Exercise sheet 4
Theoretical Physics 3: WS2023/2024

22.11.2023

Exercise 0

How much time did you take to complete this homework sheet?

Exercise 1. Double δ-potential (55 points)

Consider the following one-dimensional model potential for a molecule with one doubly degenerate state:

$$V(x) = -V_0 a \left(\delta(x-a) + \delta(x+a)\right),$$

Where V_0 and a are real parameters.

a) *(5 p.)* Apply the Fourier transform to the corresponding Schrödinger equation, $\hat{H}(x)\psi(x) = E\psi(x)$. Show that in the momentum space it becomes:

$$\frac{\hbar^2 k^2}{2m}\phi(k) - \frac{V_0 a}{\sqrt{2\pi}}\left(\psi(a)e^{-ika} + \psi(-a)e^{ika}\right) = E\phi(k),$$

Where:

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ikx}\psi(x) \quad \text{and} \quad \psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}k\, e^{ikx}\phi(k)$$

b) *(15 p.)* Using the obtained Schrödinger equation in the momentum space, find the bound states of the system in the coordinate space. How many bound states does the system have?
Hint: The solution must be consistent at the two points $x = \pm a$.

c) *(10 p.)* For $V_0 a = \frac{\hbar^2}{ma}$, find the energies of the stationary states and sketch the corresponding wave functions.
Hint: Use the fact that there are odd and even solutions.

d) *(10 p.)* Discuss the role of the parameter a on the stationary states (consider $a \to 0$ and $a \to \infty$).

e) *(15 p.)* Find the reflection and transmission coefficients for a beam of particles on this potential.

Exercise 2. One-dimensional infinite crystal (25 points)

Consider a one-dimensional infinite crystal. In a first approximation, it can be represented by a sequence of ions separated by some fixed distance a. We are interested in the electron energy levels in this crystal. An electron will see a periodic potential generated by the sequence of ions. For a periodic potential $V(x+a) = V(x)$, Bloch's theorem tells us that the solutions to the Schrödinger equation satisfy

$$\Psi(x+a) = e^{iKa}\Psi(x).$$

This means that we have to solve the Schrödinger equation for $0 \leq x \leq a$ only, *i.e.* one cell of the crystal. The wave function outside this cell is then given by Bloch's theorem. What remains to be fixed is the boundary condition. One usually uses the periodic boundary condition, which consists in considering a large but finite number of ions N and in imposing to the wave function the condition

$$\Psi(x + Na) = \Psi(x).$$

In the limit of infinite number of ions $N \to \infty$, we recover the infinite crystal.

a) *(5 p.)* Using Bloch's theorem and the periodic boundary condition, derive the allowed values of K. What happens in the limit $N \to \infty$?

b) *(20 p.)* Consider that the potential seen by the electron is the so-called Dirac comb

$$V(x) = \alpha \sum_{j=0}^{N-1} \delta(x - ja),$$

where is a real constant. Solve the Schrödinger equation for $0 \leq x \leq a$ and show that the allowed values of the energy E are determined by the condition

$$\cos Ka = \cos ka + \frac{m\alpha}{\hbar^2 k} \sin ka, \qquad k = \frac{\sqrt{2mE}}{\hbar}.$$

Show that the energy levels are grouped into bands for sufficiently large N.

Exercise 3. Matrices: eigenvalues and eigenvectors (20 points)

a) *(3 p.)* Consider three Pauli matrices:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Compute σ_x^2, σ_y^2, σ_z^2, and the commutators $[\sigma_x, \sigma_y]$, $[\sigma_y, \sigma_z]$, $[\sigma_z, \sigma_x]$.

b) *(5 p.)* Find the eigenvalues and eigenvectors of σ_x, σ_y and σ_z.

c) *(5 p.)* Find the eigenvalues and eigenvectors of the 2D rotation and hyperbolic rotation matrices, correspondingly:

$$\begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \cosh\phi & \sinh\phi \\ \sinh\phi & \cosh\phi \end{bmatrix}$$

d) *(7 p.)* Find the eigenvalues and eigenvectors of the following 3×3 matrices:

$$\begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 0 & 0 \\ 2 & 2 & 0 \\ 2 & 2 & 2 \end{bmatrix}$$