Homework #3 — Phys625 — Spring 2002
Deadline: Thursday, February 21, 2002.
Turn in homework in the class or put it in the box on the door of Phys 2314 by 10 a.m.

Victor Yakovenko, Associate Professor
Office: Physics 2314
Phone: (301)-405-6151
E-mail: yakovenk@physics.umd.edu
Web page: http://www2.physics.umd.edu/~yakovenk/teaching/phys625.spring2002

Do not forget to write your name and the homework number!
Equation numbers with the period, like (3.25), refer to the equations of the textbook.
Equation numbers without period, like (5), refer to the equations of this homework.

Green's Functions of Noninteracting Particles (§§7-11)

In this homework, we consider noninteracting particles characterized by a Hamiltonian $\hat{H}$, which has a complete set of one-particle energy eigenfunctions $\psi_n(\mathbf{r})$ with the eigenvalues ε_n: $\hat{H}\psi_n(\mathbf{r}) = \varepsilon_n\psi_n(\mathbf{r})$.

1. **[4 points]** *Complete basis*

Starting from the definition of Green's function (7.10) and the expansion $\hat{\psi}(\mathbf{r},t) = \sum_n \psi_n(\mathbf{r})e^{-i(\varepsilon_n-\mu)t}\hat{a}_n$, perform the Fourier transform in time and derive the following expression for Green's function:

$$G(\omega,\mathbf{r}_1,\mathbf{r}_2) = \sum_n \frac{\psi_n(\mathbf{r}_1)\,\psi_n^*(\mathbf{r}_2)}{\omega-\varepsilon_n+\mu+i0\,\mathrm{sgn}(\varepsilon_n-\mu)}, \tag{1}$$

where μ is the chemical potential.

Check that function (1) satisfies the equation $(\omega-\hat{H}+\mu)\,G(\omega,\mathbf{r}_1,\mathbf{r}_2) = \delta(\mathbf{r}_1-\mathbf{r}_2)$. Thus, $G = (\omega-\hat{H}+\mu+i0\,\mathrm{sgn}\,\omega)^{-1}$.

2. **[8 points]** *Green's functions of fermions in $D = 1$ and 3*

Using Eq. (1) in the basis of plane waves with momenta $\mathbf{p}$ and performing integration over $\mathbf{p}$, calculate Green's function $G(\omega,\mathbf{r}_1-\mathbf{r}_2)$ of an ideal Fermi gas in the dimensions $D = 1$ and 3. In each case, do the calculations for the parabolic dispersion $\varepsilon(p) = p^2/2m$ and for the approximate dispersion $\varepsilon(p) = v_F(p-p_F)$, which is valid near the Fermi surface, and compare the results. Describe the wave vector of Green's function oscillations.

3. *Density oscillations in 1D*

Consider 1D electron gas occupying semi-infinite space $x > 0$ with impenetrable boundary at $x = 0$. The energy dispersion is $\varepsilon(p) = p^2/2m$.

(a) **[4 points]** Calculate Green's function $G(\omega,x_1,x_2)$. To satisfy the vanishing boundary condition at $x = 0$, you can use the basis functions $\sin(px)$ in Eq. (1) or the method of images.

(b) **[4 points]** Using the formula

$$n(x) = -2i\int G(\omega,x,x)\,e^{-i0\,\omega}\,\frac{d\omega}{2\pi}, \tag{2}$$

calculate electron density $n(x)$. Compare the period of oscillation in x (the so-called Friedel oscillations) with the average distance between electrons.

Hint: You may either integrate $G(\omega,x,x)$ found in Part 3a over ω, or integrate Eq. (1) over ω first and then over p.

4. *Bound state in 1D*

(a) **[4 points]** Now let us add a static potential $U(\mathbf{r})$, so that the Hamiltonian of the system becomes $\hat{H} = \hat{H}_0 + U(\mathbf{r})$. Show that Green's function satisfies the integral equation

$$G(\omega,\mathbf{r}_1,\mathbf{r}_2) = G_0(\omega,\mathbf{r}_1-\mathbf{r}_2) + \int d^3\mathbf{r}'\,G_0(\omega,\mathbf{r}_1-\mathbf{r}')\,U(\mathbf{r}')\,G(\omega,\mathbf{r}',\mathbf{r}_2), \tag{3}$$

where G_0 is the unperturbed Green's function for $U = 0$.

Hint: Use the equation $(\omega - \hat{H} + \mu)\, G(\omega, \mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2)$.

(b) **[6 points]** Let us apply Eq. (3) to the 1D case with the potential $U(x) = -\gamma\delta(x)$, where $\gamma > 0$. Using this equation, determine the energy ε_0 and the wave $\psi_0(x)$ of the bound state. (For simplicity, set $\mu = 0$.)

Hint: When $\omega \to \varepsilon_0$, the term $n = 0$ in Eq. (1) diverges, whereas the other terms can be neglected, thus $G(\omega, x_1, x_2) \approx \psi_0(x_1)\psi_0^*(x_2)/(\omega - \varepsilon_0)$. The unperturbed Green's function G_0 is finite at $\omega \to \varepsilon_0 < 0$, so the first term in the r.h.s. of Eq. (3) can be also neglected. Thus Eq. (3) becomes (derive it!)

$$\psi_0(x) = -G_0(\varepsilon_0, x)\, \gamma\, \psi_0(0). \tag{4}$$

Setting $x = 0$ in Eq. (4) gives an equation for $\varepsilon_0 < 0$, then Eq. (4) gives $\psi_0(x)$.

5. *Friedel oscillations and RKKY*

(a) **[8 points]** Let us treat the potential $U(\mathbf{r})$ in Eq. (3) as a small perturbation. It gives the following corrections to Green's function δG and to electron density δn:

$$\delta G(\omega, \mathbf{r}_1, \mathbf{r}_2) = \int d^3\mathbf{r}'\, G_0(\omega, \mathbf{r}_1 - \mathbf{r}')\, U(\mathbf{r}')\, G_0(\omega, \mathbf{r}' - \mathbf{r}_2), \tag{5}$$

$$\delta n(\mathbf{r}) = -2i \int \frac{d\omega}{2\pi}\, e^{-i0\,\omega} \int d^3\mathbf{r}'\, G_0^2(\omega, \mathbf{r} - \mathbf{r}')\, U(\mathbf{r}'). \tag{6}$$

For a point-like perturbation (an impurity), $U(\mathbf{r}) = \gamma\delta(\mathbf{r})$. In this case, Eq. (6) gives

$$\delta n(\mathbf{r}) = -2i\gamma \int \frac{d\omega}{2\pi}\, e^{-i0\,\omega}\, G_0^2(\omega, \mathbf{r}). \tag{7}$$

Substituting Green's functions found in Part 2 into Eq. (7), calculate $\delta n(\mathbf{r})$ for $D = 3$ and 1 using both the parabolic dispersion $\varepsilon(p) = p^2/2m$ and for the approximate dispersion $\varepsilon(p) = v_F(p - p_F)$. Comment on the Friedel oscillations and the behavior of $\delta n(\mathbf{r})$ at $\mathbf{r} \to 0$ and ∞.

(b) **[2 points]** Suppose there is a magnetic impurity at $\mathbf{r} = 0$, which has exchange interaction with electron gas:

$$\hat{H}_{el-S} = J\, \mathbf{S} \cdot \hat{\mathbf{s}}(0), \tag{8}$$

where $\mathbf{S}$ is the spin of the impurity, and $\hat{\mathbf{s}}(\mathbf{r})$ is the spin operator of electrons, which is taken at the point $\mathbf{r} = 0$. Selecting the spin quantization axis along $\mathbf{S}$, the electron spin operator can be written as $\hat{s}_z(\mathbf{r}) = \hat{\psi}_\uparrow^+(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r}) - \hat{\psi}_\downarrow^+(\mathbf{r})\hat{\psi}_\downarrow(\mathbf{r})$.

Calculate the average spin density $s_z(\mathbf{r}) = \langle \hat{s}_z(\mathbf{r}) \rangle$ at the distance $\mathbf{r}$ from the impurity. You don't need to do any new calculations; just use the results of Part 5a.

(c) **[2 points]** Suppose there are two magnetic impurities located at $\mathbf{r}_1$ and $\mathbf{r}_2$, which do not interact between themselves directly, but have exchange interaction (8) with electrons:

$$\hat{H}_{el-S} = J\, \mathbf{S}_1 \cdot \hat{\mathbf{s}}(\mathbf{r}_1) + J\, \mathbf{S}_2 \cdot \hat{\mathbf{s}}(\mathbf{r}_2). \tag{9}$$

Calculate how the effective interaction $f(\mathbf{r}_1 - \mathbf{r}_2)$ between the two impurity spins via exchange with the electron gas depends on $|\mathbf{r}_1 - \mathbf{r}_2|$:

$$\hat{H}_{eff} = f(\mathbf{r}_1 - \mathbf{r}_2)\, \mathbf{S}_1 \cdot \mathbf{S}_2. \tag{10}$$

You don't need to do any new calculations; just use the results of Part 5b. Eq. (10) is called the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction.