PHZ 7428 Fall 2004 – Homework 1

Due by 4:05 p.m. on Friday, October 22.

Answer all questions. Please write neatly and include your name on the front page of your answers. You must also clearly identify all your collaborators on this assignment. To gain maximum credit you should explain your reasoning and show all working.

1. *Spectral density.* A finite system of identical fermions is described by the Hamiltonian

$$\hat{H} = \sum_k \epsilon_k c_k^\dagger c_k + \sum_{k,k'} V_{k,k'} c_k^\dagger c_{k'},$$

where c_k annihilates a particle in single-particle state $|\phi_k\rangle$, with $\langle\phi_k|\phi_{k'}\rangle = \delta_{k,k'}$. (The label k is used to represent all good quantum numbers of the single-particle states. You should not assume that k is necessarily a wave vector or that $|\phi_k\rangle$ is a momentum eigenket.) This is an example of a quadratic Hamiltonian: each term in $\hat{H}$ is the product of one creation and one annihilation operator. For any such Hamiltonian, there exists a unitary transformation $\hat{U}$ such that the operators $d_q = \sum_k U_{q,k} c_k$ diagonalize the Hamiltonian, i.e., $\hat{H} = \sum_q \varepsilon_q d_q^\dagger d_q$.

Suppose that this system is in thermal and chemical equilibrium with a reservoir of temperature T and chemical potential μ. Working in the Lehmann representation, calculate the single-particle spectral density $A(k,\omega) = -\pi^{-1}\mathrm{Im}\, G^R(k,\omega)$, where $G^R(k,\omega)$ is the temporal Fourier transform of

$$G^R(k, t-t') = -i\theta(t-t') \left\langle \{c_k(t), c_k^\dagger(t')\} \right\rangle.$$

Show that $A(k,\omega)$ is independent of temperature. (This is generally not the case for an interacting system described by a nonquadratic Hamiltonian.)

2. *Real-space retarded Green's functions in three dimensions.* The retarded single-particle Green's function for free fermions is

$$G^{(0)}(\mathbf{k}, \omega + i\eta) = \frac{1}{\omega - \omega_{\mathbf{k}} + i\eta},$$

where $\hbar\omega_{\mathbf{k}} = \hbar^2|\mathbf{k}|^2/2m - \mu$, and $\mu \approx \epsilon_F = \hbar^2 k_F^2/2m$ at low temperatures.

For a three-dimensional system, it is a standard exercise in contour integration (e.g., see Merzbacher 3rd edition pp. 291–293, Sakurai revised edition pp. 381–382, or Shankar 2nd edition pp. 541–543) to show that for $h\omega \geq -\epsilon_F$, the corresponding real-space Green's function is

$$G^{(0)}(\mathbf{r}-\mathbf{r}', \omega + i\eta) = -\frac{m}{h|\mathbf{r}-\mathbf{r}'|} \exp\left(i\sqrt{k_F^2 + 2m\omega/\hbar}\, |\mathbf{r}-\mathbf{r}'| \right).$$

You should familiarize yourself with this calculation, because you will have to reproduce it with suitable modifications in parts (a)–(c) below.

(a) Find the form of $G^{(0)}(\mathbf{r}-\mathbf{r}', \omega + i\eta)$ for $\hbar\omega < -\epsilon_F$.

(b) Consider scattering of noninteracting fermions from the zero-range impurity potential $V_i(\mathbf{r}) = V_0 a^3 \delta^3(\mathbf{r})$. Working in the Born limit and ignoring the real-part of the self-energy, the disorder-averaged retarded Green's function is

$$\bar{G}(\mathbf{k}, \omega + i\eta) = \frac{1}{\omega - \omega_{\mathbf{k}} + i/2\tau(\omega) + i\eta},$$

where $\hbar\tau^{-1}(\omega) = 2\pi n_i V_0^2 a^6 N(\hbar\omega) \geq 0$. Here n_i is the impurity concentration and $N(\epsilon - \epsilon_F)$ is the single-particle density of states per unit volume at energy ϵ. The $i\eta$ in the denominator is needed only when $\tau^{-1}(\omega) = 0$.

Show that the real-space version of this Green's function can be written

$$\bar{G}(\mathbf{r}-\mathbf{r}', \omega + i\eta) = -\frac{m}{h|\mathbf{r}-\mathbf{r}'|} \exp(ik_+|\mathbf{r}-\mathbf{r}'|),$$

where k_+ is the location in the upper half of the complex-$|\mathbf{k}|$ plane of the pole in $\bar{G}(\mathbf{k}, \omega + i\eta)$.

(c) Show that for $\hbar/2\tau \ll \epsilon_F$ and $\hbar|\omega| \ll \epsilon_F$,

$$\bar{G}(\mathbf{r}-\mathbf{r}', \omega + i\eta) = G^{(0)}(\mathbf{r}-\mathbf{r}', \omega + i\eta) e^{-|\mathbf{r}-\mathbf{r}'|/2l(\omega)},$$

and provide an expression for the mean free path $l(\omega)$.

(d) It is a common approximation to linearize the free-electron dispersion about the Fermi level, i.e., to set

$$\omega_{\mathbf{k}} = v_F(|\mathbf{k}| - k_F),$$

where $v_F = \hbar k_F/m$ is the Fermi velocity.

Using this approximation, repeat the calculation of $\bar{G}(\mathbf{r}-\mathbf{r}', \omega+i\eta)$, and compare the result with that obtained above using the full dispersion.

3. *Real-space Matsubara Green's functions in one dimension.* Consider once again scattering of noninteracting electrons by the zero-range impurity potential from question 2. Ignoring the real-part of the self-energy, the disorder-averaged Matsubara Green's function is approximately

$$\bar{G}(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n - \omega_{\mathbf{k}} + i\,\mathrm{sgn}\omega_n/2\tau}, \tag{1}$$

where τ is the scattering time for electrons near the Fermi surface.

(a) Show using contour integration that in one dimension, Eq. (1) implies the real-space Matsubara Green's function can be written

$$\bar{G}(x - x', i\omega_n) = -i\frac{m}{\hbar k_+} \exp(ik_+|x - x'|),$$

where k_+ is the location in the upper half of the complex-k plane of the pole in $\bar{G}(k, i\omega_n)$.

(b) In describing one-dimensional systems, it is again common practice to linearize the free-electron dispersion about the Fermi energy. Since the one-dimensional "Fermi surface" consists of just two points, we can write

$$\omega_k = \begin{cases} v_F(k - k_F) & \text{for } k > 0, \\ v_F(-k - k_F) & \text{for } k < 0. \end{cases}$$

The Fourier transformation of $\bar{G}(x - x', i\omega_n)$ is simplified if each of the two branches of the linearized dispersion is extended from a half line ($0 < k < \infty$ or $-\infty < k < 0$) to a full line ($-\infty < k < \infty$). The price for this simplification is the creation of unphysical free-electron states extending to arbitrarily large negative energies.

Use the extended linearized dispersion to calculate $\bar{G}(x - x', i\omega_n)$. Determine the range of ω_n over which this result provides a good approximation to the exact result described in part (a).

(c) Show that the temporal Fourier transform of your result from (b) yields

$$\bar{G}(x, \tau) = \frac{1}{\pi l_T} \operatorname{Im} \{\exp(ik_F x) \operatorname{cosech} [(x + iv_F\tau)/l_T]\} \exp(-|x|/2l), \qquad (2)$$

where $l_T = \hbar v_F/(\pi k_B T)$ is a *thermal length* (not to be confused with the mean free path l). Over what range of x and τ do you expect this result to be valid?

(d) Use Eq. (2) to calculate the disorder-averaged electron number density $n(x)$. Do the impurities affect the number density (on average)?

4. *Electron density near an impenetrable barrier.* Consider a noninteracting one-dimensional Fermi gas confined by an impenetrable barrier to the half-line $x > 0$. For electrons free to move on the entire line, we can write the field operator

$$\hat{\psi}(x) = \int_{-\infty}^{\infty} dk\, e^{ikx}\, c_k,$$

but in the presence of the barrier we must choose one-particle basis functions that vanish at $x = 0$, i.e.,

$$\hat{\psi}_{\text{half}}(x) = \sqrt{2} \int_{-\infty}^{\infty} dk\, \sin(kx)\, c_k.$$

(The factor of $\sqrt{2}$ is chosen to ensure that the average number density is the same in the two sets of basis states.)

(a) Based on the above analysis, show that the unperturbed single-particle Matsubara Green's function on the half-line is

$$\begin{aligned} G^{(0)}_{\text{half}}(x, x', \tau) \;=\; & \frac{1}{2} \left[G^{(0)}(x, x', \tau) - G^{(0)}(x, -x', \tau) \right. \\ & \left. - G^{(0)}(-x, x', \tau) + G^{(0)}(-x, -x', \tau) \right], \end{aligned}$$

where $G^{(0)}(x, x', \tau)$ is the corresponding Green's function on the full line.

(b) Prove that $G^{(0)}(x, x', \tau) = G^{(0)}(|x - x'|, \tau)$, and hence that

$$G^{(0)}_{\text{half}}(x, x', \tau) = G^{(0)}(x - x', \tau) - G^{(0)}(x + x', \tau). \tag{3}$$

Note that $G^{(0)}_{\text{half}}(x, x', \tau) \neq G^{(0)}_{\text{half}}(x - x', \tau)$, which should not be surprising given that the barrier breaks translational invariance.

(c) Combine Eq. (3) with the zero-scattering limit of Eq. (2) to obtain the electron number density $n(x)$ in the presence of the barrier. You should find that $n(x)$ exhibits *Friedel oscillations* at wavevector $2k_F$, modulated by an exponential decay with increasing distance from the barrier. Analyze separately the behavior in the limits (i) $x \to 0$ and (ii) $T \to 0$.