Exercise Sheet 3 **Theoretische Physik 4: Quantenmechanik**

SoSe 2025 Prof. Dr. C. Gros

Posted 12.05.2025, due by 12:00pm 19.05.2025.

Exercise 1 (5 points) PROPERTIES OF BOUND STATES AND THE δ-POTENTIAL

We will be concerned with solving the time-independent Schrödinger equation $\hat{H}\psi(x) = E\psi(x)$ of a one particle Hamiltonian operator $\hat{H} = \hat{p}^2/2m + V(\hat{x})$. The time-independent Schrödinger equation can admit two broad categories of solutions:

• Unbound solutions, usually running wave solutions $\psi(x) \propto \mathrm{e}^{\pm ipx/\hbar}$, also called the continuum because they hold for densely many and unbound from above values of p. Such solutions cannot be normalized at infinity.
• Bound state solutions, which are "localized" in space, unlike running waves which run off to infinity. They must have a controlled finite real space spread $\Delta x < \infty$ that characterizes their localization. This makes them normalizable.

Bound state solutions have energy eigenvalues that are smaller than the potential at infinity, so they are bound from above $E < V(\infty)$. They are also bound from below.

1. (2/5) Use the expectation value $\langle \hat{H} \rangle$ to show that bound state energy eigenvalues E must be bound from bellow $V_{\min} < E$, where $V_{\min}$ the minimum value of the potential $V(x)$.

Now consider a specific case, the δ-potential $V(x) = -\lambda\delta(x)$, where $\lambda > 0$ a constant.

2. (1/5) Argue that if you are looking for bound states of this potential, then you only need to consider $E < 0$.
3. (2/5) What are the units of the constant λ? Is there a way to think of this potential as a limiting case of the finite square well potential

$$V(x) = \begin{cases} -V_o & |x| < L/2 \\ 0 & |x| > L/2 \end{cases} \tag{1}$$

with $V_o > 0$? What would be the limit and what should be the relation of λ, V_o, and L for this to work?

Exercise 2 (3 points) BOUND STATES OF THE δ-POTENTIAL

Consider the one dimensional δ-potential $V(x) = -\lambda\delta(x)$, where $\lambda > 0$ a constant.

1. (3/3) Following the same procedure as the lectures, and considering the continuity conditions of the previous exercise sheet, show that there is only one bound state in this potential, and show that the bound state energy eigenvalue is $E = -\kappa^2\hbar^2/(2m) = -m\lambda^2/(2\hbar^2)$ and the corresponding normalized eigenvector is $\psi(x) = N\mathrm{e}^{-\lambda|x|\kappa}$, with $\kappa = m\lambda/\hbar^2$ and $N = \sqrt{\kappa} = \sqrt{m\lambda}/\hbar$.

Exercise 3 (4 points) REFLECTION AND TRANSMISSION IN THE δ-POTENTIAL

Lets examine what happens in the δ-potential $V(x) = -\lambda\delta(x)$ if we consider $E > 0$. In this case we will have a continuum of unbound states, described by running waves $\mathrm{e}^{\pm ikx}$ (it may be useful to you to consider the comparison to the bound state solution, and why $E < 0$ vs $E > 0$ gives you real vs imaginary exponentials respectively). Let us imagine an experiment, of shooting particles in from $-\infty$, and scattering at $x = 0$ off the delta peak. Some particles may scatter back and some may go through. Putting it all together, this experiment may be described, up to an overall normalization constant, by the wavefunction

$$\psi_k(x) \propto \begin{cases} \mathrm{e}^{ikx} + R\mathrm{e}^{-ikx} & x < 0 \\ T\mathrm{e}^{ikx} & x > 0 \end{cases}. \tag{2}$$

where R is the reflection coefficient, and T the transmitted coefficient. One way to rationalize this unnormalizable running wave wavefunction is with the probability current.

1. (1/4) Calculate the probability current $J(x)$ for a running wave $\psi(x) = A\mathrm{e}^{\pm ikx}$ with $k > 0$, and argue why the "+(−)" exponential can be understood as a particle density ρ_o, travelling with velocity $v = +(-)\hbar k/m$, moving to the right(left). What is the particle density ρ_o of this running wave? Using this interpretation, explain what do the exponentials and coefficients in the $\psi_k(x)$ represent?

2. (1/4) Using the continuity equation $\partial_t \rho(x,t) + \partial_x J(x,t) = 0$ show that the probability density $\rho(x,t)$ does not accumulate at any point in space, or in other words, you are trying to show that at any point $x = x_o$ in space all the incoming and outgoing probability currents balance out and you have $J(x_o - \epsilon, t) = J(x_o + \epsilon, t)$ for arbitrary small $\epsilon > 0$.

3. (1/4) Using the previous result, apply it to the wavefunction $\psi_k(x)$, to show that $|R|^2 + |T|^2 = 1$, which allows you to interpret $|R|^2$ and $|T|^2$ as the probability of reflection and transmittion.

4. (1/4) Given the continuity conditions at $x = 0$, show that $R = iK/(1 - iK)$ and $T = 1/(1 - iK)$, where $K = \kappa/k = m\lambda/(\hbar^2 k)$. Verify that $|R|^2 + |T|^2 = 1$ indeed holds for this result.

Exercise 4 (8 points) **SPREAD OF THE BOUND STATE OF THE δ-POTENTIAL**

Bound state solutions are localized in space so they have a finite $\Delta x < \infty$ that characterizes the amount of localization. From the uncertainty principle $\Delta x \Delta p \geq \hbar/2$ this means that the bound state momentum spread is also finite $\Delta p < \infty$. Lets see this in action for the bound state of the δ-potential $V(x) = -\lambda\delta(x)$.

1. (2/8) Find $\Delta x \Delta p$ graphically for the bound state. To do this you will need also the Fourier transform $\widetilde{\psi}(p)$ of $\psi(x) = N\mathrm{e}^{-\lambda|x|\kappa}$, but actually you should already know this Fourier transform from last weeks exercise as the Lorentzian $\widetilde{\psi}(p) = \dfrac{1}{\sqrt{2\pi}} \dfrac{2\kappa N}{\kappa^2 + (p/\hbar)^2}$. Now do the following:

   Set $\lambda = \hbar^2/m$ for simplicity, and plot the probability density $\rho(x) = |\psi(x)|^2$ in the range range $x \in [-2, 2]$, and the momentum probability density $\widetilde{\rho}(p/\hbar) = |\widetilde{\psi}(p/\hbar)|^2$ in the range $p/\hbar \in [-2, 2]$. Find where and and what is the maximum probability $P_{\max}$ for both cases. Argue graphically at what points does the probability drop to $P_{\max}/2$. From here the spreads Δx and Δp follow, and you should be able to show that $\Delta x \Delta p \sim \hbar$.

Now lets do this calculation more seriously. To find the spread of a physical observable $\hat{\mathcal{O}}$ in a specific state $\psi(x)$ we need to calculate $\Delta\mathcal{O} = \langle \mathcal{O}^2 \rangle - \langle \mathcal{O} \rangle^2$.

2. (1/8) Making use of the oddness of the integration, show that $\langle \hat{x} \rangle = 0$ and $\langle \hat{p} \rangle = 0$.

3. (1/8) Show that for the δ-potential bound state $\langle \hat{x}^2 \rangle = h^4/(2m^2\lambda^2)$.

   (Hint: $\int_0^{+\infty} \mathrm{d}x x^2 \mathrm{e}^{-cx} = \dfrac{2}{c^3}$ for $c > 0$)

To evaluate $\langle \hat{p}^2 \rangle = \int_{-\infty}^{+\infty} \mathrm{d}x \psi^*(x) \hat{p}^2 \psi(x)$ for the bound state $\psi(x)$ some care is needed because there is a singular issue. Let us identify the issue first.

4. (1/8) Evaluate $\hat{p}\psi(x) = -i\hbar\partial_x \psi(x)$ as a piece wise function for $x < 0$ and $x > 0$. You will notice a problem at $x = 0$ which does not allow you to continue with a second derivative, *what is the problem?*.

5. (2/8) Show that you can avoid this issue and find that $\langle \hat{p}^2 \rangle = m^2\lambda^2/h^2$.

6. (1/8) Show that $\Delta x \Delta p = \hbar/\sqrt{2}$. Is this result reasonable? Compare to the graphical estimation you did before, was the prediction any good and why?