Exercise sheet 4 Theoretical Physics 3 : QM SS2018 Lecturer : Prof. M. Vanderhaeghen

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Exercise 0.

How much time did it take to complete the task?

Exercise 1. Fourier transform. (15 points)

Calculate the Fourier transforms of the following equations using the definition given in the lecture

- c) (4 p.) $f(x) = \cos(x)$
- d) (7 p.) $f(x) = \begin{cases} 1 |t|, & |t| \le 1\\ 0, & |t| > 1 \end{cases}$

Exercise 2. Double δ -potential. (45 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

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

Hint: Use $\int_{-\infty}^{\infty} \mathrm{d}x \, x e^{ax} = \frac{\partial}{\partial a} \int_{-\infty}^{\infty} \mathrm{d}x \, e^{ax}$

- b) (10 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) (5 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 3. Matrices. (40 points)

Recall that the matrix multiplication is a non-commutative operation. We define the commutator of two matrices A and B as [A, B] = AB - BA.

a) (10 p.) Prove the following identities for arbitrary matrices A, B and C:

$$[A, BC] = [A, B]C + B[A, C],$$
$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0.$$

b) (10 p.) Consider a specific case when [A, [A, B]] = [B, [A, B]] = 0. Prove by induction, that

$$[A, B^n] = [A, B]nB^{n-1}.$$

c) (10 p.) We define a function of a matrix variable f(A) through the Maclaurin series expansion (assuming it is possible):

$$f(A) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} A^n.$$

In the case [A, [A, B]] = [B, [A, B]] = 0 show that

$$[A, F(B)] = [A, B]F'(B),$$

where F' is the function obtained by differentiation of F.

d) (10 p.) Consider the same case [A, [A, B]] = [B, [A, B]] = 0, and prove the Glauber formula

$$e^{A} e^{B} = e^{A+B} e^{\frac{1}{2}[A,B]}$$

Hint: Consider the function $F(t) = e^{tA} e^{tB}$. Show that it has to satisfy the differential equation $\frac{dF(t)}{dt} = (A+B+t[A,B])F(t)$. Then solve the equation by noting that (A+B) and [A,B] commute, and, hence, can be treated as mere numbers.

(Bonus) Exercise 4. (30 points)

During the lecture, you have learned that a free particle can be described by the wave packet

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \,\phi(k) e^{i(kx - \hbar k^2 t/(2m))}.$$

As was demonstrated, if k is narrowly distributed around k_0 a wave packet is evenly moving with a so-called group velocity $v_g = \frac{d\omega_k}{dk}$ which coincides with the classical value. Let us pretend for a moment we are physicists living many years ago and we are not sure about the

Let us pretend for a moment we are physicists living many years ago and we are not sure about the physical meaning of $\|\psi(x,t)\|^2$. The obtained result provide a hypothesis that a group of de Broglie waves forms a particle. In this way, our goal is to check if $\|\psi(x,t)\|^2$ can be interpreted as the mass density of a particle. To answer this question you are supposed to solve the following tasks.

Consider a wave packet with

$$\phi(k) = C e^{-(k-k_0)^2/(4\Delta^2)},$$

where C is the normalization factor.

a) (10 p.) Performing integration, show that

$$\psi(x,t) \propto e^{ik_0 x - i\omega_{k_0} t} \sqrt{\frac{4\pi\Delta^2}{1 + i2\hbar\Delta^2 t/m}} \exp\left[-\frac{\Delta^2 (x - v_g t)^2}{1 + i2\hbar\Delta^2 t/m}\right]$$

Hint: $\int_{-\infty}^{\infty} dx \, e^{-ax^2 + bx} = \sqrt{\frac{\pi}{a}} e^{b^2/(4a)}$, Re a > 0.

b) (10 p.) Using properties of complex numbers, write the obtained wave function in the form

$$\psi(x,t) = e^{ik_0 x - i\omega_{k_0} t} e^{i(\alpha - \phi/2)} \frac{\exp\left[-\frac{(x - v_g t)^2}{4\langle \Delta x^2 \rangle}\right]}{(2\pi \langle \Delta x^2 \rangle)^{1/4}}, \quad \text{where} \quad \langle \Delta x^2 \rangle = \frac{1}{4\Delta^2} \left[1 + \left(\frac{2\hbar\Delta^2 t}{m}\right)^2\right]$$

and $\phi = \arctan(2\hbar\Delta^2 t/m)$.

- c) (5 p.) Assume at t = 0 an electron is localized in an area $\sqrt{\langle \Delta x^2 \rangle} \sim 1$ Å. Estimate the localization region after one second.
- d) (5 p.) Can $||\psi(x,t)||^2$ be interpreted as the mass density of a particle? Why?