561 F 2005 Homework 3
assigned Tuesday, September 22, 2005; Due Thursday, October 6, 2005

1. One-electron Greens Function

The time-ordered one-electron Greens function in the Fourier space representation is given by

$$G(k,t;k',t') = -i\langle T[c_k(t)c_{k'}^+(t')]\rangle \tag{1}$$

The Greens function in real space can be written by transforming to operators that create or annihilate particles at points in space

$$\psi(x,t) = \sum_k c_k(t)e^{ikx} \quad and \quad \psi^+(x,t) = \sum_k c_k^+(t)e^{-ikx} \tag{2}$$

and we can define

$$G(x,t;x',t') = -i\langle T[\psi(x,t)\psi^+(x',t')]\rangle \tag{3}$$

a. For a homogeneous system, show that G is a function only of the differences,

$$G(x,t;x',t') = G(x-x',t-t'). \tag{4}$$

b. Show that for a non-interacting homogeneous system, G^0 satisfies the equation for the time-dependent Schrodinger equation:

$$\left(i\frac{d}{dt} + \frac{1}{2m}\frac{d^2}{dx^2}\right)G^0(x,t) = \delta(x)\delta(t), \tag{5}$$

which shows $G^0(x,t)$ is indeed a Greens function for the time-dependent Schrodinger Eq.

c. For the case of a homogeneous 1-dimensional system with no electrons in the vacuum state, show that the Greens Function is a Gaussian in imaginary time,

$$G^0(x,t) = -i\int_{-\infty}^{\infty} dk e^{-i(kx-\frac{k^2}{2m}t)} = e^{-i\frac{3\pi}{4}}\left(\frac{2\pi m}{t}\right)^{\frac{1}{2}} e^{i\frac{mx^2}{2t}} \tag{6}$$

(This is the equivalent of a Gaussian in space for imaginary time, i.e., it is equivalent to the well-known fact that at finite temperature the free-particle Green's function has a Gauussian distribution that is related to the de Broglie wavelength.)

2. The meaning of time-ordered exponential operator expressions

(This is the same as Problem 2-1 of Mahan.) Show explicitly that

$$\frac{1}{3!}\int_0^t dt_1\int_0^t dt_2\int_0^t dt_3 T[\widehat{V}(t_1)\widehat{V}(t_2)\widehat{V}(t_3)] = \int_0^t dt_1\int_0^{t_1} dt_2\int_0^{t_2} dt_3 \widehat{V}(t_1)\widehat{V}(t_2)\widehat{V}(t_3) \tag{7}$$

3. The equal-time one-electron Green's function in the non-interacting case

Show that the time-ordered one-electron Green's function transformed to a function of energy satisfies

$$-i\int_{-\infty}^{\infty} dE G^0(p,E) = n_F(\epsilon_p), \tag{8}$$

where n_F is the Fermi function at $T=0$. This can be done by contour integration, and it requires care that the integral is defined to converge in the proper half-plane.

4. Hartree-Fock Self-energy

a. Draw the Feynman diagrams for the proper self-energy $\Sigma^{\star}_{HF}(k,E)$ in the Hartree-Fock approximation for the homogeneous electron gas. Show the equations in both time and energy forms with the proper rules applied to the conservation laws at the vertices.

b. Give the corresponding expression for $\Sigma^{\star}_{HF}(k,E)$ in terms of an integral over the Green's function $G^0(k,E)$ for non-interacting electrons. Using the expression form the previous problem, show that this leads to the expression for the Hartree-Fock eigenvalues that we have derived before.

5. Properties of the self energy

In this problem you are asked to describe the form of the Greens function $G_\lambda(E)$ near a resonance $E = \epsilon_\lambda$ where there is some broadening due to many-body effects. Use the general expression for the Green's function in terms of the proper self-energy

$$G_\lambda(E) = \frac{1}{E - \epsilon^0_\lambda - \Sigma^{\star}_\lambda(E)} \tag{9}$$

and expand the self-energy $\Sigma^{\star}_\lambda(E)$ in powers of the energy difference $E - \epsilon_\lambda$. From this show that near $E = \epsilon_\lambda$ the Greens function is approximated by

$$G_\lambda(E) = \frac{Z_\lambda}{E - \epsilon_\lambda - i\gamma_\lambda}, \tag{10}$$

where

$$\epsilon_\lambda = \epsilon^0_\lambda + Re\Sigma^{\star}_\lambda(E = \epsilon_\lambda), \tag{11}$$

$$Z_\lambda = \left[1 - \frac{d\ Re\Sigma^{\star}_\lambda(E)}{dE}\right]^{-1}_{E=\epsilon_\lambda}, \tag{12}$$

and

$$\gamma_\lambda = Z_\lambda Im\Sigma^{\star}_\lambda(E = \epsilon_\lambda) \tag{13}$$

Note that solution of this problem requires only simple algebraic manipulation of the terms. It does NOT require and knowledge of the details of the self-energy.

6. Properties of the self energy - continued

Show that the proper self-energy is itself a complex function of energy that has the same form as G (retarded, advanced, time-ordered). To answer this question, it is sufficient to show that the sign of $Im\Sigma^{\star}_\lambda(E)$ is the same as the sign of $ImG_\lambda(E)$, since it is the signs of the imaginary parts that distinguishes the different (retarded, advanced, and time-ordered functions. This may be shown either algebraically from Eq. 9 or from the original definition definition of the proper self-energy.

Extra suggested problem - DO NOT TURN IN.

Pines Problem 3-5. This very similar to what we have done in class. The purpose of this exercise is to show that the general definitions of response functions we have given in class are equivalent to appropriate formulas in Pines. In particular, Pines defines a "propagating response function" Kp. From the definition given and from the signs of the infinitesimal imaginary energies, you should be able to deduce the relation of this function to a time ordered Green's function.