $\epsilon_n^- - \mu$, in practice summation over n smears these poles and turns them into cuts, just as in the one-particle Green's function case. However, if there are special discrete states such that there are no states nearby at at this energy, then the Green's function will have a pole. We say that there exists a well defined quasiparticle at this energy. Since in the Fourier space the Green's function looks like

$$G(p,E) = (2\pi)^d \sum_n \left[\frac{\left|\langle n| \hat{\psi}^\dagger |0\rangle\right|^2 \delta(P_n - p)}{E + i0 - (\epsilon_n^+ - \mu)} - \frac{\left|\langle 0| \hat{\psi}^\dagger |n\rangle\right|^2 \delta(P_n + p)}{E - i0 - (\epsilon_n^- - \mu)} \right]. \tag{5.29}$$

the equation for the quasiparticles is

$$G^{-1}(p,E) = 0. \tag{5.30}$$

5.4 Green's function of a free Bose gas

Free Bose gas is somewhat pathological: in the ground state all the particles sit in the ground state, forming a Bose condensate. The Green's function studies particles which are not in the ground state, thus it coincides with the the single particle Green's function

$$G_0(p,E) = \frac{1}{E - \frac{p^2}{2m} + \mu + i0}. \tag{5.31}$$

6 Fermions

6.1 Fermion creation and annihilation operators

Fermion creation and annihilation operators are similar to the ones for bosons. However, no two fermions can occupy one state, thus

$$\left(\hat{a}^\dagger\right)^2 = 0, \hat{a}^2 = 0. \tag{6.1}$$

Exchanging two fermions changes sign of their wave function, thus

$$\hat{a}_k^\dagger \hat{a}_q + \hat{a}_q \hat{a}_k^\dagger = \delta_{kq}, \;\; \hat{a}_k \hat{a}_q + \hat{a}_q \hat{a}_k = 0. \tag{6.2}$$

Similarly,

$$\hat{\psi}^\dagger(x)\hat{\psi}(x) + \hat{\psi}(x)\hat{\psi}^\dagger(x) = \delta(x-y). \tag{6.3}$$

$\hat{a}^\dagger \hat{a}$ still counts the total number of fermions, and the free fermion Hamiltonian is still

$$\hat{H} = \sum_k \frac{k^2}{2m} \hat{a}_k^\dagger \hat{a}_k. \tag{6.4}$$

6.2 Fermion Green's functions

Fermion retarded Green's function is defined by

$$G^R(x_f, x_i; t_f, t_i) = -i\left\langle \hat{\psi}(x_f,t_f)\hat{\psi}^\dagger(x_i,t_i) + \hat{\psi}^\dagger(x_i,t_i)\hat{\psi}(x_f,t_f)\right\rangle \theta(t_f - t_i). \tag{6.5}$$

The only difference with the case of bosons (5.14) is the plus sign.

However, more interesting is the fermion time ordered Green's function

$$G(x_f, x_i; t_f, t_i) = -i\left\langle T\hat{\psi}(x_f,t_f)\hat{\psi}^\dagger(x_i,t_i)\right\rangle. \tag{6.6}$$

defined in the same way as in the case of bosons. However, time ordered symbol is defined taking into account the fermionic nature

$$T\hat{\psi}(x_f,t_f)\hat{\psi}^\dagger(x_i,t_i) = \hat{\psi}(x_f,t_f)\hat{\psi}^\dagger(x_i,t_i) \text{ if } t_f > t_i, \tag{6.7}$$

$$T\hat{\psi}(x_f,t_f)\hat{\psi}^\dagger(x_i,t_i) = -\hat{\psi}^\dagger(x_i,t_i)\hat{\psi}(x_f,t_f) \text{ if } t_i > t_f. \tag{6.8}$$

Note the minus sign when compared to (5.20).

Let's determine the Green's function of a free fermi gas. In a ground state of such a gas, all states with momentum $p \le p_f$ are filled, while those of $p > p_f$ are empty.

$$G(p,t) = -ie^{-i\left(\frac{p^2}{2m}-\mu\right)t}\theta(p > p_f), \; t > 0. \tag{6.9}$$

$$G(p,t) = ie^{-i\left(\frac{p^2}{2m}-\mu\right)t}\theta(p < p_f), \; t < 0. \tag{6.10}$$

Fourier transform of that gives

$$G(p,E) = \frac{1}{E - \frac{p^2}{2m} + \mu + i0 \,\mathrm{sign}\, E}. \tag{6.11}$$

This means that for $p^2/(2m) > \mu$, this function is retarded. For $p^2/(2m) < \mu$ the function is advanced. This is because it describes the propagation of holes, in addition to particles.

Finally, we can derive a decomposition for the Green's function in general (interacting) case similar to (5.28). It looks like

$$G(x,E) = \sum_n \left[\frac{\left|\langle n|\,\hat{\psi}^\dagger\,|0\rangle\right|^2 e^{iP_n x}}{E + i0 - (\epsilon_n^+ - \mu)} + \frac{\left|\langle 0|\,\hat{\psi}^\dagger\,|n\rangle\right|^2 e^{-iP_n x}}{E - i0 - (\epsilon_n^- - \mu)} \right]. \tag{6.12}$$

Notice the *plus* sign as the only difference with the bosonic case. It is due to the minus sign in time ordering operation.

Finally, suppose we calculate the Green's function. What do we do next? We can look for its poles to determine the dispersion of the quasiparticles. Or we could find the density of particles

$$\rho = \pm\frac{i}{V}\lim_{t_f \to t_i - 0}\int dx\; G(x,x;t_f,t_i) \equiv \frac{1}{V}\int dx\,\left\langle \hat{\psi}^\dagger(x,t_i)\hat{\psi}(x,t_i)\right\rangle \tag{6.13}$$

(the upper sign is for the bosons, the lower sign for the fermions). Since G depends on μ, this gives us μ as a function of N. Inverting this relation, we find μ as a function of N, which in turn gives us the ground state energy if we solve $dE_0/dN = \mu$.