# Quantum theory of condensed matter I

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| Tue | 10:00 - 12:00 | H33 |
| Thu | 10:00 - 12:00 | H33 |
| Tue | 12:00 - 14:00 | 9.2.01 |

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**Sheet 1**

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## 1. Penetration lengths

Consider a one-dimensional finite potential well defined as:

$$V(x) = \begin{cases} V_0 & \text{if} \quad |x| \leq L/2 \\ 0 & \text{if} \quad |x| > L/2 \end{cases} \tag{1}$$

with $V_0 < 0$.

1. Find the eigenstates of the time independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{2}$$

   with the potential given above and associated to negative energies (the bound states). **(2 Points)**

2. The bound states wave function decays exponentially in the classically forbidden regions. Discuss the behavior of the penetration length of the bound states as a function of the the absolute value of its eigenenergy (i.e. as a function of the binding energy). **(2 Points)**

3. Calculate the penetration length associated to a binding energy of 5 and 50 eV. **(1 Point)**

## 2. The $\delta$ sum rules for crystals

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

$$x_j = -\frac{L}{2} + j\Delta x, \quad j = 0, \ldots, N-1, \tag{3}$$

and consider the sampling $f(x_j)$ of a periodic function $f(x) = f(x+L)$. The points of the reciprocal lattice are:

$$k_n = -\frac{\pi}{\Delta x} + n\Delta k = \frac{2\pi}{L}\left(-\frac{N}{2} + n\right), \quad n = 0, \ldots, N-1. \tag{4}$$

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

$$\tilde{f}(k_n) = \sum_{j=0}^{N-1} \Delta x \exp(-\mathrm{i}k_n x_j) f(x_j). \tag{5}$$

1. Verify the identities

$$\frac{1}{N}\sum_{j=0}^{N-1} \exp[\mathrm{i}x_j(k_n - k_m)] = \delta_{nm} \quad \text{and} \quad \frac{1}{N}\sum_{n=0}^{N-1} \exp[\mathrm{i}k_n(x_i - x_j)] = \delta_{ij} \tag{6}$$

and prove with them the validity of the inverse DFT:

$$f(x_i) = \frac{1}{2\pi} \sum_{n=0}^{N-1} \Delta k \exp(\mathrm{i} k_n x_i) \tilde{f}(k_n). \tag{7}$$

**(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. (5) $\to$ first of (6) $\to$ (7) $\to$ second of (6).
**(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 a periodic function

$$f_p(x) = \sum_{n \in \mathbb{Z}} f_c(x - nL) \tag{8}$$

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

$$\sum_{n \in \mathbb{Z}} \delta(x/L - n) = \sum_{m \in \mathbb{Z}} \exp(\mathrm{i} k_m x) \tag{9}$$

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

$$f_p(x) = \frac{1}{L} \sum_{m \in \mathbb{Z}} \tilde{f}(k_m) \exp(\mathrm{i} k_m x). \tag{10}$$

Use the previous equation to prove the relation

$$\frac{\pi}{\alpha} \coth \frac{\pi}{\alpha} = \sum_{m \in \mathbb{Z}} \frac{1}{1 + \alpha^2 m^2} \tag{11}$$

4. **(Oral)**
As a last step, extend the definition of Fourier transform to continuous functions without periodicity.
Hint: Now both the coordinate and wave vector (or time and frequency) are continuous, and span the whole real axis.
Calculate the Fourier transforms of a plane wave $f(x) = \exp(iqx)$, of a constant $f(x) = c$, and of a step function $[f(x) = 1, x > 0$ and $f(x) = 0, x < 0]$. Relate these results to each other and interpret them qualitatively.

## Frohes Schaffen!