Theoretical Physics II B – Quantum Mechanics

Lecture 6

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Solutions to previous control questions

5.1 (a) Normalisation (with $\langle\psi_1|\psi_2\rangle = 0$):

$$\langle\psi|\psi\rangle = |c_1|^2\,\langle\psi_1|\psi_1\rangle + |c_2|^2\,\langle\psi_2|\psi_2\rangle \longrightarrow |c_1|^2 + |c_2|^2 \stackrel{!}{=} 1$$

(b) Possilbe energies: $E_1 = \hbar\omega$ or $E_2 = 2\hbar\omega$ with probabilities

$$\mathcal{P}(E_1) = |c_1|^2 \quad \text{and} \quad \mathcal{P}(E_2) = |c_2|^2 = 1 - |c_1|^2 .$$

(c) Expectation values:

$$\begin{aligned}\left\langle\psi\left|\hat{H}\right|\psi\right\rangle &= \hbar\omega\left(|c_1|^2 + 2|c_2|^2\right) = \hbar\omega\left(1 + |c_2|^2\right)\\ \left\langle\psi\left|\hat{O}\right|\psi\right\rangle &= \mu\left(c_1^* c_2 + c_2^* c_1\right) = 2\mu\mathbf{Re}(c_1 c_2^*)\,,\end{aligned}$$

where $\mathbf{Re}(x)$ denotes the real part of the complex number x.

5.2 Goes by direct calculation. Please check yourself.

Definitions and properties of commutators

- Definition: $\left[\hat{L},\, \hat{M}\right] = -\left[\hat{M},\, \hat{L}\right] \equiv \hat{L}\hat{M} - \hat{M}\hat{L}$.
- If two operators commute, then the commutator vanishes when acting on any wave function.
- Some properties of commutators have been listed in lecture 5.
- Here, some properties relating to operator functions are added:
  (a) $\left[\hat{L},\, \hat{M}\right] = 0 \longrightarrow \left[\hat{L},\, \mathcal{F}(\hat{M})\right] = 0$, if $\mathcal{F}$ can be Taylor expanded.
  (b) $e^{\hat{L}}\, \hat{M} e^{-\hat{L}} = \sum\limits_{n=0}^{\infty} \frac{1}{n!} \left[\hat{L}, \hat{M}\right]_{(n)}$, where

  $\left[\hat{L}, \hat{M}\right]_{(0)} = \hat{M}$, $\left[\hat{L}, \hat{M}\right]_{(1)} = \left[\hat{L},\, \hat{M}\right]$, $\left[\hat{L}, \hat{M}\right]_{(2)} = \left[\hat{L},\, \left[\hat{L},\, \hat{M}\right]\right]$, and

  in general, by a recursive definition $\left[\hat{L}, \hat{M}\right]_{(n)} = \left[\hat{L}, \left[\hat{L},\, \hat{M}\right]_{(n-1)}\right]$.
  (c) $e^{\hat{L}+\hat{M}} = e^{\hat{L}} e^{\hat{M}} e^{[\hat{L},\, \hat{M}]}$ if $\left[\hat{L}\left[\hat{L}, \hat{M}\right]\right] = \left[\hat{M}\left[\hat{L}, \hat{M}\right]\right] = 0$.

- The operators related to position and momentum do not commute in general, in particular

$$[\hat{x},\, \hat{p}_x] = [\hat{y},\, \hat{p}_y] = [\hat{z},\, \hat{p}_z] = i\hbar\,,$$

while all other pairs of operators commute:

$$\boxed{[\hat{r}_j,\, \hat{p}_k] = i\hbar\delta_{jk}.}$$

Defining uncertainties

- Before discussing the uncertainty relations, a strict mathematical definition of uncertainties must be given. In the following we use the shorthand below for the expectation value of a measurement/an operator with respect to a certain state:

$$\langle \mathcal{A} \rangle_{|\psi\rangle} \equiv \langle \mathcal{A} \rangle \equiv \langle \hat{A} \rangle = \frac{\left\langle \psi \left| \hat{A} \right| \psi \right\rangle}{\langle \psi | \psi \rangle} .$$

- Then we define the unceratinty of this measurement through the squre root of the mean-square deviation, or the variance:

$$\Delta \mathcal{A} = \sqrt{\left\langle \left(\mathcal{A} - \langle \mathcal{A} \rangle \right)^2 \right\rangle} \longleftrightarrow (\Delta \mathcal{A})^2 = \langle \mathcal{A}^2 \rangle - \langle \mathcal{A} \rangle^2 .$$

Some helpers

- Introduce Hermitean operators $\overline{A} \equiv \hat{A} - \langle \mathcal{A} \rangle \, \hat{\mathbf{1}}$ also known as the *dispersion operator* corresponding to $\hat{A}$, for which $\langle \overline{A}^2 \rangle = (\Delta \mathcal{A})^2$.
- Introduce three lemma's:

Lemma 1: Schwarz inequality $\langle \alpha|\alpha \rangle \langle \beta|\beta \rangle \geq |\langle \alpha|\beta \rangle|^2$.

(aka triangle inequality)

Proof: $\forall \lambda \in \mathbf{C}: \quad (\langle \alpha| + \lambda^* \langle \beta|)(|\alpha\rangle + \lambda |\beta\rangle) \geq 0$
because all kets have non-negative length: $\langle \psi|\psi \rangle \geq 0 \;\; \forall |\psi\rangle$.
Identify $\lambda = -\langle \beta|\alpha \rangle / \langle \beta|\beta \rangle$ to complete the proof.

Lemma 2: The expecation value of a Hermitean operator is real.
Proof: Remember that the expecation value is a weighted average of eigenvalues of the respective operator.

Lemma 2: The expecation value of an anti-Hermitean operator, defined by $\hat{C} = -\hat{C}^\dagger$, is imaginary.
Proof follows from its eigenvalues being purely imaginary.

General form of Heisenberg uncertainty relation

- Heisenberg uncertainty relation for two aribtrary observables:

$$\boxed{\langle\Delta\mathcal{A}\rangle\langle\Delta\mathcal{B}\rangle \geq \frac{1}{2}\left|\left\langle\left[\hat{A},\, \hat{B}\right]\right\rangle\right|}$$

- Example:

$$\langle\Delta\mathcal{X}\rangle\langle\Delta\mathcal{P}_x\rangle \geq \frac{1}{2}\left|\langle[\hat{x},\, \hat{p}_x]\rangle\right| = \left|\frac{i\hbar}{2}\right| = \frac{\hbar}{2},$$

so *in principle*, there is no way to simultaenously measure x-position and x-momentum of a particle arbitrarily precise.

Proof

- Use lemma 1 above and apply it to the kets $|\alpha\rangle = \overline{A}\,|\rangle$ and $|\beta\rangle = \overline{B}\,|\rangle$, where $|\rangle$ denotes *any* ket. Then
$$\langle\overline{A}^2\rangle\langle\overline{B}^2\rangle \geq \left|\langle\overline{A}\cdot\overline{B}\rangle\right|^2$$
- From its definition, any operator product can be expressed as
$$\hat{L}\hat{M} = \frac{1}{2}\left[\hat{L},\,\hat{M}\right] + \frac{1}{2}\left\{\hat{L},\,\hat{M}\right\}$$
Note that the commutator of two Hermitean operators is anti-Hermitean, while its anticommutator is Hermitean, then the expectation value of the first term above is purely imaginary, and of the second term it is purely real.
- Therefore the right hand side of the inequaltiy above reads
$$\left|\langle\overline{A}\cdot\overline{B}\rangle\right|^2 = \frac{1}{4}\left|\left\langle\left[\hat{A},\,\hat{B}\right]\right\rangle\right|^2 + \frac{1}{4}\left|\left\langle\left\{\hat{A},\,\hat{B}\right\}\right\rangle\right|^2 \geq \frac{1}{4}\left|\left\langle\left[\hat{A},\,\hat{B}\right]\right\rangle\right|^2,$$
and omitting the second term, as indicated, thus makes the inequality even stronger.
- Inserting the commutator in this inequality and taking its squareroot finishes the proof if the Heisenberg uncertainty relation.

Example: Minimal uncertainty wave-packet (1-dimensional)

- Consider a Gaussian wave packet represented by $|\psi\rangle$. In x-space and concentrating on one dimension only it is given by
$$\langle x|\psi\rangle \equiv \psi(x) = \left[\frac{1}{(\pi d^2)^{1/4}}\right] \exp\left[ip_x x - \frac{x^2}{2d^2}\right] \text{ with } d \in \mathbf{R}.$$
- Use the x-representation of the position operator, which in general $\left\langle x' \left|\hat{x^n}\right| x''\right\rangle = x'^n\delta(x'-x'')$, to calculate the expectation value

$$\begin{aligned}
\langle\hat{x}\rangle_{|\psi\rangle} &= \int\limits_{-\infty}^{\infty} \mathrm{d}x'\mathrm{d}x'' \langle\psi|x'\rangle \langle x'|\hat{x}|x''\rangle \langle x''|\psi\rangle \\
&= \int\limits_{-\infty}^{\infty} \mathrm{d}x'\mathrm{d}x'' \psi^*(x') \left[x'\delta(x'-x'')\right] \psi(x'') \\
&= \frac{1}{\sqrt{\pi}\, d} \int\limits_{-\infty}^{\infty} \mathrm{d}x'\, x' \exp\left[-\frac{x^2}{d^2}\right] = 0 \quad \text{(symmetry: odd function)}\,,
\end{aligned}$$

Example: Minimal uncertainty wave-packet (1-dimensional)

- Similarly $\langle \hat{x}^2 \rangle_{|\psi\rangle} = \frac{1}{\sqrt{\pi}\,d} \int\limits_{-\infty}^{\infty} \mathrm{d}x'\, x'^2 \exp\left[-\frac{x^2}{d^2}\right] = \frac{d^2}{2}$
- Therefore $(\Delta \mathcal{X})^2 = \langle \overline{x}^2 \rangle = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 = \frac{d^2}{2}$
- To calculate $\langle \hat{p}_x^n \rangle$ remember $\langle x \,|\hat{p}_x|\, \psi \rangle = -i\hbar \frac{\partial}{\partial x} \langle x|\psi \rangle$.

$$\langle \hat{p}_x \rangle_{|\psi\rangle} = \hbar p_x \quad \text{and} \quad \langle \hat{p}_x^2 \rangle_{|\psi\rangle} = \hbar^2 p_x^2 + \frac{\hbar^2}{2d^2}$$

- Therefore $(\Delta \mathcal{P}_x)^2 = \langle \overline{p}_x^2 \rangle = \langle \hat{p}_x^2 \rangle - \langle \hat{p}_x \rangle^2 = \frac{\hbar^2}{2d^2}$ and

$$\boxed{(\Delta \mathcal{X})(\Delta \mathcal{P}_x) = \frac{\hbar}{2}}$$

the minimally possible uncertainty.

Learning outcomes

- Definition and properties of commutators.
- Definition of uncertainty in measurements.
- Special role of commutators, especially for Heisenberg uncertainty relations in their general form.

Control questions

6.1 Prove that $e^{\hat{L}}\,\hat{M}\,e^{-\hat{L}} = \sum_{n=0}^{\infty}\frac{1}{n!}\left[\hat{L},\,\hat{M}\right]_{(n)}$.

(Cf. slide 5 for a definition of the terms $\left[\hat{L},\,\hat{M}\right]_{(n)}$.)

To this end, consider an operator $\hat{F}(\alpha_0) = e^{\alpha_0\hat{L}}\,\hat{M}\,e^{-\alpha_0\hat{L}}$ and expand it in a Taylor series with terms $\hat{F}(\alpha) = \sum_n (\alpha-\alpha_0)^n/n!\mathrm{d}^n\hat{F}(\alpha_0)/\mathrm{d}\alpha_0^n$.

By choosing suitable α and α_0 you will finish the proof.

6.2 Consider the spin operators $\hat{S}_{x,y,z} = \frac{\hbar}{2}\hat{\sigma}_{x,y,z}$ related to the Pauli matrices $\hat{\sigma}_{x,y,z} = \hat{\sigma}_{1,2,3}$. Using the commutators of the Pauli matrices, given by $[\hat{\sigma}_i,\,\hat{\sigma}_j] = 2i\epsilon_{ijk}\sigma_k$, calculate the commutators of the spin operators (see also control question to lecture 5!).
With this result prove that

$$
\begin{aligned}
e^{\frac{i\omega t}{\hbar}\hat{S}_z}\hat{S}_x e^{-\frac{i\omega t}{\hbar}\hat{S}_z} &= \cos(\omega t)\hat{S}_x - \sin(\omega t)\hat{S}_y \quad \text{and}\\
e^{\frac{i\omega t}{\hbar}\hat{S}_z}\hat{S}_y e^{-\frac{i\omega t}{\hbar}\hat{S}_z} &= \cos(\omega t)\hat{S}_y + \sin(\omega t)\hat{S}_x\,.
\end{aligned}
$$

Control questions (cont'd)

6.3 Calculate, for the Gaussian Wave Packet, the dispersion $(\Delta\mathcal{P}_x)^2$, and in particular show by explicit calculation that

$$\langle\hat{p}_x\rangle_{|\psi\rangle} = \hbar p_x \quad \text{and} \quad \langle\hat{p}_x^2\rangle_{|\psi\rangle} = \hbar^2 p_x^2 + \frac{\hbar^2}{2d^2}$$

For this you will need the following integrals, already used in the lecture when calculating $(\Delta\mathcal{X})^2$,

$$\int\limits_{-\infty}^{\infty} \mathrm{d}x \left\{ \begin{array}{c} 1 \\ x^2 \end{array} \right\} e^{-a^2x^2} = \frac{\sqrt{\pi}}{a} \left\{ \begin{array}{c} 1 \\ 1/(2a^2) \end{array} \right\}$$