

---

# 1. Exercise on QFT for many-body systems

---

Sommersemester 2023

**TUTORIUM: Friday, 24.03.2023.****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  $\varepsilon$  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

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

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

- 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?
- 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?
- 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 numerically<sup>1</sup> 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  $\varepsilon$  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

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

---

<sup>1</sup>using, e.g. Mathematica/Python/Julia or Fortran/C in combination with a plotting program, e.g. gnuplot.