
1. Exercise on QFT for many-body systems

Sommersemester 2020

TUTORIUM: Friday, 13.03.2020.**1. Getting familiar with the Density of States***1+1+2+2=6 points*

The calculation of thermodynamic quantities, response functions and Feynman diagrams in QFT for condensed matter systems often requires the evaluation of integrals or sums over all momenta \mathbf{k} (typically over the first Brillouin Zone). An important simplification of these \mathbf{k} -summations is possible, however, when the integrand \mathcal{F} depends on the **energy only**. In this case the integration/sum is best performed by using the energy ε as a variable. In the case of a cubic lattice of volume L^d in d dimensions, for a given observable F , we have:

$$F = \frac{1}{L^d} \sum_{\mathbf{k}} \mathcal{F}(\varepsilon_{\mathbf{k}}) = \frac{1}{(2\pi)^d} \frac{(2\pi)^d}{L^d} \sum_{\mathbf{k}} \mathcal{F}(\varepsilon_{\mathbf{k}}) = \int d\varepsilon \mathcal{N}(\varepsilon) \mathcal{F}(\varepsilon)$$

or, for the continuous case, $F = \frac{1}{(2\pi)^d} \int d^d k \mathcal{F}(\varepsilon_{\mathbf{k}}) = \int d\varepsilon \mathcal{N}(\varepsilon) \mathcal{F}(\varepsilon),$

where $\mathcal{N}(\varepsilon)$, i.e. the so-called **Density of States (DOS)**, which can be defined by comparison of the different expressions as

$$\mathcal{N}(\varepsilon) = \frac{1}{L^d} \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}}) \quad \text{or, for the continuous case,} \quad (2a)$$

$$\mathcal{N}(\varepsilon) = \frac{1}{(2\pi)^d} \int d^d k \delta(\varepsilon - \varepsilon_{\mathbf{k}}). \quad (2b)$$

- a) Consider the two cases of particles which can move freely and particles whose motion is bound to an infinite lattice with lattice spacing a . Which of the above expressions (eqn. (2a) or (2b)) do you have to use in the first and second case, respectively? Is the integral/summation restricted to certain \mathbf{k} -vectors? How does the result change, if one considers a one-dimensional, finite lattice (N lattice points, lattice spacing a) with periodic boundary conditions?
- b) Calculate and plot the explicit expression for $\mathcal{N}(\varepsilon)$ for free, non-interacting particles of mass m (so that $\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$) in one, two and three dimensions. How do the corresponding Fermi surfaces look like in these cases?
- c) Consider the following one-dimensional tight-binding Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} \left[c_{i,\sigma}^\dagger c_{j,\sigma} + h.c. \right]$$

with hopping ($t > 0$) restricted to neighboring sites, where $c_{i,\sigma}^\dagger$ and $c_{i,\sigma}$ are the creation/annihilation operators for one electron with spin $\sigma = \uparrow, \downarrow$ at the position $x_i = i a$ with $i = 0, 1, \dots, N-1$ and a being the lattice spacing. Assuming periodic boundary conditions ($x_0 = x_N$), compute the corresponding eigenenergies, e.g., using the following basis transformation (from real to momentum space) $c_{k,\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{x_i} e^{-ikx_i} c_{i,\sigma}^\dagger$ for the fermionic operators.

- d) How can one extend the results of **1c)** to arbitrary dimensions $d > 1$? Plot numerically¹ the DOS $\mathcal{N}(\varepsilon)$ for the cases $d = 1, 2, 3$ with $\hbar = m = t = a = 1$. Which are the most prominent features of these DOS functions and at which energies ε do they occur? How would the corresponding Fermi surfaces look like for the cases $d = 1, 2$, e.g. if one has an average density of one electron per site (*half-filled system*)?

2. Screened and unscreened Coulomb Potentials

1.5+2.5=4 points

- a) From the integral representation of the delta function,

$$\delta(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}}$$

and the fact that the Coulomb potential $\phi(\mathbf{r}) = -e/r$ satisfies Poisson's equation,

$$-\nabla^2 \phi(\mathbf{r}) = -4\pi e \delta(\mathbf{r}),$$

show that the electronic pair potential, $V(\mathbf{r}) = -e\phi(\mathbf{r}) = e^2/r$, can be written in the form

$$V(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} V(\mathbf{k}),$$

where the Fourier transform $V(\mathbf{k})$ is given by

$$V(\mathbf{k}) = \frac{4\pi e^2}{k^2}$$

- b) Show that the Fourier transform of the screened Coulomb interaction $V_s(\mathbf{r}) = (e^2/r)e^{-k_{TF}r}$ is

$$V_s(\mathbf{k}) = \frac{4\pi e^2}{k^2 + k_{TF}^2} \quad (3)$$

by substituting eqn. (3) into the Fourier integral

$$V_s(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} V_s(\mathbf{k}),$$

and evaluating that integral in spherical coordinates (*Hint*: The radial integral is best done as a contour integral.). Finally, deduce from eqn. (3) that $V_s(\mathbf{r})$ satisfies

$$(-\nabla^2 + k_{TF}^2) V_s(\mathbf{r}) = 4\pi e^2 \delta(\mathbf{r})$$

¹using, e.g. Mathematica, Python or Fortran in combination with gnuplot (<http://www.gnuplot.info/>) or matplotlib (<http://matplotlib.org/>)