Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

Blatt 7

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Das Übungsblatt wird in Gruppen von maximal 3 Personen bearbeitet. Die Abgabe erfolgt digital über ILIAS.

Aufgabe 1. Coherent States and the Displacement Operator (9 Punkte)

In the lecture you were introduced to the coherent states, which may be defined as the eigenvectors of the annihilation operator, $\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle$. We can write the coherent states as a series in the number eigenstate basis as:

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\,|n\rangle\,.$$

It was also possible to define the coherent state as a displaced vacuum state, $\hat{D}(\alpha)\,|0\rangle = |\alpha\rangle$, where $\hat{D}(\alpha)$ is the displacement operator:

$$\hat{D}(\alpha) = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} = e^{-\frac{1}{2}|\alpha|^2} e^{\alpha\hat{a}^\dagger} e^{-\alpha^*\hat{a}} = e^{\frac{1}{2}|\alpha|^2} e^{-\alpha^*\hat{a}} e^{\alpha\hat{a}^\dagger}.$$

The different expressions for $\hat{D}(\alpha)$ come from the fact that for two operators with constant commutator, $[A, B] =$ const, the exponential of the operators may be written as $e^{A+B} = e^A e^B e^{-[A,B]/2}$ (this is an application of the Baker-Campbell-Hausdorff formula, also just called "BCH").

1. (1 Punkt) Show that the adjoint of the displacement operator is a displacement of opposite magnitude, $\hat{D}^\dagger(\alpha) = \hat{D}(-\alpha)$. As a result of this, the displacement operator is a unitary operator.
2. (1 Punkt) Show the following property of the displacement operator:

$$\hat{D}(\alpha)\hat{D}(\beta) = e^{(\alpha\beta^* - \alpha^*\beta)/2}\hat{D}(\alpha + \beta).$$

   Hint: use the BCH formula provided in the introduction.
3. (3 Punkte) For this problem we will use another identity related to BCH. For two arbitrary operators Z and Y:

$$e^Z Y e^{-Z} = Y + [Z, Y] + \frac{1}{2!}[Z, [Z, Y]] + \frac{1}{3!}[Z, [Z, [Z, Y]]] + \ldots$$

   The series of nested commutators continues in a predictable manner. This formula is very useful when applying unitary transformations to operators. Use it to show how $\hat{D}(\alpha)$ "displaces" the creation and annihilation operators, that is calculate:
   (a) $\hat{D}^\dagger(\alpha)\hat{a}\hat{D}(\alpha)$
   (b) $\hat{D}^\dagger(\alpha)\hat{a}^\dagger\hat{D}(\alpha)$
   (c) $\hat{D}^\dagger(\alpha)\hat{a}^\dagger\hat{a}\hat{D}(\alpha)$.
4. (1 Punkt) Calculate the displacement of a coherent state $\hat{D}(\beta)\,|\alpha\rangle$.

5. (3 Punkte) Remember that we can write the position and momentum operators in terms of creation and annihilation operators as $\hat{x} = (\hat{a}^\dagger + \hat{a})/\sqrt{2}$ and $\hat{p} = i(\hat{a}^\dagger - \hat{a})/\sqrt{2}$ (where all other physical parameters are taken to be 1). Calculate the standard deviation of the position and momentum operators, Δx and Δp, and the uncertainty, $\Delta x \Delta p$, for a coherent state $|\alpha\rangle$. What do you notice about the value of the uncertainty? (Hint: use $\langle\alpha|\,\hat{a}^\dagger = \alpha^* \langle\alpha|$ and $[\hat{a}, \hat{a}^\dagger] = 1$ to simplify these calculations.)

Lösung Aufgabe 1.

1. Here we just take the complex conjugate of the displacement operator

$$\hat{D}^\dagger(\alpha) = \left(\exp[\alpha\hat{a}^\dagger - \alpha^*\hat{a}]\right)^\dagger = \exp[\alpha^*\hat{a} - \alpha\hat{a}^\dagger] \qquad \hat{D}(-\alpha) = \exp[-\alpha\hat{a}^\dagger + \alpha^*\hat{a}]$$

   These are the same, so $\hat{D}^\dagger(\alpha) = \hat{D}(-\alpha)$.

2. We can use the BCH formula for operators with a constant commutator, $e^{[A,B]/2}e^{A+B} = e^A e^B$, to combine the exponential of the operators. We just need to calculate

$$[\alpha\hat{a}^\dagger - \alpha^*\hat{a}, \beta\hat{a}^\dagger - \beta^*\hat{a}] = -\alpha\beta^*[\hat{a}^\dagger, \hat{a}] - \alpha^*\beta[\hat{a}, \hat{a}^\dagger] = \alpha\beta^* - \alpha^*\beta$$

   where we have used the fact that $[\hat{a}, \hat{a}^\dagger] = -[\hat{a}^\dagger, \hat{a}] = 1$, and the fact that all other commutators are 0. Therefore we can write

$$\begin{aligned}\hat{D}(\alpha)\hat{D}(\beta) &= e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}e^{\beta\hat{a}^\dagger - \beta^*\hat{a}} = e^{[\alpha\hat{a}^\dagger - \alpha^*\hat{a}, \beta\hat{a}^\dagger - \beta^*\hat{a}]/2}e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a} + \beta\hat{a}^\dagger - \beta^*\hat{a}} \\ &= e^{(\alpha\beta^* - \alpha^*\beta)/2}e^{(\alpha+\beta)\hat{a}^\dagger - (\alpha+\beta)^*\hat{a}} = e^{(\alpha\beta^* - \alpha^*\beta)/2}\hat{D}(\alpha + \beta)\end{aligned}$$

   where in the last line we have used the definition of the displacement operator and the previously computed commutator.

3. Since the commutator $[\hat{a}, \hat{a}^\dagger] = 1$ is constant, all higher order terms in the infinite series of nested commutators will vanish. We therefore only need to calculate:

$$e^B A e^{-B} = A + [A, B]$$

   Since $e^B = \hat{D}^\dagger(\alpha) = \hat{D}(-\alpha)$, we have that $B = -\alpha\hat{a}^\dagger + \alpha^*\hat{a}$ from the definition of the displacement operator. We can now calculate the transformation of these operators.

   (a) $\hat{D}^\dagger(\alpha)\hat{a}\hat{D}(\alpha) = \hat{a} + [-\alpha\hat{a}^\dagger + \alpha^*\hat{a}, \hat{a}] = \hat{a} + \alpha$

   (b) $\hat{D}^\dagger(\alpha)\hat{a}^\dagger\hat{D}(\alpha) = \hat{a}^\dagger + [-\alpha\hat{a}^\dagger + \alpha^*\hat{a}, \hat{a}^\dagger] = \hat{a}^\dagger + \alpha^*$

   (c) Here we can use the previous two expressions and the fact that the displacement operator is unitary, and hence $\hat{D}(\alpha)\hat{D}^\dagger(\alpha) = \mathbb{1}$.

$$\hat{D}^\dagger(\alpha)\hat{a}^\dagger\hat{a}\hat{D}(\alpha) = \left(\hat{D}^\dagger(\alpha)\hat{a}^\dagger\hat{D}(\alpha)\right)\left(\hat{D}^\dagger(\alpha)\hat{a}\hat{D}(\alpha)\right) = (\hat{a}^\dagger + \alpha^*)(\hat{a} + \alpha) = \hat{a}^\dagger\hat{a} + \alpha^*\hat{a} + \alpha\hat{a}^\dagger + |\alpha|^2.$$

   It is fine if the students do not expand the product $(\hat{a}^\dagger + \alpha^*)(\hat{a} + \alpha)$.

4. This is just an application of the result from 1.2. We start by using the definition of the coherent state as a displaced vacuum state $\hat{D}(\alpha)|0\rangle = |\alpha\rangle$ then just combine the displacement operators.

$$\hat{D}(\beta)|\alpha\rangle = \hat{D}(\beta)\hat{D}(\alpha)|0\rangle = e^{(\beta\alpha^* - \beta^*\alpha)/2}\hat{D}(\alpha + \beta)|0\rangle = e^{(-\alpha\beta^* + \alpha^*\beta)/2}|\alpha + \beta\rangle$$

   Note that we have to swap α and β in the exponential as compared to 1.2.

5. Since $\hat{a}^\dagger|\alpha\rangle$ is not trivial to evaluate, but $\langle\alpha|\,\hat{a}^\dagger$ is, we want to rearrange all operators so that the creation operators $\hat{a}^\dagger$ are always on the left and the annihilation operators $\hat{a}$ are always on the right in an operator product. This is called "normal ordering." In order to put the operators in normal order we will use the

commutator $[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1$. In this way the inner products become easy to evaluate. We will start with the expectation values for $\hat{x}$ and $\hat{p}$:

$$\langle \hat{x} \rangle = \langle \alpha|\hat{x}|\alpha\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle\alpha|\hat{a}^\dagger + \hat{a}|\alpha\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\big(\langle\alpha|\hat{a}^\dagger|\alpha\rangle + \langle\alpha|\hat{a}|\alpha\rangle\big) = \sqrt{\frac{\hbar}{2m\omega}}(\langle\alpha|\alpha^*|\alpha\rangle + \langle\alpha|\alpha|\alpha\rangle) = \sqrt{\frac{\hbar}{2m\omega}}(\alpha^* + \alpha)$$
$$\langle \hat{p} \rangle = \langle \alpha|\hat{p}|\alpha\rangle = i\sqrt{\frac{\hbar m\omega}{2}}\,\langle\alpha|\hat{a}^\dagger - \hat{a}|\alpha\rangle = i\sqrt{\frac{\hbar m\omega}{2}}(\alpha^* - \alpha)$$

Next we must calculate $\langle \hat{x}^2\rangle$ and $\langle \hat{p}^2\rangle$. First, we write the operators in terms of the creation an annihilation operators in normal order:

$$\hat{x}^2 = \frac{\hbar}{2m\omega}(\hat{a}^\dagger + \hat{a})^2 = \frac{\hbar^2}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger + (\hat{a}^\dagger)^2 + \hat{a}^2) = \frac{\hbar}{2m\omega}(2\hat{a}^\dagger\hat{a} + 1 + (\hat{a}^\dagger)^2 + \hat{a}^2)$$
$$\hat{p}^2 = -\frac{\hbar m\omega}{2}(\hat{a}^\dagger - \hat{a})^2 = \frac{\hbar m\omega}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger - (\hat{a}^\dagger)^2 - \hat{a}^2) = \frac{\hbar m\omega}{2}(2\hat{a}^\dagger\hat{a} + 1 - (\hat{a}^\dagger)^2 - \hat{a}^2)$$

where we have used $\hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1$. The expectation values can be written directly:

$$\langle \hat{x}^2\rangle = \frac{\hbar}{2m\omega}\,\langle\alpha|(2\hat{a}^\dagger\hat{a} + 1 + (\hat{a}^\dagger)^2 + \hat{a}^2)|\alpha\rangle = \frac{\hbar}{2m\omega}(2|\alpha|^2 + 1 + \alpha^{*2} + \alpha^2)$$
$$\langle \hat{p}^2\rangle = \frac{\hbar m\omega}{2}\,\langle\alpha|(2\hat{a}^\dagger\hat{a} + 1 - (\hat{a}^\dagger)^2 - \hat{a}^2)|\alpha\rangle = \frac{\hbar m\omega}{2}(2|\alpha|^2 + 1 - \alpha^{*2} - \alpha^2)$$

We can now calculate the standard deviations:

$$\Delta x = \sqrt{\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2} = \sqrt{\frac{\hbar}{2m\omega}(2|\alpha|^2 + 1 + \alpha^{*2} + \alpha^2) - \frac{\hbar}{2m\omega}(\alpha^* + \alpha)^2}$$
$$= \sqrt{\frac{\hbar}{2m\omega}}\sqrt{(2|\alpha|^2 + 1 + \alpha^{*2} + \alpha^2) - (2|\alpha|^2 + \alpha^{*2} + \alpha^2)} = \sqrt{\frac{\hbar}{2m\omega}}$$
$$\Delta p = \sqrt{\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2} = \sqrt{\frac{\hbar m\omega}{2}(2|\alpha|^2 + 1 - \alpha^{*2} - \alpha^2) + \frac{\hbar m\omega}{2}(\alpha^* - \alpha)^2}$$
$$= \sqrt{\frac{\hbar m\omega}{2}}\sqrt{(2|\alpha|^2 + 1 - \alpha^{*2} - \alpha^2) + (-2|\alpha|^2 + \alpha^{*2} + \alpha^2)} = \sqrt{\frac{\hbar m\omega}{2}}$$

We therefore have that the standard deviations are $\Delta x = \sqrt{\hbar/2m\omega}$ and $\Delta p = \sqrt{\hbar m\omega/2}$. The product of the standard deviations is then:

$$\Delta x\Delta p = \frac{\hbar}{2}.$$

The product of the standard deviations is related to the uncertainty of the state; coherent states therefore have the lowest possible uncertainty since $\hbar/2$ is the minimum value of the uncertainty allowed by quantum mechanics.

Aufgabe 2. (6 Punkte)

Recall that the eigenenergies for the quantum harmonic oscillator Hamiltonian, $\hat{H} = \hat{p}^2/2m + m\omega^2\hat{x}^2/2 = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2)$, have the form $E_n = \hbar\omega(n + 1/2)$. The associated eigenvectors are called the "number eigenstates" and are written as $|n\rangle$. The corresponding orthonormal wavefunctions in the position basis, $\psi_n(x) = \langle x|n\rangle$, are written as

$$\psi_n(x) = \left(\frac{1}{\sqrt{2\pi}2^n n! x_{\mathrm{ZPF}}}\right)^{1/2} e^{-x^2/4x_{\mathrm{ZPF}}^2} H_n\left(\frac{x}{\sqrt{2}x_{\mathrm{ZPF}}}\right), \quad \text{where} \quad x_{\mathrm{ZPF}} = \sqrt{\frac{\hbar}{2m\omega}}.$$

1. (2 Punkte) Calculate the standard deviation of $\hat{x}$ for the ground state wavefunction, $\langle x|0\rangle = \psi_0(x)$, and show that it is equal to x_{ZPF} (you may use known results for the integrals to avoid explicit calculations). This is why we call this constant the "zero point fluctuation": the "zero point" refers to the ground state (the $n = 0$ state), and the "fluctuation" refers to the standard deviation. You may also notice that the standard deviation of $\hat{x}$ for $|0\rangle$ is the same as for a coherent state $|\alpha\rangle$ from question 1.5. This is because the ground state of the quantum harmonic oscillator is just a coherent state with no displacement, $\alpha = 0$.

2. (2 Punkte) The Hermite polynomials can be defined using the following generating function:

$$e^{-s^2+2s\chi} = \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(\chi).$$

Differentiate this with respect to s and χ, and demand that terms of the same order of s in the sum be equal, to obtain the following recurrence relations:

(a) $H_{n+1}(\chi) - 2\chi H_n(\chi) + 2nH_{n-1}(\chi) = 0$

(b) $\frac{d}{d\chi} H_n(\chi) = 2nH_{n-1}(\chi)$.

3. (2 Punkte) For this part you may assume that $x_{\text{ZPF}} = 1/\sqrt{2}$ for simplicity. We know that the number eigenstates are orthonormal, $\langle m|n\rangle = \delta_{m,n}$. This inner product can be expressed in integral form as

$$\int_{-\infty}^{\infty} dx\, \psi_m^*(x)\psi_n(x) = \delta_{m,n}.$$

Using the explicit forms for the wavefunctions, we can arrive at the following integral:

$$\int_{-\infty}^{\infty} dx\, e^{-x^2} H_m(x) H_n(x) = \sqrt{\pi} 2^n n! \delta_{m,n}.$$

Working in the position basis, show that the expectation values of the position and momentum operators are zero for any number eigenstate (you should use the above integrals to avoid solving the other integrals explicitly).

Lösung Aufgabe 2.

1. The ground state wavefunction has the following form:

$$\psi_0(x) = \left(\frac{1}{\sqrt{2\pi} x_{\text{ZPF}}}\right)^{1/2} e^{-x^2/4x_{\text{ZPF}}^2}, \qquad \text{where} \qquad x_{\text{ZPF}} = \sqrt{\frac{\hbar}{2m\omega}}$$

since $H_0(x) = 1$. Next calculate the expectation value for $\hat{x}$:

$$\langle x\rangle = \langle 0|\hat{x}|0\rangle = \int_{-\infty}^{\infty} dx\, \psi_0^*(x) x \psi_0(x) = \left(\frac{1}{\sqrt{2\pi} x_{\text{ZPF}}}\right) \int_{-\infty}^{\infty} dx\, x e^{-x^2/2x_{\text{ZPF}}^2} = 0$$

which we know to be true since the integrand is odd over the interval. And now the expectation value for $\hat{x}^2$:

$$\langle x^2\rangle = \int_{-\infty}^{\infty} dx\, \psi_0^*(x) x^2 \psi_0(x) = \left(\frac{1}{\sqrt{2\pi} x_{\text{ZPF}}}\right) \int_{-\infty}^{\infty} dx\, x^2 e^{-x^2/2x_{\text{ZPF}}^2} = \left(\frac{1}{\sqrt{2\pi} x_{\text{ZPF}}}\right) \sqrt{2\pi} x_{\text{ZPF}}^3 = x_{\text{ZPF}}^2$$

The standard deviation is then just

$$\Delta x = \sqrt{\langle \hat{x}^2\rangle - \langle \hat{x}\rangle^2} = x_{\text{ZPF}}$$

and we get $\Delta x = x_{\text{ZPF}}$ as desired.

2. This is just matching terms in the series on the left and right hand sides for identical orders of the variable s.

(a) First we differentiate with respect to s. First the left hand side:

$$\frac{d}{ds} e^{-s^2+2s\chi} = 2(-s+\chi) e^{-s^2+2s\chi} = 2(-s+\chi) \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(\chi) = \left(\sum_{n=0}^{\infty} 2\chi \frac{s^n}{n!} H_n(\chi)\right) - \left(\sum_{n=0}^{\infty} 2\frac{s^{n+1}}{n!} H_n(\chi)\right)$$

$$= \left(\sum_{n=0}^{\infty} 2\chi \frac{s^n}{n!} H_n(\chi)\right) - \left(\sum_{n=0}^{\infty} 2\frac{s^n}{(n-1)!} H_{n-1}(\chi)\right) = \sum_{n=0}^{\infty} \frac{s^n}{n!} \left(2\chi H_n(\chi) - 2nH_{n-1}(\chi)\right)$$

Where we have reindexed the sum in the last line; this still holds since the Hermite polynomials are taken to be zero for negative integers. Now the right hand side

$$\frac{d}{ds}\sum_{n=0}^{\infty}\frac{s^n}{n!}H_n(\chi)=\sum_{n=1}^{\infty}\frac{s^{n-1}}{(n-1)!}H_n(\chi)=\sum_{n=0}^{\infty}\frac{s^n}{n!}H_{n+1}(\chi)$$

Now we set the sums to be equal (and claim that the coefficients for identical orders of s must be identical)

$$\sum_{n=0}^{\infty}\frac{s^n}{n!}\left(2\chi H_n(\chi)-2nH_{n-1}(\chi)\right)=\sum_{n=0}^{\infty}\frac{s^n}{n!}H_{n+1}(\chi)\Rightarrow H_{n+1}(\chi)-2\chi H_n(\chi)+2nH_{n-1}(\chi)=0.$$

(b) Now we differentiate with respect to χ, first the left hand side:

$$\frac{d}{d\chi}e^{-s^2+2s\chi}=2se^{-s^2+2s\chi}=\sum_{n=0}^{\infty}\frac{s^{n+1}}{n!}2H_n(\chi)=\sum_{n=0}^{\infty}\frac{s^n}{(n-1)!}2H_{n-1}(\chi)=\sum_{n=0}^{\infty}\frac{s^n}{n!}2nH_{n-1}(\chi).$$

And then the right hand side

$$\frac{d}{d\chi}\sum_{n=0}^{\infty}\frac{s^n}{n!}H_n(\chi)=\sum_{n=0}^{\infty}\frac{s^n}{n!}\frac{d}{d\chi}H_n(\chi).$$

We therefore have

$$\sum_{n=0}^{\infty}\frac{s^n}{n!}\frac{d}{d\chi}H_n(\chi)=\sum_{n=0}^{\infty}\frac{s^n}{n!}2nH_{n-1}(\chi)\Rightarrow\frac{d}{d\chi}H_n(\chi)=2nH_{n-1}(\chi).$$

3. For $x_{\text{ZPF}}=1/\sqrt{2}$ the wavefunctions become

$$\psi_n(x)=\left(\frac{1}{\sqrt{\pi}2^n n!}\right)^{1/2}e^{-x^2/2}H_n(x)$$

which will simplify the following calculations. This question just uses the previously obtained recurrence relations for the Hermite polynomials. We will start by calculating $\langle\hat{x}\rangle$:

$$\begin{aligned}
\langle\hat{x}\rangle&=\int_{-\infty}^{\infty}dx\,\psi_n^*(x)x\psi_n(x)=\left(\frac{1}{\sqrt{\pi}2^n n!}\right)\int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)\left(xH_n(x)\right)\\
&=\left(\frac{1}{\sqrt{\pi}2^n n!}\right)\int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)\left(\frac{1}{2}H_{n+1}(x)+nH_{n-1}(x)\right)\quad\text{we have used } H_{n+1}(x)-2\chi H_n(x)+2nH_{n-1}(x)=0\\
&=\left(\frac{1}{\sqrt{\pi}2^n n!}\right)\left(\frac{1}{2}\int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)H_{n+1}(x)+n\int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)H_{n-1}(x)\right)\\
&=0
\end{aligned}$$

The last line follows as a result of the orthonormality of the number eigenstates (and the integral we can obtain showing the orthogonality of the Hermite polynomials with respect to the weight function e^{-x^2}).

Next, we calculate the expectation value for the momentum operator:

$$\begin{aligned}
\langle\hat{p}\rangle&=\int_{-\infty}^{\infty}dx\,\psi_n^*(x)\left(-i\hbar\frac{d}{dx}\psi_n(x)\right)=\left(\frac{1}{\sqrt{\pi}2^n n!}\right)\int_{-\infty}^{\infty}dx\,e^{-x^2/2}H_n(x)\left(-i\hbar\frac{d}{dx}e^{-x^2/2}H_n(x)\right)\\
&=-i\hbar\left(\frac{1}{\sqrt{\pi}2^n n!}\right)\int_{-\infty}^{\infty}dx\,e^{-x^2/2}H_n(x)e^{-x^2/2}\left(-xH_n(x)+\frac{d}{dx}H_n(x)\right)\\
&=-i\hbar\left(\frac{1}{\sqrt{\pi}2^n n!}\right)\left(-\int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)\left(xH_n(x)\right)+\int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)\frac{d}{dx}H_n(x)\right)\\
&=-i\hbar\left(\frac{1}{\sqrt{\pi}2^n n!}\right)\int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)\frac{d}{dx}H_n(x)\quad\text{we know the first integral is 0 from calculating }\langle x\rangle\\
&=-i\hbar\left(\frac{1}{\sqrt{\pi}2^n n!}\right)2n\int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)H_{n-1}(x)\quad\text{using the other recurrence relation}\\
&=0
\end{aligned}$$

where we have used the same logic as before. Therefore $\langle \hat{x} \rangle = \langle \hat{p} \rangle = 0$ for the number eigenstates.

Aufgabe 3. Pauli-Matrizen (5 Punkte)

Die Pauli-Matrizen sind definiert über

$$\sigma_x = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \text{und} \qquad \sigma_z = \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1}$$

Später in der Vorlesung lernen wir, dass die Pauli-Matrizen mit dem Spin der Elektronen verbunden sind. Für jetzt reicht es zu wissen, dass wir ein zwei-Level System beschreiben über die Operatoren

$$\vec{S} = \begin{pmatrix} \hat{S}_x \\ \hat{S}_y \\ \hat{S}_z \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} = \frac{\hbar}{2} \vec{\sigma}. \tag{2}$$

1. (1 Punkt) Zunächst untersuchen wir die Eigenschaften der Pauli-Matrizen. Beweisen Sie die Formel

$$\sigma_j \sigma_k = \mathbb{1}_2 \delta_{jk} + i\epsilon_{jkl}\sigma_l \tag{3}$$

   wobei $\mathbb{1}_2 = \mathrm{diag}(1, 1)$. Leiten Sie daraus

$$\{\sigma_j, \sigma_k\} = 2\mathbb{1}_2 \delta_{jk} \qquad\qquad [\sigma_j, \sigma_k] = 2i\epsilon_{jkl}\sigma_l \tag{4}$$

   her und zeigen Sie, dass $[\hat{S}_j, \hat{S}_k] = i\hbar\epsilon_{jkl}\hat{S}_l$ gilt. Die Operatoren $\hat{S}_i$ erfüllen eine sogenannte Drehimpulsalgebra.

2. (1 Punkt) Beweisen Sie für beliebige $\vec{a}, \vec{b} \in \mathbb{C}^3$, dass

$$(\vec{a} \cdot \vec{\sigma})(\vec{b} \cdot \vec{\sigma}) = (\vec{a} \cdot \vec{b})\mathbb{1}_2 + i(\vec{a} \times \vec{b}) \cdot \vec{\sigma}. \tag{5}$$

3. (1 Punkt) Bestimmen Sie die normierten Eigenzustände/ Eigenvektoren und Eigenwerte der $\hat{S}_i$.

4. (1 Punkt) Bestimmen Sie $\hat{S}^2$ und zeigen Sie, dass die Eigenzustände von $\vec{S}_i$ auch Eigenzustände von $\vec{S}^2$ sind. Welche Eigenwerte besitzt $\vec{S}^2$?

5. (1 Punkt) Seien $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ und $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ nun die Eigenzustände zu $\hat{S}_z$. Bestimmen Sie die Matrixdarstellung der Leiteroperatoren $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$ und deren Wirkung auf $|\uparrow\rangle, |\downarrow\rangle$.

Aufgabe 3. Pauli-Matrizen (5 Punkte)

1. (1 Punkt) Wir berechnen explizit

$$\sigma_x\sigma_x = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \mathbb{1}_2$$
$$\sigma_x\sigma_y = \begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix} = i\sigma_z = i\epsilon_{123}\sigma_z$$
$$\sigma_x\sigma_z = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} = -i\sigma_y = i\epsilon_{132}\sigma_y$$
$$\sigma_y\sigma_x = \begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix} = -i\sigma_z = i\epsilon_{213}\sigma_z$$
$$\sigma_y\sigma_y = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \mathbb{1}_2$$
$$\sigma_y\sigma_z = \begin{pmatrix}0 & i\\ i & 0\end{pmatrix} = i\sigma_x = i\epsilon_{231}\sigma_x$$
$$\sigma_y\sigma_z = \begin{pmatrix}0 & i\\ i & 0\end{pmatrix} = i\sigma_x = i\epsilon_{231}\sigma_x$$
$$\sigma_z\sigma_x = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix} = i\sigma_y = i\epsilon_{312}\sigma_y$$
$$\sigma_z\sigma_y = \begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix} = -i\sigma_x = i\epsilon_{321}\sigma_x$$
$$\sigma_z\sigma_z = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \mathbb{1}_2,$$

sodass

$$\sigma_j\sigma_k = \mathbb{1}_2\delta_{jk} + i\epsilon_{jkl}\sigma_l. \tag{6}$$

Damit folgt direkt

$$[\sigma_j, \sigma_k] = \sigma_j\sigma_k - \sigma_k\sigma_j = i\epsilon_{jkl}\sigma_l - i\epsilon_{kjl}\sigma_l = 2i\epsilon_{jkl}\sigma_l \tag{7}$$
$$\sigma_j, \sigma_k = \sigma_j\sigma_k + \sigma_k\sigma_j = 2\delta_{jk}\mathbb{1}_2 + i\epsilon_{jkl}\sigma_l + i\epsilon_{kjl}\sigma_l = 2\delta_{jk}\mathbb{1}_2 \tag{8}$$

und

$$[\hat{S}_j, \hat{S}_k] = \frac{\hbar^2}{4}[\sigma_j, \sigma_k] = \frac{\hbar^2}{4}2i\epsilon_{jkl}\sigma_l = i\hbar\epsilon_{jkl}\frac{\hbar\sigma_l}{2} = i\hbar\epsilon_{jkl}\hat{S}_l. \tag{9}$$

2. (1 Punkt) Wir nutzen (6), um zu zeigen, dass

$$(\vec{a}\cdot\vec{\sigma})(\vec{b}\cdot\vec{\sigma}) = a_j b_k \sigma_j\sigma_k \tag{10}$$
$$= a_j b_k \mathbb{1}_2\delta_{jk} + i a_j b_k \epsilon_{jkl}\sigma_l \tag{11}$$
$$= (\vec{a}\cdot\vec{b})\mathbb{1}_2 + i(\vec{a}\times\vec{b})\cdot\vec{\sigma}. \tag{12}$$

3. (1 Punkt) Die normierten Eigenzustände und Eigenwerte der Operatoren $\hat{S}_i$ sind gerade

$$\hat{S}_x: \quad \vec{a}_x^1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix},\ \vec{a}_x^2\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \quad s_x^1 = \frac{\hbar}{2},\ s_x^2 = -\frac{\hbar}{2} \tag{13}$$
$$\hat{S}_y: \quad \vec{a}_y^1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix},\ \vec{a}_y^2\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} \quad s_y^1 = \frac{\hbar}{2},\ s_y^2 = -\frac{\hbar}{2} \tag{14}$$
$$\hat{S}_z: \quad \vec{a}_z^1 = \begin{pmatrix}1\\0\end{pmatrix},\ \vec{a}_z^2\begin{pmatrix}0\\1\end{pmatrix} \quad s_z^1 = \frac{\hbar}{2},\ s_z^2 = -\frac{\hbar}{2}. \tag{15}$$

4. Wir nutzen die Formel (6), um zu zeigen, dass

$$\vec{S}^2 = \sum_i \hat{S}_i \cdot \hat{S}_i = \frac{\hbar^2}{4} \sum_i \sigma_i \sigma_i = \frac{\hbar^2}{4} \mathbb{1}_2 \sum_i \delta_i i = \frac{3}{4} \hbar \mathbb{1}_2, \tag{16}$$

wobei wir die Summe trotz Summenkonvention schreiben, um klar zu machen, dass wir am Ende wirklich noch summieren müssen. Da $\vec{S}^2 \sim \mathbb{1}_2$ ist jeder beliebige Vektor $\vec{a} \in \mathbb{C}^2$ ein Eigenzustand zu $\vec{S}^2$ mit dem Eigenwert $3/4\hbar^2$, also auch die Eigenzustände der $\hat{S}_i$.
Alternativ können wir zeigen, dass $[\vec{S}^2, \hat{S}_i] = 0$ und damit $\vec{S}^2$ und $\hat{S}_i$ gemeinsame Eigenzustände besitzen.

5. Die Leiteroperatoren sind gegeben als

$$\hat{S}_+ = \hat{S}_x + i\hat{S}_y = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{17}$$

$$\hat{S}_- = \hat{S}_x - i\hat{S}_y = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{18}$$

$$\tag{19}$$

und damit gilt für $|\uparrow\rangle \mathrel{\hat{=}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ und $|\downarrow\rangle \mathrel{\hat{=}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\hat{S}_+ |\uparrow\rangle = 0 \tag{20}$$

$$\hat{S}_+ |\downarrow\rangle = \hbar |\uparrow\rangle \tag{21}$$

$$\hat{S}_- |\uparrow\rangle = \hbar |\downarrow\rangle \tag{22}$$

$$\hat{S}_- |\downarrow\rangle = 0. \tag{23}$$