Karlsruher Institut für Technologie

Moderne Physik für Lehramtskandidaten

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Lösung 09

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Aufgabe 1: Operatoren in der Quantenmechanik (10 P)

(a) Der Kommutator für zwei lineare Operatoren A und B ist definiert durch

$$[A, B] \coloneqq AB - BA$$

Zeigen Sie die folgende Eigenschaften des Kommutators, wenn A, B, C lineare Operatoren und $\lambda \in \mathbb{R}$ sind:

- Antisymmetrie: $[A, B] = -[B, A]$
- Linearität: $[\lambda A + B, C] = \lambda[A, C] + [B, C]$
- Prodktregel: $[A, BC] = [A, B]C + B[A, C]$
- Jacobi-Indentität:

$$\big[A, [B, C]\big] + \big[B, [C, A]\big] + \big[C, [A, B]\big] = 0$$

(b) In der Quantenmechanik werden die physikalischen Observablen als Operatoren identifiziert. Die Ortskoordinaten und Impulse von Teilchen werden nun durch den Ortsoperator X bzw. Impulseoperator P dargestellt, die auf die Wellenfunktion $\psi(\boldsymbol{x}, t)$ wirken. Dies ist eine Eigenwertgleichung:

$$X_i \psi(\boldsymbol{x}, t) = x_i \psi(\boldsymbol{x}, t)$$
$$P_i \psi(\boldsymbol{x}, t) = p_i \psi(\boldsymbol{x}, t)$$

wobei $x_i, p_i \in \mathbb{R}$ den gemessen Orten bzw. Impulsen entspricht. In der *Ortsraumdarstellung* gilt:

$$X_i \psi(\boldsymbol{x}, t) = x_i \psi(\boldsymbol{x}, t)$$
$$P_i \psi(\boldsymbol{x}, t) = -\mathrm{i}\hbar \frac{\partial}{\partial x_i} \psi(\boldsymbol{x}, t)$$

(i) Zeigen Sie in dieser Darstellung die *kanonischen Vertauschungsrealtionen*

$$\big[X_i, P_i\big] \psi(\boldsymbol{x}, t) = \mathrm{i}\hbar \delta_{ij} \psi(\boldsymbol{x}, t)$$

(ii) Der Hamilton Operator für ein freies Teilchen lautet $H = \sum_i P_i^2/2m$. Zeigen Sie

$$\big[X_i, H\big] \psi(\boldsymbol{x}, t) = \frac{\mathrm{i}\hbar}{m} P_k \psi(\boldsymbol{x}, t)$$

Solution to Aufgabe 1:

In quantum mechanics, observables (real values that one can obtain by performing measurements on a quantum system) are mathematically described by linear operators of a Hilbert space.

Why Hilbert spaces?

Physical states of a system are described as vectors in a Hilbert space. $|\psi\rangle \in \mathcal{H}$ and Hilbert spaces are complete (vollständige), thus have a complete basis (a set of linearly independent basis vectors) so a basis representation is possible. Hilbert spaces also have a natural definition of the scalar product and hence normalization - extremely important concepts of quantum mechanics.

Consider the equation:

$$\hat{X}\,|\psi\rangle = x_i\,|\psi\rangle$$

This is an eigenvalue equation, with $\hat{X}$ being the operator, $|\psi\rangle$ the physical state of the system, and $x_i \in \mathbb{R}$ being the eigenvalue of the operator.

So, measurements in QM correspond to determination of the eigenvalue of the corresponding operator.

(a) Commutator of two operators:

$$[A, B] = AB - BA$$

For linear operators, the commutator is generally **not** vanishing: $[A, B] \neq 0$.

To so the properties of the commutator:

- Anti-symmetry:

$$[A, B] = AB - BA = -(BA - AB) = -[B, A]$$

- Bi-linearity:

$$\begin{aligned}[\lambda A + B, C] &= (\lambda A + B)C - C(\lambda A + B)\\ &= \lambda AC + BC - C\lambda A - CB\\ &= \lambda(AC - CA) + BC - CB\\ &= \lambda[A, C] + [B, C]\end{aligned}$$

- Product rule:

$$\begin{aligned}[A, BC] &= ABC - BCA\\ &= ABC - BCA + BAC - BAC\\ &= ABC - BAC + BAC - BCA\\ &= (AB - BA)C + B(AC - CA)\\ &= [A, B]C + B[A, C]\end{aligned}$$

- Jacobi identity (defines the Lie-algebra):

$$\begin{aligned}\big[A, [B, C]\big] &= [A, BC - CB]\\ &= [A, BC] - [A, CB]\\ &= [A, B]C + B[A, C] - [A, C]B - C[A, B]\end{aligned}$$

Expanding the other two terms: $[B, [C, A]]$ and $[C, [A, B]]$, and adding all 12 terms together we see that they all cancel, leading to 0, i.e. the Jacobi identity

(b) Position representation of $\hat{X}, \hat{P}$:

$$\hat{X} : L^2 \to \mathbb{R}, \quad \hat{X}\psi(x) = x_i\psi(x)$$

where:

- L^2 is a square-integrable function
- $\psi(x,t)$ is the wavefunction
- $|\psi(x,t)|^2$ is the probability density
- $\int_{\mathbb{R}} \mathrm{d}x |\psi(x,t)|^2 = 1$ normalization condition
- Momentum operator $\hat{P} = -\mathrm{i}\hbar\frac{\partial}{\partial x}$

Bra-ket notation:

$$|\psi\rangle \in \mathcal{H} \leftarrow \text{ket}$$
$$\langle\psi| \in \mathcal{H}^* \leftarrow \text{bra}$$

where the bra lives in the dual Hilbert space.

The wavefunction $\psi(x)$ is given by:

$$\psi(x) = \langle x|\psi\rangle$$

i.e. a projection into the position space.

We have the following:

$$\langle x|\, \hat{X}\, |\psi\rangle = \langle x|\, x_i\, |\psi\rangle = x_i\, \langle x|\psi\rangle = x_i\psi(x)$$
$$\langle x|\, \hat{P}\, |\psi\rangle = -\mathrm{i}\hbar\frac{\partial}{\partial x}\, \langle x|\psi\rangle = -\mathrm{i}\hbar\frac{\partial}{\partial x}\psi(x)$$

What is the commutator of $\hat{X}$ and $\hat{P}$?

$$\begin{aligned}
\big[\hat{X}_i, \hat{P}_j\big]\psi(x,t) &= -\mathrm{i}\hbar\big(x_i\frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_j}x_i\big)\psi(x,t) \\
&= -\mathrm{i}\hbar\big(x_i\frac{\partial}{\partial x_j}\psi(x,t) - \frac{\partial}{\partial x_j}\big[x_i\psi(x,t)\big]\big) \\
&= -\mathrm{i}\hbar\big(x_i\frac{\partial}{\partial x_j}\psi(x,t) - \big[\delta_{ij}\psi(x,t) + x_i\frac{\partial}{\partial x_j}\psi(x,t)\big]\big) \\
&= \mathrm{i}\hbar\delta_{ij}\psi(x,t) \quad \forall\psi(x,t) \in L^2 \\
\Rightarrow \big[\hat{X}_i, \hat{P}_j\big] &= \mathrm{i}\hbar\delta_{ij}
\end{aligned}$$

This relation is known as the canonical commutation relation (kanonische Vertauschungsrelation).

(c) Consider the Hamilton operator:

$$\hat{H} = \sum_i \frac{\hat{P}_i^2}{2m}$$

with the eigenvalue equation (also known as the stationary or time-independent Schrödinger equation):

$$\hat{H}\psi(x) = E\psi(x)$$

We have the following:

$$
\begin{aligned}
[\hat{X}_i, \sum_j \frac{\hat{P}_j^2}{2m}] &= \sum_j \frac{1}{2m}[\hat{X}_i, \hat{P}_j^2] \\
&= \sum_j \frac{1}{2m}\Big([\hat{X}_i, \hat{P}_j]\hat{P}_j + \hat{P}_j[\hat{X}_i, \hat{P}_j]\Big) \\
&= \sum_j \frac{1}{2m}\Big(\mathrm{i}\hbar\delta_{ij}\hat{P}_j + \hat{P}_j\mathrm{i}\hbar\delta_{ij}\Big) \\
&= \sum_j \frac{1}{m}\mathrm{i}\hbar\delta_{ij}\hat{P}_j \\
&= \frac{\mathrm{i}\hbar}{m}\hat{P}_i
\end{aligned}
$$

Aufgabe 2: 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:

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

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?

Aufgabe 2: Gaussian Wavepacket

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 $t = 0$:

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

Let the exponential's argument be E:

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

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:

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

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:

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

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

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

For arbitrary times:

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

where we have used the dispersion relation for ω:

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

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:

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

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:

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

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

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

So overall, the Uncertainty Relation is given by:

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

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