Tutorial : uncertainty in quantum mechanics

1. Standard deviation and interpretation

Let A denote an observable and $\hat{A}$ be the associated hermitian operator. When a quantum system is in the normalized state $|\Psi\rangle$, the expectation values for A and A^2 read $\langle A\rangle_\Psi = \langle\Psi|\hat{A}|\Psi\rangle$ and $\langle A^2\rangle_\Psi = \langle\Psi|\hat{A}^2|\Psi\rangle$, respectively. The standard deviation $\left(\Delta A\right)_\Psi$ is defined as follows,

$$\left(\Delta A\right)_\Psi = \sqrt{\langle A^2\rangle_\Psi - \langle A\rangle_\Psi^2}.$$

The purpose of the exercise is to show that the standard deviation is a mathematical tool that quantifies the uncertainty in the value of A before measurement.

1. Show that $\langle A^2\rangle_\Psi - \langle A\rangle_\Psi^2 = \left\langle \Psi \middle| \left(\hat{A} - \langle A\rangle_\Psi\right)^2 \middle| \Psi \right\rangle$. Conclude that the standard deviation is well defined.

2. Let $|\Psi_a\rangle$ denote a normalized eigenstate of $\hat{A}$ with eigenvalue a. Show that $\left(\Delta A\right)_{\Psi_a} = 0$. What value would be measured for A if the system were in the quantum state $|\Psi_a\rangle$ just before measurement.

3. We assume in the following that the quantum state of the system $|\Psi\rangle$ is a linear combination of two orthonormal states $|\Psi_a\rangle$ and $|\Psi_b\rangle$ that are eigenstates of $\hat{A}$ with eigenvalues a and b, respectively:

$$|\Psi\rangle = \frac{1}{\sqrt{1+\delta^2}}\Big(|\Psi_a\rangle + \delta|\Psi_b\rangle\Big),$$

where $\delta > 0$. Explain why $|\Psi_a\rangle$ and $|\Psi_b\rangle$ are necessarily orthogonal when $a \neq b$ and verify that $|\Psi\rangle$ is normalized. Show that, in this particular case, the standard deviation can be simplified as follows,

$$\left(\Delta A\right)_\Psi = \frac{\delta|b-a|}{1+\delta^2}.$$

Comment on this result.

2. Heisenberg inequalities

We consider in this exercise the particular case of a particle described by the normalized wavefunction $\Psi(\mathbf{r})$. We will show that the product of standard deviations for the position x and the x component of the momentum p_x has a lower bound that is equal to $\hbar/2$:

$$(\Delta x)_\Psi (\Delta p_x)_\Psi \geq \frac{\hbar}{2}.$$

This relation is one of the famous Heisenberg inequalities.

1. Give a physical interpretation to the above inequality.

2. Let α be a real number that we use to construct the following (α-dependent) quantum state,

$$|\Psi(\alpha)\rangle = \Big[(\hat{p_x} - \langle p_x\rangle_\Psi) + \mathrm{i}\alpha(\hat{x} - \langle x\rangle_\Psi)\Big]|\Psi\rangle,$$

where $\mathrm{i}^2 = -1$. Show that the square norm $N(\alpha) = \langle\Psi(\alpha)|\Psi(\alpha)\rangle$ can be written as

$$N(\alpha) = (\Delta x)_\Psi^2\,\alpha^2 + (\Delta p_x)_\Psi^2 - \mathrm{i}\alpha\langle\Psi|[\hat{x}, \hat{p_x}]|\Psi\rangle,$$

where $[\hat{x}, \hat{p_x}] = \hat{x}\hat{p_x} - \hat{p_x}\hat{x}$ is the commutator of $\hat{x}$ and $\hat{p_x}$.

3. Show that $[\hat{x}, \hat{p_x}] = \mathrm{i}\hbar$. [**Hint**: apply the operator $[\hat{x}, \hat{p_x}]$ to a trial wavefunction $\varphi(\mathbf{r})$]

4. Deduce from question **3.** that

$$N(\alpha) = (\Delta x)_\Psi^2\,\alpha^2 + \hbar\alpha + (\Delta p_x)_\Psi^2 = (\Delta x)_\Psi^2\left[\left(\alpha + \frac{\hbar}{2(\Delta x)_\Psi^2}\right)^2 + \frac{1}{(\Delta x)_\Psi^2}\left((\Delta p_x)_\Psi^2 - \frac{\hbar^2}{4(\Delta x)_\Psi^2}\right)\right].$$

5. Explain why $N(\alpha) \geq 0$ for any α value. Conclude by considering the particular case $\alpha = -\dfrac{\hbar}{2(\Delta x)_\Psi^2}$.

Ecart type et interprétation

1. $\langle\psi|(\hat{A}-\langle A\rangle_\psi)^2|\psi\rangle = \langle(\hat{A}-\langle A\rangle_\psi)^\dagger\psi|\hat{A}-\langle A\rangle_\psi|\psi\rangle$

Définition de l'opérateur adjoint

Formules utiles :

① $\forall |\psi\rangle, |\varphi\rangle \quad \langle\psi|\hat{A}|\varphi\rangle = \langle\hat{A}^\dagger\psi|\varphi\rangle = \langle\varphi|\hat{A}^\dagger|\psi\rangle^*$

② $\forall |\psi\rangle, |\varphi\rangle \quad \langle\psi|\hat{A}+\hat{B}|\varphi\rangle = \langle\psi|\hat{A}|\varphi\rangle + \langle\psi|\hat{B}|\varphi\rangle$

$$= \langle\hat{A}^\dagger\psi|\varphi\rangle + \langle\hat{B}^\dagger\psi|\varphi\rangle$$

$$= \langle\underbrace{(\hat{A}^\dagger+\hat{B}^\dagger)}_{(\hat{A}+\hat{B})^\dagger}\psi|\varphi\rangle$$

soit $\boxed{(\hat{A}+\hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger}$

③ $\forall \alpha \in \mathbb{C}, \forall |\psi\rangle, |\varphi\rangle$

$$\langle\psi|\alpha\hat{A}|\varphi\rangle = \alpha\langle\psi|\hat{A}|\varphi\rangle = \alpha\langle\hat{A}^\dagger\psi|\varphi\rangle$$

$$= \langle\alpha^*\hat{A}^\dagger\psi|\varphi\rangle$$

soit $\boxed{(\alpha\hat{A})^\dagger = \alpha^*\hat{A}^\dagger}$

$\hat{A}-\langle A\rangle_\psi$ est une notation simple pour

$\hat{A}-\langle A\rangle_\psi\hat{\mathbb{1}}$ → opérateur identité ($\hat{\mathbb{1}}|\psi\rangle = |\psi\rangle$)

D'après la formule ②

$$(\hat{A}-\langle A\rangle_\psi\hat{\mathbb{1}})^\dagger = \hat{A}^\dagger + (-\langle A\rangle_\psi\hat{\mathbb{1}})^\dagger$$

$$= \hat{A}^\dagger - \langle A\rangle_\psi^* \underbrace{\hat{\mathbb{1}}^\dagger}_{\hat{\mathbb{1}}} \leftarrow \text{formule ③}$$

Comme $\hat{A}$ est hermitique $\hat{A}^\dagger = \hat{A}$ et

$$\langle A\rangle_\psi^* = \langle\psi|\hat{A}|\psi\rangle^* = \langle\hat{A}\psi|\psi\rangle$$

$$= \langle\hat{A}^\dagger\psi|\psi\rangle$$

$$= \langle\psi|\hat{A}|\psi\rangle$$

$$= \langle A\rangle_\psi$$

donc $(\hat{A}-\langle A\rangle_\psi)^\dagger = \hat{A} - \langle A\rangle_\psi$

et $\langle\psi|(\hat{A}-\langle A\rangle_\psi)^2|\psi\rangle = \langle(\hat{A}-\langle A\rangle_\psi)\psi|(\hat{A}-\langle A\rangle_\psi)|\psi\rangle$

$$= \|(\hat{A}-\langle A\rangle_\psi)|\psi\rangle\|^2 \geq 0$$

- Comme $(\hat{A}-\langle A\rangle_\psi)^2 = \hat{A}^2 - 2\langle A\rangle_\psi\hat{A} + \langle A\rangle_\psi^2$

il vient

$$\langle\psi|(\hat{A}-\langle A\rangle_\psi)^2|\psi\rangle = \langle\psi|\hat{A}^2|\psi\rangle - 2\langle A\rangle_\psi \underbrace{\langle\psi|\hat{A}|\psi\rangle}_{\langle A\rangle_\psi} + \langle A\rangle_\psi^2 \underbrace{\langle\psi|\psi\rangle}_{1}$$

$$= \langle A^2\rangle_\psi - 2\langle A\rangle_\psi^2 + \langle A\rangle_\psi^2$$

donc $\langle A^2\rangle_\psi - \langle A\rangle_\psi^2 = \langle\psi|(\hat{A}-\langle A\rangle_\psi)^2|\psi\rangle \geq 0$

L'écart type est donc bien défini.

2. • $\hat{A}|\psi_a\rangle = a|\psi_a\rangle \Rightarrow \langle\psi_a|\hat{A}|\psi_a\rangle = \langle A\rangle_{\psi_a} = a\langle\psi_a|\psi_a\rangle = a$

car $|\psi_a\rangle$ est normé

• $\hat{A}^2|\psi_a\rangle = \hat{A}(\hat{A}|\psi_a\rangle) = a\hat{A}|\psi_a\rangle = a^2|\psi_a\rangle$

$\Rightarrow \langle\psi_a|\hat{A}^2|\psi_a\rangle = a^2\langle\psi_a|\psi_a\rangle = a^2 = \langle A^2\rangle_{\psi_a} = \langle A\rangle_{\psi_a}^2$

soit $(\Delta A)_{\psi_a} = 0$

3. $|\psi\rangle = \frac{1}{\sqrt{1+\delta^2}}(|\psi_a\rangle + \delta|\psi_b\rangle)$

$$\langle\psi|\psi\rangle = \frac{1}{(1+\delta^2)}\langle\psi_a+\delta\psi_b|\psi_a+\delta\psi_b\rangle$$

$$= \frac{1}{(1+\delta^2)}\Big[\underbrace{\langle\psi_a|\psi_a\rangle}_{1} + \delta\underbrace{\langle\psi_a|\psi_b\rangle}_{0} + \underbrace{\delta^*}_{\delta}\underbrace{\langle\psi_b|\psi_a\rangle}_{0} + \delta^2\underbrace{\langle\psi_b|\psi_b\rangle}_{1}\Big]$$

soit $\langle\psi|\psi\rangle = 1.$

• $\hat{A}|\psi\rangle = \frac{1}{\sqrt{1+\delta^2}}(\hat{A}|\psi_a\rangle + \delta\hat{A}|\psi_b\rangle)$

$$= \frac{1}{\sqrt{1+\delta^2}}(a|\psi_a\rangle + \delta b|\psi_b\rangle)$$

$$\langle A\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle = \frac{1}{1+\delta^2}\langle\psi_a+\delta\psi_b|a\psi_a+\delta b\psi_b\rangle$$

$$= \frac{1}{1+\delta^2}\Big[a\langle\psi_a|\psi_a\rangle + \delta b\langle\psi_a|\psi_b\rangle + \delta^* a\langle\psi_b|\psi_a\rangle + \underbrace{|\delta|^2}_{\delta^2} b\langle\psi_b|\psi_b\rangle\Big]$$

car δ est réel

donc $\boxed{\langle A\rangle_\psi = \frac{a+b\delta^2}{1+\delta^2}}$

$$\langle A\rangle_\psi^2 = \frac{a^2+2ab\delta^2+b^2\delta^4}{(1+\delta^2)^2}$$

• $\hat{A}^2|\psi\rangle = \hat{A}(\hat{A}|\psi\rangle)$

$$= \frac{1}{\sqrt{1+\delta^2}}(a\hat{A}|\psi_a\rangle + \delta b\hat{A}|\psi_b\rangle)$$

Soit

$$\hat{A}^2|\psi\rangle = \frac{1}{\sqrt{1+\delta^2}}(a^2|\psi_a\rangle + \delta b^2|\psi_b\rangle)$$

$$\langle \psi | \hat{A}^2 | \psi \rangle = \frac{1}{(1+\delta^2)} \langle \psi_a + \delta \psi_b | a^2 \psi_a + \delta b^2 \psi_b \rangle$$

$$\shortparallel$$

$$\langle A^2 \rangle_\psi = \frac{1}{(1+\delta^2)} \left[a^2 + b^2 \delta^2 \right]$$

D'où $(\Delta A)^2_\psi = \dfrac{1}{(1+\delta^2)^2} \Big[\underbrace{(a^2+b^2\delta^2)(1+\delta^2)}_{\cancel{a^2}+\delta^2 a^2 + b^2\delta^2 + \cancel{b^2\delta^4}} - \cancel{a^2} - 2ab\delta^2 - \cancel{b^2\delta^4} \Big]$

Ainsi

$$(\Delta A)^2_\psi = \frac{1}{(1+\delta^2)^2} \left[\delta^2 \right] \left(a^2 + b^2 - 2ab \right) = \frac{\delta^2 (a-b)^2}{(1+\delta^2)^2}$$

$$\Rightarrow \boxed{(\Delta A)_\psi = \frac{\delta |a-b|}{(1+\delta^2)}}$$

$|\psi\rangle$ n'est état propre de $\hat{A}$ que lorsque $\delta = 0$ ou $\delta \to +\infty$ puisque $a \neq b$. Dans ces deux situations, le résultat de la mesure de A est connu. Ce sera a $(\delta = 0)$ ou b $(\delta \to +\infty)$. Pour $0 < \delta < +\infty$, la probabilité de mesurer a est $|\langle \psi_a | \psi \rangle|^2 = \dfrac{1}{1+\delta^2}$

et celle de mesurer b est $|\langle \psi_b | \psi \rangle|^2 = \dfrac{\delta^2}{1+\delta^2}$, et

$(\Delta A)_\psi \neq 0$ Il rend compte de l'incertitude avant la mesure.

Relations d'incertitude d'Heisenberg

1. Mesurer simultanément x et p_x revient à dire que, juste après la mesure, x et p_x sont connus et donc qu'il n'y a aucune incertitude sur leurs valeurs. Ainsi le système (ici la particule) serait dans un état quantique $|\psi\rangle$ tel que $(\Delta x)_\psi = 0$ ET $(\Delta p_x)_\psi = 0$

Soit $(\Delta x)_\psi (\Delta p_x)_\psi = 0 \longleftarrow$ impossible d'après la relation d'incertitude d'Heisenberg.

2. $$N(\alpha) = \langle \psi(\alpha)|\psi(\alpha)\rangle = \langle \hat\Delta(\alpha)\psi | \hat\Delta(\alpha)\psi\rangle$$

où $\hat\Delta(\alpha) = \hat p_x - \langle p_x\rangle_\psi + i\alpha(\hat x - \langle x\rangle_\psi)$

Formule utile : $\hat A$ opérateur quelconque.

$$\forall |\psi\rangle, |\varphi\rangle \quad \langle \hat A\psi|\varphi\rangle = \langle\varphi|\hat A\psi\rangle^* = (\langle A^\dagger\varphi|\psi\rangle)^* = \langle\psi|A^\dagger|\varphi\rangle$$

donc $\boxed{(\hat A^\dagger)^\dagger = \hat A}$

Ainsi $N(\alpha) = \langle\psi|\hat\Delta^\dagger(\alpha)\hat\Delta(\alpha)|\psi\rangle$

où $$\hat\Delta^\dagger(\alpha) = \underbrace{\hat p_x^\dagger}_{\hat p_x} - \underbrace{\langle p_x\rangle_\psi^*}_{\langle p_x\rangle_\psi} - i\underbrace{\alpha^*}_{\alpha \text{ puisque } \alpha \text{ est réel}}(\overbrace{\hat x^\dagger}^{\hat x} - \overbrace{\langle x\rangle_\psi^*}^{\langle x\rangle_\psi})$$

⚠

soit $\hat\Delta^\dagger(\alpha) = \hat p_x - \langle p_x\rangle_\psi - i\alpha(\hat x - \langle x\rangle_\psi)$

et $$\hat\Delta^\dagger(\alpha)\hat\Delta(\alpha) = \left(\hat p_x - \langle p_x\rangle_\psi - i\alpha(\hat x - \langle x\rangle_\psi)\right) \cdot \left(\hat p_x - \langle p_x\rangle_\psi + i\alpha(\hat x - \langle x\rangle_\psi)\right)$$

$$= \hat p_x^2 - \langle p_x\rangle_\psi \hat p_x + i\alpha(\hat p_x\hat x - \langle x\rangle_\psi \hat p_x) - \langle p_x\rangle_\psi\hat p_x + \langle p_x\rangle_\psi^2 - i\alpha(\langle p_x\rangle_\psi \hat x - \langle p_x\rangle_\psi\langle x\rangle_\psi)$$
$$+\alpha^2(\hat x^2 - 2\langle x\rangle_\psi \hat x + \langle x\rangle_\psi^2)$$
$$-i\alpha(\hat x - \langle x\rangle_\psi)(\hat p_x - \langle p_x\rangle_\psi)$$

donc

$$N(\alpha) = \underbrace{\langle p_x^2\rangle_\psi - \langle p_x\rangle_\psi^2} + i\alpha\langle\psi|\hat p_x\hat x|\psi\rangle - i\alpha\langle x\rangle_\psi\cancel{\langle p_x\rangle_\psi} - \cancel{\langle p_x\rangle_\psi^2} + \cancel{\langle p_x\rangle_\psi^2}$$
$$-i\alpha\cancel{\langle p_x\rangle_\psi}\langle x\rangle_\psi + i\alpha\cancel{\langle p_x\rangle_\psi}\langle x\rangle_\psi$$
$$+\alpha^2\langle x^2\rangle_\psi - 2\alpha^2\langle x\rangle_\psi^2 + \alpha^2\langle x\rangle_\psi^2$$
$$-i\alpha\langle\psi|\hat x\hat p_x|\psi\rangle + i\alpha\cancel{\langle p_x\rangle_\psi}\langle x\rangle_\psi$$
$$+i\alpha\langle x\rangle_\psi\cancel{\langle p_x\rangle_\psi} - i\alpha\cancel{\langle x\rangle_\psi}\langle p_x\rangle_\psi$$

$$N(\alpha) = (\Delta p_x)_\psi^2 + \alpha^2(\Delta x)_\psi^2 + i\alpha\langle\psi|\hat p_x\hat x - \hat x\hat p_x|\psi\rangle$$

$$\boxed{N(\alpha) = (\Delta x)_\psi^2\, \alpha^2 - i\alpha \langle\psi|[\hat{x},\hat{p_x}]|\psi\rangle + (\Delta p_x)_\psi^2}$$

3. Comme $[\hat{x},\hat{p_x}] = i\hbar$

$$N(\alpha) = (\Delta x)_\psi^2\, \alpha^2 + \alpha\hbar + (\Delta p_x)_\psi^2$$

$$= (\Delta x)_\psi^2 \left[\alpha^2 + \frac{\hbar\alpha}{(\Delta x)_\psi^2} + \frac{(\Delta p_x)_\psi^2}{(\Delta x)_\psi^2} \right]$$

$$= (\Delta x)_\psi^2 \left[\left(\alpha + \frac{\hbar}{2(\Delta x)_\psi^2}\right)^2 + \frac{(\Delta p_x)_\psi^2}{(\Delta x)_\psi^2} - \frac{\hbar^2}{4(\Delta x)_\psi^4} \right]$$

donc

$$N(\alpha) = (\Delta x)_\psi^2 \left[\left(\alpha + \frac{\hbar}{2(\Delta x)_\psi^2}\right)^2 + \frac{1}{(\Delta x)_\psi^2}\left[(\Delta p_x)_\psi^2 - \frac{\hbar^2}{4(\Delta x)_\psi^2}\right] \right]$$

$$N\left(-\frac{\hbar}{2(\Delta x)_\psi^2}\right) = (\Delta p_x)_\psi^2 - \frac{\hbar^2}{4(\Delta x)_\psi^2} \geqslant 0$$

puisque $N(\alpha) = \langle\psi(\alpha)|\psi(\alpha)\rangle$

norme au carré !

d'où $(\Delta p_x)_\psi^2 \geqslant \dfrac{\hbar^2}{4(\Delta x)_\psi^2} \Rightarrow (\Delta p_x)_\psi^2 (\Delta x)_\psi^2 \geqslant \dfrac{\hbar^2}{4}$

soit $\boxed{(\Delta x)_\psi (\Delta p_x)_\psi \geqslant \dfrac{\hbar}{2}}$