Universität Bonn
Physikalisches Institut
Prof. Dr. J. Kroha, M. Kajan, M. Lenk, M. Turaev

17.04.2019
Summer semester 2019
http://www.kroha.uni-bonn.de

Advanced Theoretical Condensed Matter Physics
Exercise 1

(Submission date: 02.05.19, discussion: 03.05.19)
Note: Submit your solutions until 12h in room PI 1.055

1.1 Green's functions for non-interacting electrons (2+2+4+3+4=15 points)

In the lecture, the position-dependent Green's function was defined in terms of field operators. In a similar way one can define the momentum dependent, retarded Green's function

$$G^R_{\boldsymbol{k}\sigma}(t,t') = -\mathrm{i}\Theta(t-t')\frac{1}{Z_G}\mathrm{tr}\left\{\mathrm{e}^{-\beta(H-\mu N)}\left[c_{\boldsymbol{k}\sigma}(t), c^\dagger_{\boldsymbol{k}\sigma}(t')\right]_+\right\} \tag{1}$$

The advanced and time-ordered, momentum-dependent Green's functions are defined analogously. We consider a system of non-interacting electrons,

$$\mathcal{H}_0 = H_0 - \mu N = \sum_{\boldsymbol{k}\sigma}(\epsilon_{\boldsymbol{k}} - \mu)c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma} \tag{2}$$

a) Determine the time-dependence of $c_{\boldsymbol{k}\sigma}(t)$ and $c^\dagger_{\boldsymbol{k}\sigma}(t')$ in the Heisenberg picture.

b) Derive the equation of motion for the retarded Green's function $G^R_{\boldsymbol{k}\sigma}(t,t') \equiv G^{(0)R}_{\boldsymbol{k}\sigma}(t-t')$ for the non-interacting system $\mathcal{H}_0$ using the results of a).

c) Calculate the Fourier transform with respect to time $(t-t')$. Discuss, in particular, why an infinitesimal imaginary part $i\eta$ must be added to the energy in order to make the Fourier integral convergent and determine the sign of η. Similarly, calculate the advanced Green's function $G^{(0)A}_{\boldsymbol{k}\sigma}(\omega)$ and determine the sign of η in this case.

   Result for G^R:

$$G^{(0)R}_{\boldsymbol{k}\sigma}(\omega) = \int_{-\infty}^{\infty} d(t-t')\, G^{(0)R}_{\boldsymbol{k}\sigma}(t-t')\,\mathrm{e}^{\mathrm{i}\omega(t-t')} = \frac{1}{\omega + \mu - \epsilon_{\boldsymbol{k}} + \mathrm{i}\eta}\ , \quad \eta \to 0^+\ . \tag{3}$$

d) Another important quantity can be obtained from the retarded Greens function by taking the imaginary part and tracing over the quantum numbers. Which quantity do you obtain in this way? To proceed further, take the continuum limit of the momentum sum and assume that the dispersion ϵ_k only depends on the absolute value of $\boldsymbol{k}$.

In the general, interacting case, the retarded Green's function contains a non-infinitesimal imaginary part in the denominator,

$$G^R_{\boldsymbol{k}\sigma}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\boldsymbol{k}} + \mathrm{i}/(2\tau)}$$

e) Use complex contour integration to calculate the time-dependent Green's function by Fourier transformation. How does the Green's function behave for large $(t-t')$? Give a physical interpretation for τ and try to explain why a finite τ may occur.

1.2 Contour integrals $(3+3+3+2+4=15 \text{ points})$

In order to evaluate energy integrals, it is often helpful to use complex contour integration. This exercise should help you recall the methods you have learnt earlier in your studies and prepare you for applying them to calculations in the present course.

a) Consider a function $f(z)$, which is analytic everywhere in the complex plane, except at $z = x_0, x_0 \in \mathbb{R}$, where it has a **simple pole**. In order to evaluate the integral along the contour in Fig. 1, factorize out the simple pole at $z = x_0$ and relate the integral along the full contour $\mathcal{C} = \mathcal{C}_1 + \mathcal{C}_2 + \mathcal{C}_3$ in the limit of $r \to \infty$ and $\epsilon \to 0$ to the Cauchy principal value integral of $f(z)$. What is the condition for a vanishing contribution of $\mathcal{C}_1$?

b) How can the expression obtained in a) be related to the case, where the pole is at $z = x_0 - i\eta$ with $\eta > 0$? Following the same train of thought, what is the contour that you would use for the case $z = x_0 + i\eta$ instead? For both cases, **draw a sketch** of the contour and mark the pole.

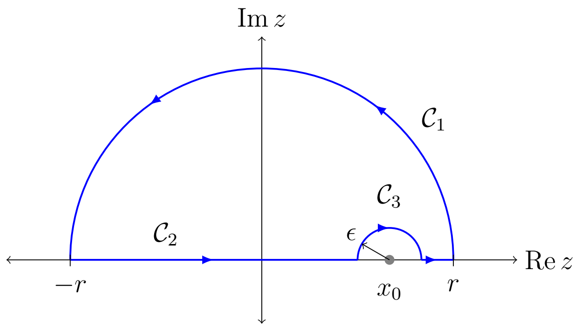

Figure 1: Integration contour for 1.1 a), radius of curve $\mathcal{C}_3$ is ϵ.

What you have found in a) & b) is a version of the Kramers-Kronig relation. By separating $f(z)$ into its real and imaginary part, you can find a relation between them.

Now consider the function $G(z) = \int_{-\infty}^{+\infty} dk \ 1/(z - \epsilon_k)$, which is analytic everywhere, except on the real axis (it has a line of poles whose positions depend on ϵ_k). Assume, that ϵ_k is a surjective function of some variable k (i.e. it covers the whole real axis). In terms of many-body Green's functions, this means that the system has a continuous spectrum. We are interested in integrals enclosing the entire complex plane, except the real axis. The line of poles at $z = \epsilon_k$ has to be considered a branch cut, so we have to avoid "hitting" it with the contour. The contour thus has to be chosen similar to Fig. 2.

c) Evaluate the sum of the integrals along $\mathcal{C}_1$ and $\mathcal{C}_2$ from Fig. 2 in the limit $r \to \infty$. For this, assume that you can multiply $G(z)$ with $e^{\pm z 0^+}$ in order to make the arcs vanish.

d) Compare your results to Eq. (1) from exercise 1.1. What are the two contributions you have found in the language of Green's functions?

e) Determine the poles and calculate the residues of the Fermi-Dirac distribution function $f(z) = 1/(e^{\beta z} + 1)$ and the Bose-Einstein distribution function $b(z) = 1/(e^{\beta z} - 1)$, where $z \in \mathbb{C}$.

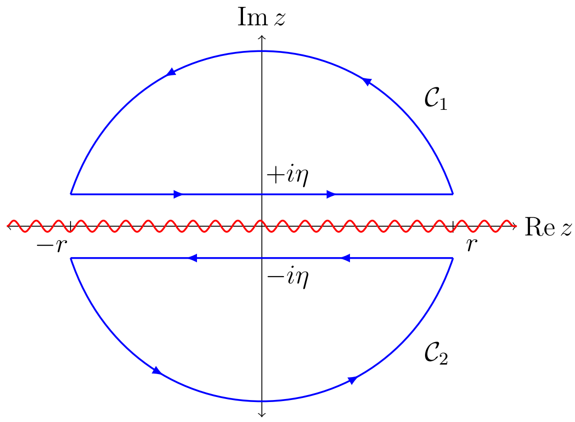

Figure 2: Integration contour for 1.3 d)

In the lecture, you will learn how to use the results from d) and e) for the evaluation of Feynman diagrams in field theory.

1.3 Nonlinear response functions and discrete symmetries (5+5=10 points)

We consider the nonlinear response of a system to an external optical laser pulse. In leading order, the laser field couples to the system via electric dipole coupling, $\delta\mathcal{H} = -\boldsymbol{d}\cdot\boldsymbol{E}$, where $\boldsymbol{d}$ is the dipole operator of the system. The system's response is an emitted light pulse, proportional to its induced dipole moment $\delta\boldsymbol{d}$. The quadratic response equation then reads

$$\delta d_i(t) = \int \mathrm{d}t_1\,\mathrm{d}t_2\,\chi^{(2)}_{d_i,d_j,d_k}(t,t_1,t_2)E_j(t_1)E_k(t_2)\;, \tag{4}$$

where the subscripts i, j, k denote the x, y, or z components. With the non-linear response function $\chi^{(2)}_{d_i,d_j,d_k}(t,t_1,t_2)$ given by

$$\chi^{(2)}_{d_i,d_j,d_k}(t,t_1,t_2) = (-\mathrm{i})^2\Theta(t-t_1)\Theta(t_1-t_2)\left\langle\left[\left[d_i(t),d_j(t_1)\right],d_k(t_2)\right]\right\rangle_0 \tag{5}$$

The average is taken here over the equilibrium distribution of the system, indicated by the subscript zero. In equilibrium, the system is described by the Hamiltonian $\mathcal{H}_0$, which also reflects the symmetries of the system.

a) We now want to study the symmetry properties of $\chi^{(2)}$. $\boldsymbol{E}$ and $\boldsymbol{d}$ have odd parity under space inversion : $\hat{\mathrm{P}}\boldsymbol{E} = -\boldsymbol{E}$, $\hat{\mathrm{P}}\boldsymbol{d} = -\boldsymbol{d}$. Show that for a system invariant under space inversion the non-linear response function $\chi^{(2)}$ vanishes.
Hint: You can show this either by analyzing the space inversion behavior of Eq. (4) or of the expectation value in Eq. 5.

By an elementary, but tedious, calculation one can explicitly show that the quadratic response $\chi^{(2)}$ only depends on two time differences,

$$\chi^{(2)}_{d_i,d_j,d_k}(t,t_1,t_2) = \chi^{(2)}_{d_i,d_j,d_k}(t-t_1,t_1-t_2)\;. \tag{6}$$

b) Calculate the change of the dipole moment as a function of frequency $\delta d_i(\omega)$, by performing the Fourier transform of Eq. (4) with the help of Eq. (6).
Show that for a monochromatic incident light beam the response is at twice the frequency.