Prof. Dr. J. von Delft, Dr. O. Yevtushenko, F. Kugler Oct. 28, 2019

Problem Set 3: Kubo formula, free energy of Fermi gas

Exercise 1. Kubo formula: Conductivity in a weak external electromagnetic field

We consider N particles in an external electromagnetic field $(\phi, \mathbf{A})$ described by the Hamiltonian

$$H = \sum_{i=1}^{N} \left[\frac{1}{2m} \big(\hat{\mathbf{p}}_i - \frac{e}{c} \mathbf{A}(\hat{\mathbf{x}}_i, t) \big)^2 + e\phi(\hat{\mathbf{x}}_i, t) \right], \tag{1}$$

where we use the notation $\hat{\mathbf{O}} = (\hat{O}_x, \hat{O}_y, \hat{O}_z)^T$.

(a) Consider the following first-quantized operators,

$$\hat{n}(\mathbf{x}) = \sum_{i=1}^{N} \delta(\mathbf{x} - \hat{\mathbf{x}}_i), \tag{2}$$

$$\hat{\mathbf{j}}(\mathbf{x}) = \frac{e}{2m} \sum_{i=1}^{N} \Big[\hat{\mathbf{p}}_i \delta(\mathbf{x} - \hat{\mathbf{x}}_i) + \delta(\mathbf{x} - \hat{\mathbf{x}}_i) \hat{\mathbf{p}}_i \Big], \tag{3}$$

$$\hat{\mathbf{j}}_A(\mathbf{x}) = \frac{e}{2m} \sum_{i=1}^{N} \Big[\big(\hat{\mathbf{p}}_i - \frac{e}{c} \mathbf{A}(\hat{\mathbf{x}}_i, t) \big) \delta(\mathbf{x} - \hat{\mathbf{x}}_i) + \delta(\mathbf{x} - \hat{\mathbf{x}}_i) \big(\hat{\mathbf{p}}_i - \frac{e}{c} \mathbf{A}(\hat{\mathbf{x}}_i, t) \big) \Big], \tag{4}$$

where $\hat{\mathbf{p}}_i = -i\nabla_{\mathbf{x}_i}$, and the current $\hat{\mathbf{j}}_A(\mathbf{x})$ is composed of a paramagnetic and diamagnetic contribution, $\hat{\mathbf{j}}_A(\mathbf{x}) = \hat{\mathbf{j}}(\mathbf{x}) - \frac{e^2}{mc} \hat{n}(\mathbf{x}) \mathbf{A}$. The latter is responsible for the diamagnetic effect occuring in the presence of an external magnetic field in diamagnetic materials. In paramagnetic materials the former contribution dominates the current.

Rewrite H such that the parts linear in the external fields couple to $\hat{\mathbf{j}}_A(\mathbf{x})$ and $\hat{n}(\mathbf{x})$.

(b) Show that the linear response of $\langle \hat{\mathbf{j}}_A(\mathbf{x}, t) \rangle$ to an external electromagnetic perturbation $(\phi, \mathbf{A})$ is given by

$$\begin{aligned} \langle \hat{j}_{A,\mu}(\mathbf{x}, t) \rangle = \int \mathrm{d}^3x' \mathrm{d}t' \Big[& -\frac{1}{c} \chi_{j_\mu, j_\nu}(\mathbf{x} - \mathbf{x}', t - t') A_\nu(\mathbf{x}', t') \\ & + e\chi_{j_\mu, n}(\mathbf{x} - \mathbf{x}', t - t') \phi(\mathbf{x}', t') \Big] - \frac{e^2 n}{mc} A_\mu(\mathbf{x}, t), \end{aligned} \tag{5}$$

with the retarded susceptibilities

$$\chi_{j_\mu, j_\nu}(\mathbf{x} - \mathbf{x}', t - t') = -i\Theta(t - t') \, \langle \, [\hat{j}_\mu^{H_0}(\mathbf{x}, t), \, \hat{j}_\nu^{H_0}(\mathbf{x}', t')] \, \rangle, \tag{6}$$

$$\chi_{j_\mu, n}(\mathbf{x} - \mathbf{x}', t - t') = -i\Theta(t - t') \, \langle \, [\hat{j}_\mu^{H_0}(\mathbf{x}, t), \, \hat{n}^{H_0}(\mathbf{x}', t')] \, \rangle. \tag{7}$$

Here, the superscript H_0 on an operator indicates that its time dependence is given in the interaction picture, i.e., w.r.t. the unperturbed Hamiltonian.

(c) Now, we choose the gauge $\phi = 0$ and consider a particle in a spatially constant external electric field of the form $\mathbf{E} = -\frac{1}{c}\partial_t \mathbf{A}$.

Show that $\langle \hat{j}_{A,\mu}(\omega)\rangle = \sigma_{\mu\nu}|_{\mathbf{p}=\mathbf{0}}(\omega) E_\nu(\omega)$, where $\mathbf{p}$ denotes momentum and

$$\sigma_{\mu\nu}|_{\mathbf{p}=\mathbf{0}}(\omega) = \frac{i}{\omega}\Big(\chi_{j_\mu,j_\nu}(\mathbf{p}=\mathbf{0},\omega) + \frac{e^2 n}{m}\delta_{\mu\nu}\Big). \tag{8}$$

Exercise 2. Matsubara sums

The Matsubara technique usually requires calculating sums of the type

$$S = \frac{1}{\beta}\sum_n F(i\omega_n), \tag{9}$$

where $F(z)$ has simple poles at $z = z_i$, where $\mathrm{Re}(z_i) \neq 0$, and residues $R(z_i)$. In this exercise, we recall a useful technique for this, which is based on rewriting the sum as a contour integral.

(a) Consider the function ($\zeta \in \{\pm 1\}$)

$$n_\zeta(z) = \frac{1}{\exp(\beta z) - \zeta}. \tag{10}$$

What is its pole-structure (i.e., where are its poles and what are the residues)?

(b) Use this to transform S into a contour integral over $n_\zeta(z)F(z)$.

(c) Assume that F vanishes sufficiently quickly for $|z| \to \infty$ and deform the contour. Then, take a clever deformation of the contour to pick up the contributions from the poles of F. Use this to show

$$S = -\zeta \sum_i n_\zeta(z_i) R(z_i). \tag{11}$$

Exercise 3. Free energy of non-interacting fermions

The free energy of a Fermi gas described in the grand canonical ensemble reads

$$F = -\tfrac{1}{\beta}\ln \mathrm{Tr}[\rho] = -\tfrac{1}{\beta}\sum_k \ln\big[1 + \exp(-\beta\xi_k)\big], \tag{12}$$

where $\xi_k = \epsilon_k - \mu$. Let us calculate the free energy for a Fermi gas in a continuum approach as well as from a discretized field integral.

(a) In the *continuum approach*, a system of non-interacting fermions is described by the action

$$S = \int_0^\beta \mathrm{d}\tau \sum_k \bar{\psi}_k(\tau)[\partial_\tau + \xi_k]\psi_k(\tau), \tag{13}$$

with Grassmann fields $\psi_k(\tau)$. Perform a discrete Fourier transformation using Matsubara frequencies to show that

$$F = -\tfrac{1}{\beta}\ln \mathcal{Z} = -\tfrac{1}{\beta}\sum_{k,n} \ln\big[\beta(-i\omega_n + \xi_k)\big]. \tag{14}$$

(b) In order to evaluate the Matsubara frequency summation we introduce the auxiliary function $n(z) = \frac{1}{\exp(\beta z)+1}$ from Ex. 2 and consider $h(z) = \ln[-z + \xi_k]$. Assume that due to a suitable regularizer $\exp(i0^+ z)$, we can achieve that the contour integral for the sum $\sum_n \ln[\beta(-i\omega_n + \xi_k)]$ vanishes at the perimeter. Determine an integral expression for the above Matsubara sum and derive Eq. (12).

(c) The *discretized field integral* does not require any trick or regularization. We consider a discretized imaginary time axis with steps $\tau_j = j\frac{\beta}{N}$ with $0 \le j \le N-1$ and $\delta\tau_j = \tau_j - \tau_{j-1} = \frac{\beta}{N}$. The Fourier transform is then

$$\psi_{k,j} = \frac{1}{\beta}\sum_{l=0}^{N-1} \exp(-i\omega_l \tau_j)\psi_{k,\omega_l}, \qquad \psi_{k,\omega_l} = C\sum_{j=0}^{N-1} \exp(i\omega_l \tau_j)\psi_{k,j}. \tag{15}$$

What is C? Determine a discretized form of the action for non-interacting electrons in the Matsubara representation. Derive the partition sum

$$\mathcal{Z}_N(\beta) = \prod_k \prod_{l=0}^{N-1} \left[1 - \exp\left(i\omega_l \frac{\beta}{N}\right) + \frac{\beta}{N}\xi_k \exp\left(i\omega_l \frac{\beta}{N}\right)\right]. \tag{16}$$

Contrary to the expression in Eq. (14), this result is already regular. What is the origin of the regularizer that arises naturally in the discrete-integral approach?

(d) We can decompose the partition sum as

$$\ln \mathcal{Z}_N(\beta) = \ln \mathcal{Z}_N^0(\beta) + \sum_k \sum_{l=0}^{N-1} \ln\left[1 - \frac{\beta\xi_k}{N}\frac{1}{1-W_l}\right], \tag{17}$$

where $\mathcal{Z}_N^0(\beta) = \prod_{l=0}^{N-1}[1 - \exp(i\omega_l \frac{\beta}{N})]$ and $W_l = \exp(-i\pi\frac{2l+1}{N})$. Compute the first term and show that $\ln \mathcal{Z}_N^0(\beta) = \ln 2$. *Hint:* Use $\prod_{k=0}^{N-1} \sin(\frac{\pi k}{N} + x) = 2^{1-N}\sin(Nx)$.

(e) The sum over l in Eq. (17) contains values for W_l on the unit circle in discrete steps of $\exp(-i2\pi\frac{l}{N})$. We can thus split the sum as $(1 \ll \Lambda \ll N)$

$$\sum_{l=0}^{N-1} \ln\left[1 - \frac{\beta\xi_k}{N}\frac{1}{1-W_l}\right] = \tag{18}$$
$$\underbrace{\sum_{l=0}^{\Lambda/2}\left(\ln\left[1 - \frac{\beta\xi_k}{N}\frac{1}{1-W_l}\right] + \text{c.c.}\right)}_{\sum^L} + \underbrace{\sum_{l=\Lambda/2+1}^{N/2-1}\left(\ln\left[1 - \frac{\beta\xi_k}{N}\frac{1}{1-W_l}\right] + \text{c.c.}\right)}_{\sum^H}.$$

Perform the sum $\sum^L$ by expanding the argument of the logarithm for large N and using $\cosh x = \prod_{k=1}^{\infty}\left[1 + \frac{4x^2}{(2k-1)^2\pi^2}\right]$.

The denominator of $\sum^H$ has no singularity, and, for large N, the step size $\approx \frac{2\pi}{N}$ is small. We therefore replace the sum by an integral. Evaluate the integral by expanding the logarithm for large N, and show $\sum^H \approx -\beta\xi_k/2$.

Combine these results to identify the expression from Eq. (12).

Discussion of the problem set on Nov. 5, 2019.