

Condensed Matter Theory II: Many-Body Theory (TKM II) SoSe 2023

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Homework assignment 1
Deadline: 28 April 2023

1. Real-space Green's functions

(5 + 5 = 10 points)

Starting from the momentum-space retarded Green's function

$$G^R(\mathbf{k}, E) = \frac{1}{E - \frac{\hbar^2}{2m}\mathbf{k}^2 + i\delta}, \quad (1)$$

where $\mathbf{k}$ is a d -dimensional momentum, calculate the real-space retarded Green's function $G^R(\mathbf{r} - \mathbf{r}', E)$. *Hint: Integrals can usually be solved using contour integration, as practiced on sheet 0.*

(a) in one dimension, $d = 1$

Solution: The Fourier transformation convention from the lecture is

$$G^R(\mathbf{r}, E) = \int \frac{d^d k}{(2\pi)^d} \frac{\exp(i\mathbf{k}\mathbf{r})}{E - \frac{k^2}{2m} + i\delta}. \quad (2)$$

In one dimension, we have

$$G^R(r, E) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\exp(ikr)}{E - \frac{k^2}{2m} + i\delta} \quad (3)$$

$$= \left[\theta(r) \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\exp(ik|r|)}{E - \frac{k^2}{2m} + i\delta} + \theta(-r) \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\exp(-ik|r|)}{E - \frac{k^2}{2m} + i\delta} \right]. \quad (4)$$

We can now switch to contour integrals, closing the first contour upwards, the second contour downwards. The arcs vanish, as we can easily see by invoking **Jordan's lemma**. The integrand has two first order poles in the complex plane at the roots of the denominator:

$$E - \frac{k^2}{2m} + i\delta \stackrel{!}{=} 0 \quad (5)$$

$$\Rightarrow k = \pm k_0 \quad (6)$$

$$k_0 := \left(\sqrt{2mE} + i0 \right) \quad (7)$$

We find the solution using the Residue theorem (the first (second) integral picks up the residue in the upper (lower) half plane):

$$G^R(r, E) = -\sqrt{2m} \frac{2\pi i}{2\pi} \left[\theta(r) \frac{\exp\left(i\sqrt{2mE}|r|\right)}{2\sqrt{E}} + \theta(-r) \frac{\exp\left(i\sqrt{2mE}|r|\right)}{2\sqrt{E}} \right] \quad (8)$$

We find:

$$G^R(r, E) = -i\sqrt{\frac{m}{2E}} \exp(i\sqrt{2mE}|r|). \quad (9)$$

Defining $k_E = \sqrt{2mE}$ and writing out the two coordinates x and x' explicitly, we may also write this as

$$G^R(x, x', E) = -i\frac{m}{k_E} \exp(ik_E|x - x'|). \quad (10)$$

(b) in three dimensions, $d = 3$.

Solution:

$$G^R(\mathbf{r}, E) = \int \frac{d^3k}{(2\pi)^3} \frac{\exp(i\mathbf{k}\mathbf{r})}{E - \frac{k^2}{2m} + i\delta} \quad (11)$$

$$= \frac{2\pi}{(2\pi)^3} \int_0^\infty k^2 dk \int_{-1}^1 d\cos(\phi) \frac{\exp(i|k||r|\cos(\phi))}{E - \frac{k^2}{2m} + i\delta} \quad (12)$$

$$= \frac{4\pi}{(2\pi)^3} \frac{1}{|r|} \int_0^\infty k dk \frac{\sin(|k||r|)}{E - \frac{k^2}{2m} + i\delta} \quad (13)$$

$$= \frac{2\pi}{(2\pi)^3} \frac{1}{|r|} \int_{-\infty}^\infty k dk \frac{\sin(k|r|)}{E - \frac{k^2}{2m} + i\delta} \quad (14)$$

$$= \frac{2\pi}{(2\pi)^3} \frac{1}{|r|} \int_{-\infty}^\infty k dk \frac{\sin(k|r|)}{E - \frac{k^2}{2m} + i\delta} \quad (15)$$

This is the integral we solved on sheet 0, task 3. we obtain

$$G^R(\mathbf{r}, E) = -\frac{m}{2\pi} \frac{\exp(-i\sqrt{2mE}|r|)}{|r|}. \quad (16)$$

2. Green's function in graphene

(10 points)

(a) Starting with the effective Hamiltonian of electrons in one valley of graphene,

$$\hat{H} = v(\sigma_x \hat{p}_x + \sigma_y \hat{p}_y)$$

(here σ_x and σ_y are the Pauli matrices in the sublattice space), find the retarded Green's function $G^R(\varepsilon, \mathbf{p})$ for free electrons as a 2×2 matrix in the sublattice space.

Solution: The defining property of the Green's function is

$$\left(i\hbar \frac{\partial}{\partial t} - \hat{H}(\vec{r})\right) \hat{G}(\vec{r}, t; \vec{r}', t') = \delta(t - t') \delta(\vec{r} - \vec{r}') \quad (17)$$

For the case of graphene, the Hamiltonian is a matrix acting on the sublattice space and thus the Green's function has to be a matrix acting on the same sublattice space and we have to insert unity matrices σ_0 where necessary. The coordinate $\vec{r}$ acts in the two dimensional real space of the graphene sheet.

The starting point is the same as for the case of the free electron gas, i.e. we start by introducing the Fourier transform of the Green's function via

$$\hat{G}(\vec{r}, t; \vec{r}', t') = \int \int \frac{d^2k}{(2\pi)^2} \frac{d^2k'}{(2\pi)^2} \int \int \frac{dt}{(2\pi)} \frac{dt'}{(2\pi)} e^{i\vec{k} \cdot \vec{r}} e^{i\vec{k}' \cdot \vec{r}'} e^{i\omega t} e^{i\omega' t'} \hat{G}(\vec{k}, \omega; \vec{k}', \omega'). \quad (18)$$

We use this representation and plug it into the definition (17). Since the time derivative and the Hamiltonian only act on the exponentials and

$$\delta(x) = \int \frac{dk}{2\pi} e^{ikx} \quad (19)$$

we get an algebraic equation for $\hat{G}(\vec{k}, \omega; \vec{k}', \omega') = \hat{G}(\vec{k}, \omega; -\vec{k}, -\omega) = \hat{G}(\vec{k}, \omega)$:

$$[\hbar\omega\sigma_0 - v\hbar(\sigma_x k_x + \sigma_y k_y)] \hat{G}(\vec{k}, \omega) = \sigma_0. \quad (20)$$

Thus, we find

$$\hat{G}(\vec{k}, \omega) = [\hbar\omega\sigma_0 - v\hbar(\sigma_x k_x + \sigma_y k_y)]^{-1} \quad (21)$$

$$= \begin{pmatrix} \hbar\omega & -v\hbar(k_x - ik_y) \\ -v\hbar(k_x + ik_y) & \hbar\omega \end{pmatrix}^{-1} \quad (22)$$

$$= \frac{1}{\hbar^2\omega^2 - \hbar^2v^2(k_x^2 + k_y^2)} \begin{pmatrix} \hbar\omega & v\hbar(k_x - ik_y) \\ v\hbar(k_x + ik_y) & \hbar\omega \end{pmatrix}. \quad (23)$$

The retarded Green's function is found by shifting the pole: $\omega \rightarrow \omega + i\delta$, i.e.

$$\hat{G}^R(\vec{k}, \omega) = \frac{1}{\hbar^2(\omega + i\delta)^2 - \hbar^2v^2(k_x^2 + k_y^2)} \begin{pmatrix} \hbar\omega & v\hbar(k_x - ik_y) \\ v\hbar(k_x + ik_y) & \hbar\omega \end{pmatrix} \quad (24)$$

$$= \frac{\hbar\omega\sigma_0 + v\hbar(k_x\sigma_x + k_y\sigma_y)}{\hbar^2(\omega + i\delta)^2 - \hbar^2v^2(k_x^2 + k_y^2)}. \quad (25)$$

One can further convert this to $\epsilon, \vec{p}$ space by $\epsilon = \hbar\omega$ and $\vec{p} = \hbar\vec{k}$.

3. Friedel oscillations around a barrier in a 1D system (8 + 8 + 8 + 6 points)

- (a) Express the density $n(x)$ of non-interacting fermions in $D = 1$ spatial dimension at zero temperature in terms of the imaginary part of the retarded Green's function $G^R(\epsilon; x, x')$, starting from the zero temperature expression

$$n(x) = \sum_{\alpha \in \text{occupied}} |\psi_\alpha(x)|^2, \quad (26)$$

where ψ_α are the single particle wave functions and the sum is taken over all states with energy $\epsilon < \epsilon_F := 0$.

Solution:

We know from the lecture (equation (2.37)):

$$G^R(\epsilon; \mathbf{r}, \mathbf{r}) = \sum_{\alpha} \frac{|\psi_\alpha(\mathbf{r})|^2}{\epsilon - \epsilon_\alpha + i0} \quad (27)$$

And also (lecture equation (2.44))

$$\text{Im} \left(\frac{1}{x + i0} \right) = -\pi \delta(x) \quad (28)$$

We use Eq. (28) to extract the imaginary part from the spectral representation (27):

$$\text{Im} (G^R(\varepsilon; \mathbf{r}, \mathbf{r})) = -\pi \sum_{\alpha} |\psi_{\alpha}(\mathbf{r})|^2 \delta(\varepsilon - \varepsilon_{\alpha}) \quad (29)$$

We now integrate over all desired energies:

$$\int_{-\infty}^0 d\varepsilon \text{Im} (G^R(\varepsilon; \mathbf{r}, \mathbf{r})) = -\pi \sum_{\alpha} |\psi_{\alpha}(\mathbf{r})|^2 \int_{-\infty}^0 d\varepsilon \delta(\varepsilon - \varepsilon_{\alpha}) \quad (30)$$

$$= -\pi \sum_{\alpha: \varepsilon_{\alpha} < 0} |\psi_{\alpha}(\mathbf{r})|^2 \quad (31)$$

In the last equality, we used

$$\int_{-\infty}^0 d\varepsilon \delta(\varepsilon - \varepsilon_{\alpha}) = \begin{cases} 1 & \varepsilon_{\alpha} < 0 \\ 0 & \varepsilon_{\alpha} > 0 \end{cases}. \quad (32)$$

The sum now only includes energies < 0 , which correspond to the occupied states. Therefore

$$n(x) = -\frac{1}{\pi} \int_{-\infty}^0 d\varepsilon \text{Im}[G^R(\varepsilon, \mathbf{r}, \mathbf{r})] \quad (33)$$

- (b) Find $G^R(\varepsilon; x, x')$ for non-interacting one-dimensional fermions with parabolic dispersion $E = \frac{\hbar^2 k^2}{2m}$ in the presence of a δ -barrier $V(x) = V_0 a \delta(x)$.

Solution: There are two ways of solving this problem:

- One can construct the single-particle Green's function from the eigenstates.
- The δ potential is one of the cases, where one can solve the Dyson series explicitly.

The first way involves several technical steps. Therefore, we present the solution based on the Dyson equation, which is more straightforward.

In this case, the Dyson equation is

$$\begin{aligned} G^R(x, x') &= G_0^R(x, x') + \int_{-\infty}^{\infty} dx'' G_0^R(x, x'') V_0 a \delta(x'') G^R(x'', x') \\ &= G_0^R(x, x') + V_0 a G_0^R(x, 0) G^R(0, x') \end{aligned} \quad (34)$$

We have not written the energy ε here explicitly, since it is the same for all GFs. Setting $x = 0$ we get the equation

$$G^R(0, x') = G_0^R(0, x') + V_0 a G_0^R(0, 0) G^R(0, x'), \quad (35)$$

which has the solution

$$G^R(0, x') = \frac{G_0^R(0, x')}{1 - V_0 a G_0^R(0, 0)}. \quad (36)$$

Substituting this solution to Eq. (34), we find

$$G^R(x, x') = G_0^R(x, x') + \frac{G_0^R(x, 0)V_0aG_0^R(0, x')}{1 - V_0aG_0^R(0, 0)}. \quad (37)$$

Using the equation for the bare GF, we get

$$G^R(x, x') = -i\frac{m}{k_\varepsilon} \left(\exp(ik_\varepsilon|x - x'|) - \frac{iZ}{1 + iZ} \exp[ik_\varepsilon(|x| + |x'|)] \right), \quad (38)$$

where we defined $Z = maV_0/k_\varepsilon$. This solution is the same as the one obtained the other way.

- (c) Using the relation between the scattering amplitude $f(\mathbf{k}, k\mathbf{n})$ and the Green's function (see lecture notes for the relation), calculate the reflection and transmission amplitudes for the δ -barrier. *Hint: How are the reflection and transmission amplitudes related to the wave functions before and after scattering?*

Solution:

In the lecture (section (2.7) about scattering amplitudes), a formula (2.67) for the wave function after the scattering was given. This formula relates the scattered wave function to the scattering amplitude $f(\mathbf{k}, k\mathbf{n})$, which, in turn is connected to F (Eq. (2.74) in the lecture notes) which can be obtained from the Green's functions G_0 and G . Reflection and transmission coefficients are defined in terms of the scattered wave function: The ratio of amplitudes between the wave behind the barrier and the incoming wave is the transmission coefficient, and the ratio between incoming and reflected is the reflection coefficient. Therefore, we find reflection and transmission coefficients from the scattered wave function, which is determined by the scattering amplitude to be obtained from F .

The lecture expression for the scattered wave in terms of the scattering amplitude (2.67) is derived for a three dimensional system and it is different from the expression for a 1D system. Therefore, we start by rederiving this lecture relation (Lippman-Schwinger equation) for the 1D case:

$$(E - H_0)\psi = V\psi \quad (39)$$

$$(E - H_0)G_0(E, x, x') = \delta(x - x') \quad (40)$$

$$\psi_k(x) = \psi_{0,k}(x') + \int dx' G_0(E, x, x')V(x')\psi_k(x') \quad E = \frac{k^2}{2m} \quad (41)$$

where $\psi_{0,k}(x) = \exp(ikx)$ solves the free Schroedinger equation. Eq. (41) is obtained, by writing the solution to the Schroedinger equation (39) with the help of the Green's function G_0 applied to the inhomogeneity $V\psi$.

We plug in the free Green's function

$$G_0(E, x, x') = -i\frac{m}{k_E} \exp(ik_E|x - x'|) \quad (42)$$

and the result (for $|x| > |x'|$), observing the wave function away from the range of the potential

$$|x - x'| = \begin{cases} x - x' & x > 0 \\ x' - x & x < 0 \end{cases} \quad (43)$$

$$= |x| - \text{sgn}(x)x' \quad (44)$$

to obtain

$$\psi_k(x) = \psi_{0,k}(x) - i \frac{m}{k_E} \exp(ik|x|) \int dx' \exp(-ik'x') V(x') \psi_k(x') \quad k' := \text{sgn}(x)k. \quad (45)$$

In analogy to the lecture, we identify the scattering amplitude f in the scattered wave function:

$$\psi_k(x) := \psi_{0,k}(x) - i \frac{m}{k} \exp(ik|x|) f(k, k') \quad (46)$$

We see, that $f(k, k')$ fullfills a recursion relation:

$$f(k, k') := \int dx' \exp(-ik'x') V(x') \psi_k(x') \quad (47)$$

$$= \int dx' \exp(-ik'x') V(x') \exp(ikx') \quad (48)$$

$$+ \int dx' \exp(-ik'x') V(x') \int dx'' G_0(E, x', x'') V(x'') \psi_k(x'') \quad (49)$$

$$= V(k - k') + \int dx' \exp(-ik'x') V(x') \int dx'' G_0(E, x', x'') V(x'') \psi_k(x'') \quad (50)$$

$$= V(k - k') + \int dk'' V(k' - k'') \mathcal{FT} \left[\int dx'' G_0(E, x', x'') V(x'') \psi_k(x'') \right] (k'') \quad (51)$$

$$= V(k - k') + \int dk'' \frac{V(k' - k'')}{E(k) - k''^2/(2m) + i0} f(k, k'') \quad (52)$$

For the first equality, we used Eq. (41). We also used:

$$\int dx' \exp(ik''x') \int dx'' G_0(x' - x'') V(x'') \psi(x'') = G_0(k'') \mathcal{FT} [V(x'') \psi(x'')] (k'') \quad (53)$$

$$= G_0(k'') \int dx'' \exp(-ik''x'') V(x'') \psi(x'') \quad (54)$$

$$= G_0(k'') f(k, k'') \quad (55)$$

(Remember, that the Fourier transform of a multiplication is a convolution and vice-versa.)

We end up with the recursion

$$f(k, k') = V(k - k') + \int dk'' \frac{V(k' - k'')}{E(k) - k''^2/(2m) + i0} f(k, k'') \quad (56)$$

which can be seen to be equivalent to

$$f(k, k') = V(k - k') + \int dk'' \frac{V(k - k'')}{E(k) - k''^2/(2m) + i0} f(k'', k'). \quad (57)$$

To see this, consider the recursion in operator form:

$$f = V + fG_0V \quad f^{-1}(\dots)V^{-1} \quad (58)$$

$$V^{-1} = f^{-1} + G_0 \quad V(\dots)f \quad (59)$$

$$f = V + VG_0f. \quad (60)$$

(To see it graphically, draw the diagrammatic representations of the recursions.)

Comparing Eq. (57) to the definition of the function F from the lecture (lecture equation (2.72)), we recognize, that in the 1D case, a relation between F and f analogous to the 3D case holds:

$$f(k, k') = F^R(E = k^2/(2m), k, k'). \quad (61)$$

We now need to find F , to obtain the scattered wave function explicitly, using Eqs. (61) and (46).

We can identify F^R from full Green's function, which we found in subtask (b). Alternatively, we can calculate it from the definition

$$F(\varepsilon, \mathbf{p}_1, \mathbf{p}_2) = V(\mathbf{q}) + \int \frac{d\mathbf{p}_3}{2\pi} \frac{V(\mathbf{p}_1 - \mathbf{p}_3)F(\varepsilon, \mathbf{p}_3, \mathbf{p}_2)}{\varepsilon - p_3^2/(2m) + i0} \quad (62)$$

$$V(q) = \int dr \exp(-iqr)V(r) \quad (63)$$

$$= V_0a \quad (64)$$

therefore

$$F(\varepsilon) = V_0a + V_0a \int \frac{dp_3}{2\pi} \frac{F(\varepsilon)}{\varepsilon - p_3^2/(2m) + i0} \quad (65)$$

$$= V_0a \sum_{n=0}^{\infty} \left(V_0a \int \frac{dp_3}{2\pi} G^R(\varepsilon, p_3) \right)^n \quad (66)$$

$$= \frac{V_0a}{1 - V_0a \int \frac{dp_3}{2\pi} G^R(\varepsilon, p_3)} \quad (67)$$

$$= \frac{V_0a}{1 + i \frac{V_0am}{k_\varepsilon}}. \quad (68)$$

We finally determine f by evaluating F “on the mass shell”

$$f(k, k') = F(\varepsilon = k^2/2m) \quad (69)$$

$$= \frac{V_0a}{1 + i \frac{V_0am}{k}}. \quad (70)$$

To identify transmission and reflection coefficients, we consider the scattered wave function

$$\psi_k(x) = \psi_{0,k}(x) - i \frac{m}{k} f(k, k') \exp(ik|x|) \quad (71)$$

$$= \begin{cases} \exp(ikx) - i \frac{m}{k} f(k, k') \exp(-ikx) & x < 0 \\ \exp(ikx) [1 - i \frac{m}{k} f(k, k')] & x > 0 \end{cases} \quad (72)$$

$$=: \begin{cases} \exp(ikx) + r \exp(-ikx) & x < 0 \\ t \exp(ikx) & x > 0 \end{cases} \quad (73)$$

We find

$$t = \left[1 - i \frac{m}{k} f(k, k') \right] = 1 - \frac{iV_0 am}{k + iV_0 am} \quad (74)$$

$$= \frac{k}{k + iV_0 am} = \frac{1}{1 + \frac{iV_0 am}{k}} \quad (75)$$

$$r = -i \frac{m}{k} f(k, k') = -\frac{iV_0 am}{k + iV_0 am} = \frac{1}{\frac{ik}{V_0 am} - 1} \quad (76)$$

These are indeed the reflection and transmission coefficients of the δ -potential, see [https://en.wikipedia.org/wiki/Delta_potential#Solving_the_Schrdinger_equation\[1\]](https://en.wikipedia.org/wiki/Delta_potential#Solving_the_Schrdinger_equation[1]).

- (d) Calculate $n(x)$ around this barrier at zero temperature. (You can use the formula derived in part (a)).

Solution: In subtask 1a, we derived an expression for the density. Now, the spectrum shifts by μ in presence of finite chemical potential:

$$n(x) = \frac{-1}{\pi} \int_{-\infty}^0 d\varepsilon \text{Im} G^R(\varepsilon + \mu, x, x). \quad (77)$$

We are not interested in constant background charge, so we subtract it and study the perturbation:

$$\delta n(x) = \frac{-1}{\pi} \int_{-\infty}^0 d\varepsilon \text{Im} [G^R(\varepsilon + \mu, x, x) - G_0^R(\varepsilon + \mu, x, x)] \quad (78)$$

$$= \frac{-1}{\pi} \int_{-\infty}^0 d\varepsilon \text{Re} \frac{mr}{k_\varepsilon} e^{2ik_\varepsilon |x|} \quad (79)$$

Where we expressed the prefactor of the GF in terms of the reflection coefficient r . We can write this as

$$r = |r| e^{i \text{ph } r} \quad (80)$$

and combine it with the other exponential. We get

$$\delta n(x) = \frac{-1}{\pi} \int_{-\infty}^0 d\varepsilon \frac{m|r|}{k_\varepsilon} \cos(2ik_\varepsilon |x| + i \text{ph } r) \quad (81)$$

Let us now linearize around Fermi energy: $k_\varepsilon = k_F + \frac{\varepsilon - \mu}{v_F}$. For r and the k_ε in the denominator, we neglect the energy dependence completely and only take the Fermi surface value. We get

$$\delta n(x) = -\frac{m|r|}{\pi k_F} \int_0^\mu d\varepsilon \cos\left(2k_F |x| + 2\frac{\varepsilon - \mu}{v_F} |x| + \text{ph } r\right) \quad (82)$$

$$= -\frac{m|r|v_F}{\pi k_F |x|} [\sin(2k_F |x| + \text{ph } r) - \sin(\text{ph } r)] \quad (83)$$

$$(84)$$

The lower limit gives just some constant, which is not accurately reproduced in this calculation. The upper limit shows the Friedel oscillations that go with $2k_F$.