Moderne Physik für Lehramtskandidaten

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Lösung 10

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Aufgabe 1: Gaußsches Wellenpaket (10 P)

Gegeben sei ein Wellenpaket für ein freies Teilchen mit der Impulsverteilung

$$g(k) = \frac{\sqrt{a}}{(2\pi)^{1/4}} \exp\Big(-\frac{a^2k^2}{4}\Big)$$

Wir betrachten ein Wellenpaket aus ebenen Wellen mit genau dieser Verteilung:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k g(k) e^{\mathrm{i}(kx-\omega_k t)}$$

mit der Dispersionrelation $\omega_k = \hbar k^2/2m$.

(a) **(4 P)** Zunächst diskutieren wir den Zeitpunkt $t = 0$. Zeigen Sie, dass $\psi(x, 0)$ auch eine Gauß-Funktion ist und bestimmen Sie die Breite der Wahrscheinlichkeitsdichte, $|\psi|^2$. Wie hängt diese von a ab?

(b) **(3 P)** Die Standard-Abweichung einer Observablen $\mathcal{O}$ ist definiert durch:

$$\Delta\mathcal{O} \coloneqq \sqrt{\langle \mathcal{O}^2 \rangle - \langle \mathcal{O} \rangle^2}$$

wobei der Erwartungswert definiert ist durch

$$\langle \mathcal{O} \rangle (t) = \int_{-\infty}^{\infty} \mathrm{d}x \psi^\dagger(x,t) \mathcal{O} \psi(x,t)$$

Zeigen Sie für $t = 0$, dass $\psi(t = 0)$ ein Zustand minimaler Unschärfe ist, sodass folgendes gilt:

$$\Delta x \Delta p = \hbar/2$$

(c) **(3 P)** Bestimmen Sie nun $\psi(x,t)$ für beliebige Zeiten t und diskutieren Sie das Verhalten der Wahrscheinlichkeitsdichte mit der Zeit. Ist es immernoch ein Zustand minimaler Unschärfe?

Solution to Aufgabe 1

Initially, as you saw in lectures, we described a free particle as a wave, and the physical state as being a overlap of many plane waves. The problem is that the plane wave solution is not normalizable, thus the wavefunction, or more appropriately the squared wavefunction, cannot be physical.

Momentum distribution is a Gaussian distribution:

$$g(k) = \frac{\sqrt{a}}{(2\pi)^{1/4}} e^{-a^2k^2/4}$$

Wave packet:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}k g(k) e^{\mathrm{i}(kx-\omega t)}$$

This is a Fourier transform of the plane wave. Fourier transforms connect the position-space-representation and the momentum-space-representations.

For $t = 0$, we have that $\psi(x, t = 0)$ is a state with the minimal uncertainty:

$$\Delta x \cdot \Delta p = \hbar/2$$

We will take as a given that

$$\int_{\infty}^{\infty} \mathrm{d}x e^{-x^2/a^2} = a\sqrt{\pi}$$

Note: to show this, simply square the integral, using y as the label for the integration variable, and use polar coordinates (correctly changing the limits of integration while you do so).

For $t = 0$:

$$\psi(x) := \psi(x, t = 0) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}k \frac{\sqrt{a}}{(2\pi)^{1/4}} e^{-a^2k^2/4+\mathrm{i}kx}$$

Let the exponential's argument be E:

$$\begin{aligned}
E &= a^2k^2/4 - \mathrm{i}kx \\
&= (a/2)^2\big[k^2 - 4\mathrm{i}kx/a^2 + \big(\frac{2\mathrm{i}x}{a^2}\big)^2\big] - a^2\big(\frac{\mathrm{i}x}{a^2}\big)^2 \\
&= (a/2)^2\big[k - \mathrm{i}\frac{2x}{a^2}\big]^2 + (x/a)^2 \\
E &:= (a/2)^2u^2 + (x/a)^2
\end{aligned}$$

Thus:

$$\begin{aligned}
\psi(x) &= \frac{\sqrt{a}}{(2\pi)^{3/4}} \exp\big(-x^2/a^2\big) \int_k \mathrm{d}k \exp\Big[-\big(\frac{a}{2}\big)^2u^2\Big] \\
&= \frac{\sqrt{a}}{(2\pi)^{3/4}} \exp\big(-x^2/a^2\big) \int_{\mathbb{R}} \mathrm{d}u \exp\Big[-\big(\frac{a}{2}\big)^2u^2\Big]
\end{aligned}$$

So overall we have:

$$\begin{aligned}
\Rightarrow \psi(x) &= \big(\frac{2}{\pi a^2}\big)^{1/4} \exp\big(-\frac{x^2}{a^2}\big) \\
g(k) &= \frac{\sqrt{a}}{(2\pi)^{1/4}} e^{-a^2k^2/4}
\end{aligned}$$

i.e. $\psi(x)$ is a Gaussian with width $1/a$, and $g(k)$ a Gaussian with width a.

Calculating the Uncertainty:

$$\begin{aligned}
\Delta\mathcal{O} &= \sqrt{\langle\mathcal{O}^2\rangle - \langle\mathcal{O}\rangle^2} \\
\text{where } \mathcal{O} &= \int_{\mathbb{R}} \mathrm{d}x \psi^*(x)\mathcal{O}\psi(x)
\end{aligned}$$

Thus, the expectation value of the position operator:

$$\begin{aligned}\langle \hat{X} \rangle &= \int_{\mathbb{R}} \mathrm{d}x \psi^*(x) \hat{X} \psi(x) \\ &= \int_{\mathbb{R}} \mathrm{d}x \psi^*(x) x \psi(x)\end{aligned}$$

where we have used $\hat{X}\psi(x) = x\psi(x)$.

Inserting the wavepacket we have above:

$$\langle \hat{X} \rangle = (\frac{2}{\pi a^2})^{1/2} \int_{\mathbb{R}} x \exp(-\frac{2x^2}{a^2}) = 0$$

where we've used the fact that x is an antisymmetric function and the exponential term is symmetric, thus integrating over all x will yield 0.

Now the variance:

$$\begin{aligned}\langle \hat{X}^2 \rangle &= \int_{\mathbb{R}} \mathrm{d}x \psi^*(x) x^2 \psi(x) \\ &= (\frac{2}{\pi a^2})^{1/2} \int_{\mathbb{R}} x^2 \exp(-\frac{2x^2}{a^2}) \\ &= a^2/4 \\ \Rightarrow \Delta \hat{X} &= \sqrt{\langle \hat{X}^2 \rangle - \langle \hat{X} \rangle^2} = a/2\end{aligned}$$

Repeating the same analysis for the momentum operator:

$$\begin{aligned}\langle \hat{P} \rangle &= \langle \mathrm{i}\hbar \partial_x \rangle \\ &= i\hbar \int_{\mathbb{R}} \mathrm{d}x \psi^*(x) \partial_x \psi(x) \\ &= i\hbar (\frac{2}{\pi a^2})^{1/2} \int_{\mathbb{R}} \mathrm{d}x \big(-\frac{2x}{a^2}\big) \exp(-\frac{2x^2}{a^2}) = 0\end{aligned}$$

where we have used the symmtery and antisymmetry argument to evaluate it, as before.

For the variance:

$$\begin{aligned}\langle \hat{P}^2 \rangle &= -\hbar^2 \int_{\mathbb{R}} \mathrm{d}x \psi^*(x) \partial_x^2 \psi(x) \\ &= -\hbar^2 (\frac{2}{\pi a^2})^{1/2} \int_{\mathbb{R}} \mathrm{d}x \exp(-\frac{x^2}{a^2}) \partial_x^2 \Big[\exp(-\frac{x^2}{a^2}) \Big] \\ &= -\hbar^2 (\frac{2}{\pi a^2})^{1/2} \int_{\mathbb{R}} \mathrm{d}x \exp(-\frac{x^2}{a^2}) \partial_x \Big[\big(-\frac{2x}{a^2}\big) \exp(-\frac{x^2}{a^2}) \Big] \\ &= -\hbar^2 (\frac{2}{\pi a^2})^{1/2} \int_{\mathbb{R}} \mathrm{d}x \exp(-\frac{x^2}{a^2}) \Big[\big(-\frac{2}{a^2} + \frac{4x^2}{a^4}\big) \Big] \exp(-\frac{x^2}{a^2}) \\ &= \hbar^2 (\frac{2}{\pi a^2})^{1/2} \int_{\mathbb{R}} \mathrm{d}x \Big[\big(-\frac{2}{a^2} + \frac{4x^2}{a^4}\big) \Big] \exp(-\frac{2x^2}{a^2})\end{aligned}$$

First term is just a Gaussian integral, and the second is an x^2 Gaussian integral, leading to the final expression of:

$$\begin{aligned}\langle \hat{P}^2 \rangle &= \hbar^2/a^2 \\ \Rightarrow \Delta \hat{P} &= \hbar/a\end{aligned}$$

So overall, the uncertainty relationship for $t = 0$ is:

$$\Delta\hat{X}\Delta\hat{P} = \hbar/2$$

For arbitrary times:

$$\begin{aligned}\psi(x,t) &= \frac{\sqrt{a}}{(2\pi)^{3/4}}\int_{\mathbb{R}} \mathrm{d}k \exp\Big[-fraca^2k^24 + \mathrm{i}kx - \mathrm{i}\omega t\Big] \\ &= \frac{\sqrt{a}}{(2\pi)^{3/4}}\int_{\mathbb{R}} \mathrm{d}k \exp\Big[-\big(a^2 + 2\frac{\mathrm{i}\hbar t}{m}\big)\frac{k^2}{4} + \mathrm{i}kx\Big]\end{aligned}$$

where we have used the dispersion relation for ω:

$$\omega = \hbar^2k^2/2m$$

Defining:

$$a^2 + 2\frac{\mathrm{i}\hbar t}{m} := \alpha$$

leads to:

$$\psi(x,t) = \frac{\sqrt{a}}{(2\pi)^{3/4}}\int_{\mathbb{R}} \mathrm{d}k \exp\Big[-\alpha\frac{k^2}{4} + \mathrm{i}kx\Big]$$

which is analogous to a Gaussian of the form

$$\frac{\sqrt{a}}{\alpha}\big(\frac{2}{\pi\alpha^2}\big)^{1/4}\exp\big(-\frac{x^2}{\alpha^2}\big)$$

Rearranging the wavefunction:

$$\psi(x,t) = \big(\frac{2a^2}{\pi}\big)^{1/4}\frac{1}{\big(a^2 + 2\mathrm{i}\hbar t/m\big)^{1/2}}\exp\Big[-\frac{x^2}{a^2 + 2\mathrm{i}\hbar t/m}\Big]$$

Notice that the width of the distribution is dependent on time!

The probability density is then given by:

$$|\psi|^2 = \big(\frac{2}{\pi a^2}\big)^{1/2}\frac{1}{\big(1 + 4\hbar^2t^2/(m^2a^4)\big)^{1/2}}\exp\Big(-\frac{2x^2}{a^2\big(1 + 4\hbar^2t^2/(m^2a^4)\big)}\Big)$$

Remember: $\psi(x,t)$ is not an observable!!! $|\psi(x,t)|^2$ - the probability density is measurable.

Width of the probability density $|\psi|^2$ - begin by defining:

$$\beta = a\sqrt{1 + \frac{4\hbar^2}{m^2a^4}t^2}$$

You can go through exactly the same calculations we did before for the expectation values of the position and momentum operators:

$$\begin{aligned}\langle\hat{X}^2\rangle &= \frac{\beta^2}{4} \\ \langle\hat{P}^2\rangle &= \frac{\hbar^2\beta^2}{|\alpha|^2} \\ \langle\hat{X}\rangle &= \langle\hat{P}\rangle = 0\end{aligned}$$

So overall, the Uncertainty Relation is given by:

$$\Delta\hat{X}\Delta\hat{P} = \frac{\hbar}{2}\big(1 + \frac{4\hbar^2}{m^2a^4}t^2\big)^{1/2} \geq \frac{\hbar}{2}$$

where we have used the fact that the second term in square brackets is always greater than or equal to 0.

Aufgabe 2: Unendlicher Potentialtopf (10 P)
Betrachten Sie ein Teilchen im folgenden eindimensionalen Potential

$$V(x) = \begin{cases} 0, & x \in [-a/2, a/2] \\ \infty, & \text{sonst} \end{cases}$$

wobei a die Breite des Potentialtopfes parametrisiert. Lösen Sie die stationäre Schrödingergleichung für $E > 0$

$$\Big[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\Big]\psi(x) = E\psi(x)$$

Eine allgemeine Lösung der Wellengleichung ist gegeben durch

$$\psi(x) = \alpha e^{ikx} + \beta e^{-ikx}$$

wobei die Paramete α, β durch die Randbedingungen bestimmt werden können. Überlegen Sie sich dazu wie die Wellenfunktion außerhalb des Topfes aussehen und welche weitere Eigenschaften die Wellenfunktion erfüllen muss.

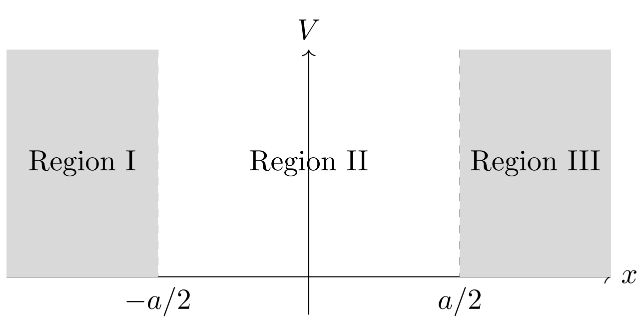
(a) Bestimmen Sie die Energieeigenwerte und die Wellenfunktionen und zeigen Sie dass die Energie *quantisiert* ist.

(b) Was passiert für Energien $E < 0$?

Solution to Aufgabe 2:
Infinite potential well described by the following potential:

$$V(x) = \begin{cases} 0, & x \in [-a/2, a/2] \\ \infty, & \text{sonst} \end{cases}$$

A sketch of the system:



(a) We begin by considering the positive energy case $E > 0$.
Recipe for potential problems:

1. Begin by dividing the problem into physical and unphysical areas. Here regions 1 and 3 are unphysical due to their infinite potential energies, while region 2 is the allowed space.

2. Ansätze for the different areas:

$$\psi_I(x) = \psi_{III}(x) = 0 \quad \forall x \in I, III$$
$$\psi_{II}(x) = \alpha e^{\mathrm{i}kx} + \beta e^{-\mathrm{i}kx}$$

Region II is the physically allowed region, so we use the ansatz of plane waves, and there are two degrees of freedom.

3. Determining the energies:

We use the Schrödinger equation:

$$\Big[-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\Big]\psi(x) = E\psi(x)$$
$$\Leftrightarrow \hat{S}\psi(x) = 0$$
$$\text{where } \hat{S} = -\frac{\hbar^2}{2m}\partial_x^2 + V(x) - E$$

Applying this operator $\hat{S}$ to the wavefunction in region II:

$$\hat{S}\psi_{II}(x) = 0$$
$$\Rightarrow -\frac{\hbar^2}{2m}\big((\mathrm{i}k)^2\alpha e^{\mathrm{i}kx} + (-\mathrm{i}k)^2\beta e^{-\mathrm{i}kx}\big) + 0 - E\psi_I I(x) = 0$$
$$\Rightarrow \Big(-\frac{\hbar^2}{2m}(\mathrm{i}k)^2 - E\Big)\psi(x) = 0 \quad \forall x \in \mathbb{R}$$
$$\Rightarrow k^2 = \frac{2mE}{\hbar^2} \;\; \forall \, x \in \text{ Region II}$$

k would become imaginary for $E < 0$!

4. Determination of the free parameters by using the boundary conditions/constraints.

Things we know about the wavefunction

- $\psi(x)$ is continuous.
- $\psi(x)$ is differentiable.
- $\int \mathrm{d}x|\psi(x)|^2 = 1$ - conservation of unit probability.

(i) Using the first quality (continuity):

$$\psi_I(x = -a/2) \overset{!}{=} \psi_{II}(x = -a/2)$$
$$\Leftrightarrow 0 = \alpha e^{-\mathrm{i}ka/2} + \beta e^{\mathrm{i}ka/2} - (1)$$

Similarly on the other side:

$$\psi_{II}(x = a/2) \overset{!}{=} \psi_{III}(x = a/2)$$
$$\Leftrightarrow 0 = \alpha e^{\mathrm{i}ka/2} + \beta e^{-\mathrm{i}ka/2} - (2)$$

Rewriting (1) and (2) and subtracting:

$$\alpha + \beta e^{\mathrm{i}ka} = 0$$
$$\alpha + \beta e^{-\mathrm{i}ka} = 0$$
$$\Rightarrow \beta\big(e^{\mathrm{i}ka} - e^{-\mathrm{i}ka}\big) = 0$$

So we could have the solutions $\beta = 0$, but then $\alpha = 0$, i.e. the wavefunction is trivially 0 everywhere. The other solution is that:

$$2i\beta \sin(ka) = 0$$
$$\Rightarrow ka = n\pi, \quad n \in \mathbb{Z}$$

and using $k = \sqrt{2mE/\hbar}$, the energy levels are given by:

$$E_n = \frac{\pi^2\hbar^2}{2ma^2}n^2, \quad n \in \mathbb{Z}$$

i.e. we have quantized energy levels! What do the energy levels look like?
The question now is: what is α? Adding (1) and (2):

$$\begin{aligned} \alpha &= -\beta \\ \Rightarrow \psi_{II}(x) &= \alpha\big(e^{ikx} - e^{-ikx}\big) \\ &= 2i\alpha \sin kx \\ &= \tilde{\alpha} \sin\big(n\pi x/a\big) \end{aligned}$$

where the $\tilde{\alpha}$ is still a free parameter.

(ii) Now we can use the normalization condition:

$$\begin{aligned} \int dx|\psi|^2 &= \int_{-a/2}^{a/2} dx|\psi_{II}(x)|^2 \\ &= \int_{-a/2}^{a/2} |\tilde{\alpha}|^2 \sin^2 kx \\ &= |\tilde{\alpha}|^2\big(\frac{a}{2} - \frac{\sin ka}{2k}\big) \end{aligned}$$

The second term on the last line will always be zero ($ka = n\pi \Rightarrow \sin ka = 0$), so we finally have:

$$\begin{aligned} 1 &= |\tilde{\alpha}|^2\frac{a}{2} \\ \Rightarrow \tilde{\alpha} &= \sqrt{2/a} \end{aligned}$$

Thus, overall, we have a wavefunction that looks like:

$$\psi(x) = \begin{cases} 0, & x \in I \\ \sqrt{2/a}\sin kx, & x \in II \\ 0, & x \in III \end{cases}$$

with energy levels given by:

$$E_n = \frac{\pi^2\hbar^2}{2ma^2}n^2$$

i.e. we have quantized energies of standing waves.

(b) For the case of negative energy $E < 0$, the negative energy solutions are unphysical and there are no such particles that can exist.

N.B. The eigenvalues, i.e. the energies E_n of the potential well should be the same regardless of the choice of coordinates, but note that $\psi(x)$ does change. This is because the translation introduces a phase-shift, which is not observable (upon taking the mod-square of the wavefunction, it yields unity).