QUANTUM MECHANICS Lecture 4

Still about linear operators The Uncertainty Principle

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D. J. Griffiths: paragraph 1.6 and 2.1

Linear operators: a first view

In the previous lecture, we have seen that

- since for a point-like particle, every mechanical quantity Q can be expressed in terms of position and linear momentum;
- since to the position and the momentum we have to associate the linear operators
  $\hat{x} \rightarrow x\cdot$
  $\hat{p} \rightarrow -i\hbar\frac{\partial}{\partial x}$

it will be possible to associate to every physical observable Q a QM operator $\mathcal{Q}$ as follows

$$\mathcal{Q}(x,p) \rightarrow \mathcal{Q}\left(\hat{x},\hat{p}\right) \equiv \mathcal{Q}\left(x, -i\hbar\frac{\partial}{\partial x}\right)$$

Linear operators: a first view

1. Let us take, f.i., the kinetic energy $T = \frac{p^2}{2m}$. According to the above rule, the QM operator $\hat{T}$ associated to T is $\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$, which means, in particular, that, as far as the expectation value of T is concerned, we have

$$< T >= \int dx\, \Psi^*(x,t) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Big(\Psi(x,t) \Big) \right]$$

2. For the potential energy, the QM operator $\hat{V}$ is simply $V(\hat{x}) = V(x)$, which means that its expectation value on the state described by the normalized w.f. $\Psi(x,t)$ will be

$$< V >= \int dx\, \Psi^*(x,t) \Big[V(x)\, \Psi(x,t) \Big]$$

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Linear operators: a first view

1. The QM operator associated to the particle hamiltonian$^{(*)}$ $H = H(p, x) = T(p) + V(x)$ is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

2. and we recognize in $\hat{H}$ the operator present in the right hand side of the Schrödinger equation, acting on the wave-function $\Psi(x, t)$ (and this is not by chance ...).

(*) From Classical Mechanics we remember that

$$\frac{dx}{dt} = \frac{\partial H}{\partial p}; \quad \frac{dp}{dt} = -\frac{\partial H}{\partial x}$$

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Linear operators: a first view

Therefore, the expectation value E of the particle total energy is given by

$$E = \ < H >= \int dx\, \Psi^*(x,t) \Big[\hat{H}\, \Psi(x,t) \Big] =$$

$$= \int dx\, \Psi^*(x,t) \left[\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi(x,t) \right] =$$

$$= \ \int dx\, \Psi^*(x,t) \left[i\hbar \frac{\partial}{\partial t} \Psi(x,t) \right]$$

where, for the last conclusion, we have used the Schrödinger equation.

Linear operators: a first view

1. Before leaving the argument, let us point out an important property of the momentum operator $\hat{p} = -i\hbar\frac{\partial}{\partial x}$.

2. Let Ψ_1 and Ψ_2 be two (wave)functions such that $\Psi_{1,2}(x) \to 0$ when $x \to \pm\infty$.
   Let us consider the quantity

$$\int dx\, \Psi_2^*(x,t)\,(\hat{p}\Psi_1)\,(x,t) \equiv -i\hbar \int dx\, \Psi_2^*\, \frac{\partial \Psi_1}{\partial x}$$

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Linear operators: a first view

1. However

$$\Psi_2^* \frac{\partial \Psi_1}{\partial x} = \frac{\partial}{\partial x}\left(\Psi_2^* \Psi_1\right) - \frac{\partial \Psi_2^*}{\partial x}\,\Psi_1$$

and the total derivative does not contribute to the integral because, by hypothesis, $\Psi_{1,2}(x) \to 0$ when $x \to \pm\infty$.

2. Therefore

$$\int dx\, \Psi_2^*(x,t)\,(\hat{p}\Psi_1)(x,t) = i\hbar \int dx \frac{\partial \Psi_2^*}{\partial x}\Psi_1 =$$

$$= \int dx \left(-i\hbar \frac{\partial \Psi_2}{\partial x}\right)^* \Psi_1 \equiv \int dx\, (\hat{p}\Psi_2)^*\, \Psi_1$$

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Linear operators: a first view

This property for which we have, in particular, that

$$\int dx\, \Psi^* \left(\widehat{p}\Psi\right) = \int dx\, \left(\widehat{p}\Psi\right)^* \Psi \qquad (1)$$

ensures that the momentum expectation value $< p >$ is, as it should be, a **real quantity !**
In fact, since

$$< p >= \int dx\, \Psi^* \left(-i\hbar \frac{\partial \psi}{\partial x}\right) \equiv \int dx\, \Psi^* \left(\widehat{p}\Psi\right)$$

then

$$< p >^* = \int dx\, \Psi \left(\widehat{p}\Psi\right)^*$$

and, because of the identity (1), $< p >$ and $< p >^*$ **do** coincide !

Linear operators: a first view

1. But every dynamical variable Q, represented by an operator $\mathcal{Q}$, **must** have a real expectation value on any physical state.
   As a matter of fact, as we will see later on, for every Q we will indeed have that

$$\int dx\, \Psi_2^* \left(\mathcal{Q}\Psi_1\right) = \int dx\, \left(\mathcal{Q}\Psi_2\right)^* \Psi_1$$

2. We will come again on this property.
   For the moment, let us only point out and remember that, because of this, **for the hamiltonian** we have

$$\int dx\, \Psi_2^* \left(\widehat{H}\Psi_1\right) = \int dx\, \left(\widehat{H}\Psi_2\right)^* \Psi_1$$

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The uncertainty principle

1. Let us consider, now, the physical state described by the normalized w.f.

$$\Psi(x,0) = \sqrt{\frac{1}{s\sqrt{2\pi}}}\, e^{-\frac{(x-a)^2}{4s^2}} \equiv A\, e^{-\frac{(x-a)^2}{4s^2}}$$

   We have already seen that, for the **position** expectation value, we have $< x >= a$ and that the corresponding standard deviation is $\sigma_x = s$.

2. But what about the **momentum** ?

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The uncertainty principle

As far as its expectation value, we have

$$
\begin{aligned}
< p > \; &= \; -i\hbar \int dx\, \Psi^* \frac{\partial \Psi}{\partial x} = \\
= -i\hbar A^2 \int dx\, e^{\frac{-(x-a)^2}{4s^2}} &\left(\frac{-2(x-a)}{4s^2} e^{\frac{-(x-a)^2}{4s^2}} \right) = \\
= -i\hbar A^2 \int dy\, e^{\frac{-y^2}{4s^2}} &(-\frac{2y}{4s^2})\, e^{\frac{-y^2}{4s^2}} = \\
= i\hbar A^2 \frac{1}{2s^2} \int dy\, e^{\frac{-y^2}{2s^2}}\, y &= 0
\end{aligned}
$$

where we have put $y \equiv x - a$.

The uncertainty principle

Concerning $< p^2 >=< -\hbar^2 \frac{\partial^2}{\partial x^2} >$, we have

$$
\begin{aligned}
< p^2 > &= -\hbar^2 \int dx\, \Psi^* \frac{\partial^2 \Psi}{\partial x^2} = \\
&= -\hbar^2 A^2 \int dx\, e^{\frac{-(x-a)^2}{4s^2}} \left(\frac{\partial^2}{\partial x^2} e^{\frac{-(x-a)^2}{4s^2}} \right) = \\
&= -\hbar^2 A^2 \int dy\, e^{\frac{-y^2}{4s^2}} \left(\frac{\partial^2}{\partial y^2}\, e^{\frac{-y^2}{4s^2}} \right)
\end{aligned}
$$

But

$$
\begin{aligned}
\frac{\partial^2}{\partial y^2}\, e^{\frac{-y^2}{4s^2}} &= \frac{\partial}{\partial y} \left(-\frac{2y}{4s^2}\, e^{\frac{-y^2}{4s^2}} \right) = \\
&= \left[-\frac{1}{2s^2} + \frac{y^2}{2s^2} \frac{1}{2s^2} \right] e^{\frac{-y^2}{4s^2}}
\end{aligned}
$$

The uncertainty principle

Therefore

$$
\begin{aligned}
< p^2 > &= -\hbar^2 A^2 \int dy\ e^{\frac{-y^2}{4s^2}} \left[-\frac{1}{2s^2} + \frac{y^2}{2s^2}\frac{1}{2s^2} \right] e^{\frac{-y^2}{4s^2}} = \\
&= -\frac{\hbar^2 A^2}{2s^2} \int dy\, e^{\frac{-y^2}{2s^2}} \left[-1 + \frac{y^2}{2s^2} \right] = \\
&= -\frac{\hbar^2 A^2}{2s^2}\, s\sqrt{2} \int dz\, e^{-z^2} \left[-1 + z^2 \right]
\end{aligned}
$$

where we have defined $z \equiv \frac{y}{s\sqrt{2}}$.
But

$$
\int dz\, e^{-z^2} = \sqrt{\pi}
$$

The uncertainty principle

whereas

$$\int dz\, e^{-z^2}\, z^2 = -\frac{d}{d\alpha}\Big|_{\alpha=1} \int dz\, e^{-\alpha z^2} = $$
$$= -\frac{d}{d\alpha}\Big|_{\alpha=1} \sqrt{\frac{\pi}{\alpha}} = \frac{1}{2}\sqrt{\pi}$$

therefore

$$< p^2 > = -\frac{\hbar^2 A^2}{2s^2}\, s\sqrt{2}\left[-\sqrt{\pi} + \frac{1}{2}\sqrt{\pi}\right] =$$
$$= A^2 \frac{\hbar^2}{\sqrt{2}s}\left[\frac{1}{2}\sqrt{\pi}\right] = \frac{1}{s\sqrt{2\pi}}\frac{\hbar^2}{\sqrt{2}s}\frac{1}{2}\sqrt{\pi} =$$
$$= \frac{\hbar^2}{4s^2}$$

The uncertainty principle

1. Since $<p>= 0$, the standard deviation for the momentum distribution is then

$$\sigma_p = \frac{\hbar}{2s}$$

and one has

$$\sigma_x \, \sigma_p = s \, \frac{\hbar}{2s} = \frac{\hbar}{2}$$

2. This result shows that, at least on the w.f. we were considering, **the position and momentum uncertainties cannot be <u>both</u> reduced as much as we want**, since their product must remain constant.

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The uncertainty principle

This is a general feature.

We will show that, for any w.f., one obtains

$$\sigma_x \, \sigma_p \geq \frac{\hbar}{2}$$

The gaussian case is the more favourable !

1. It is the Heisenberg **uncertainty principle**.

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Exercise N.2

The physical state of a particle is represented at $t = 0$ by the following w.f.

$$\begin{aligned}\Psi(x,0) &= A(x^2 - 4a^2)\ for\ |x| \leq 2a \\ \psi(x,0) &= 0\ for\ |x| > 2a\end{aligned}$$

where A and a are positive constants.

a) determine the normalization constant A;
b) calculate the expectation value of x;
c) calculate the expectation value of p;
d) find σ_x;
e) find σ_p;
f) evaluate the product $\sigma_x \sigma_p$.