Assignments to Condensed Matter Theory I
Sheet 1

G. Cuniberti (Phy 4.1.29) Room H33
A. Donarini (Phy 3.1.24) Wed 03.05 (h 13.15)

---

sheet online: `http://www-MCG.uni-R.de/teaching/`

Problem set: Lattice and beyond

1.1. The δ sum rules for crystals

Let us take a set of equally spaced points $x_0, \ldots, x_{N-1}$, on an interval of length $L = N\Delta x$,

$$x_j = j\Delta x, \quad j = 0, \ldots, N-1, \tag{1}$$

and then impose periodic boundary conditions, $x_N = x_0$. The points of the reciprocal lattice are:

$$k_n = n\Delta k = \frac{n}{N}\frac{2\pi}{\Delta x}, \quad n = 0, \ldots, N-1. \tag{2}$$

The Discrete Fourier Transform (DFT) of a function $f(x_j)$ is defined as

$$\tilde{f}(k_n) = \sum_{j=0}^{N-1} \Delta x \exp(-\mathrm{i}k_n x_j) f(x_j). \tag{3}$$

(a) Verify the identities

$$\frac{1}{N}\sum_{j=0}^{N-1} \exp(\mathrm{i}x_j(k_n - k_m)) = \delta_{nm} \quad \text{and} \quad \frac{1}{N}\sum_{n=0}^{N-1} \exp(\mathrm{i}k_n(x_i - x_j)) = \delta_{ij} \tag{4}$$

and prove with them the validity of the inverse DFT:

$$f(x_i) = \frac{1}{2\pi}\sum_{n=0}^{N-1} \Delta k \exp(\mathrm{i}k_n x_i) \tilde{f}(k_n). \tag{5}$$

(b) Extend the previous results to the case of a continuous function $f(x)$ defined on the interval $[-L/2, L/2]$ and with periodic boundary conditions $f(-L/2) = f(L/2)$.
`Hint:` Make the limits $N \to \infty$ and $\Delta x \to 0$ with $\Delta x N = L = \text{constant}$. In extending the results follow the order: Eq. (3) → first of (4) → (5) → second of (4).

(c) Let us take a function $f_c(x) : \mathbb{R} \to \mathbb{R}$, $f_c(x) = f(x)$ on the interval $[-L/2, L/2]$ and zero elsewhere . We define the continuous periodic function

$$f_p(x) = \sum_{n\in\mathbb{Z}} f_c(x - nL) \tag{6}$$

Prove the following identity for the so called *Dirac comb* distribution:

$$\sum_{n\in\mathbb{Z}} \delta\left(\frac{x}{L} - n\right) = \sum_{m\in\mathbb{Z}} \exp(\mathrm{i}k_m x) \tag{7}$$

and apply this identity to prove the so called *Poisson sum rule*

$$f_p(x) = \frac{1}{L}\sum_{m\in\mathbb{Z}} \tilde{f}(k_m)\exp(\mathrm{i}k_m x). \tag{8}$$

Use the previous equation to prove the relation

$$\frac{\pi}{\alpha}\coth\frac{\pi}{\alpha} = \sum_{m\in\mathbb{Z}} \frac{1}{1+\alpha^2 m^2}$$

(d) **[Kür]** As a last step, extend the definition of Fourier transform to continuous functions without periodicity. Should we restrict ourselves to $\mathcal{L}^2(\mathbb{R})$, the space of the square integrable functions ?

1.2. Fourier transform of the Yukawa and Coulomb potential

The 3d Yukawa potential is given as

$$V_{\mathrm{Y}}(\mathbf{r}) \equiv V_{\mathrm{Y}}(r) = \frac{A}{r}\exp(-\alpha r) \qquad (\alpha > 0)\ .$$

(a) Calculate the Fourier transform $F_{\mathrm{Y}}(\mathbf{k})$ of the Yukawa potential

$$F_{\mathrm{Y}}(\mathbf{k}) = \int \mathrm{d}\mathbf{r}\, V_{\mathrm{Y}}(\mathbf{r})\exp(-\mathrm{i}\mathbf{k}\cdot\mathbf{r})\ .$$

(b) Calculate the Fourier transform $F_{\mathrm{C}}(\mathbf{k})$ of the 3d Coulomb potential

$$V_{\mathrm{C}}(\mathbf{r}) \equiv V_{\mathrm{C}}(r) = \frac{A}{r}\ .$$

(c) Compare this result with what is obtained by Fourier transforming the Poisson equation for a point charge in 3d.

(d) **[Kür]** Discuss the 2d and 1d case: how does the Fourier transform look like then? Make plots of the Yukawa potential in the real and momentum space for different values of the parameter α.

`Note:` The Yukawa potential -as it will be seen in coming lectures- is the Thomas-Fermi screening potential for a single point charge in 3d.