Exercise sheet 5
Theoretical Physics 3 : QM SS2018
Lecturer : Prof. M. Vanderhaeghen

23.05.2018

Exercise 0.

How much time did it take to complete the task?

Exercise 1. Finite square well potential. (20 points)

A particle of mass m is moving in a finite square potential well

$$V(x) = \begin{cases} -\frac{\alpha}{2a} & \text{for } -a \le x \le a \\ 0 & \text{for } x > |a| \end{cases}.$$

The energy levels are determined by the condition

$$z \tan z = \sqrt{z_0^2 - z^2}$$

where

$$z = \frac{a}{\hbar}\sqrt{2m\left(E + \frac{\alpha}{2a}\right)}, \qquad z_0 = \frac{a}{\hbar}\sqrt{\frac{m\alpha}{a}}.$$

a) *(10 p.)* Considering the limit $a \to 0$ and assuming that E is finite in this limit, show that you recover the unique bound state of the δ potential well $E = -\frac{m\alpha^2}{2\hbar^2}$.

b) *(10 p.)* What should be the value of $m\alpha a/\hbar^2$ in order for the system to have precisely n bound states?

Exercise 2. (40 + 20 points)

Consider Schrödinger equation with the following potential:

$$V(x) = \begin{cases} 0 & x < 0 \\ -V_0 & 0 < x < a \\ V_1 & x > a. \end{cases}$$

a) *(10 p.)* Consider bound states of the system ($E < 0$). Derive the transcendental equation(s) for the energy quantum number. Notice in the case $V_1 = 0$ one should recover expressions for the finite well problem considered in the lecture.

b) *(10 p.)* Write down the eigenfunctions of the Hamiltonian for the case $0 < E < V_1$.
Sketch an eigenfunction for some intermediate value of E.

c) *(5 p.)* Show that in the limit $V_1 \to +\infty$ the eigenfunctions of the Hamiltonian vanish for $x > a$. Is it true that not only the eigenfunctions of the Hamiltonian, but *all* the wave functions must vanish for $x > a$?

d) *(15 p.)* Consider scattering states for the case $E > V_1$. Derive expressions for the reflection and transmission coefficients.

e) *(10 p.)(Bonus)* Consider the limit $V_1 \to +\infty$. Prove that the system admits no bound states if and only if $V_0 \leq \pi^2\hbar^2/(8ma^2)$.

f) *(10 p.)(Bonus)* Assume that in the limit $V_1 \to +\infty$ the system does not admit bound states ($\sqrt{2mV_0 a^2/\hbar^2} < \pi/2$), whereas it is known that for $V_1 = 0$ the system always admits at least one bound state. Determine $\bar{V_1}$ such that for $V_1 < \bar{V_1}$ the system admits at least one bound state.

Exercise 3. (20 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) *(15 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 4. Matrices: eigenvalues and eigenvectors. (20 points)

a) *(5 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) *(5 p.)* Find the eigenvalues and eigenvectors of the following 3×3 matrices:

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