University of Regensburg Summer Term 2014

Quantum Theory of Condensed Matter I

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Sheet 1

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1. Fourier transform of the Yukawa and Coulomb potential

The 3d Yukawa potential is given as

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

1. Calculate the Fourier transform $F_{\rm Y}(\mathbf{k})$ of the Yukawa potential

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

(2 Points)

2. Calculate the Fourier transform $F_{\rm C}(\mathbf{k})$ of the 3d Coulomb potential

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

(2 Points)

2. 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 $L = N\Delta x$,

$$x_j = -\frac{L}{2} + j\Delta x, \quad j = 0, \ldots, N-1, \tag{1}$$

and consider a periodic function $f(x_j)$ such that $f(x_j) = f(x_{j+N})$. The points of the reciprocal lattice are:

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

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

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

1. 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:

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

(2 Points)

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

3. **(Oral)** 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:

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

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

$$\frac{\pi}{\alpha} \coth \frac{\pi}{\alpha} = \sum_{m\in\mathbb{Z}} \frac{1}{1 + \alpha^2 m^2} \tag{9}$$

4. **(Oral)**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?

Frohes Schaffen!