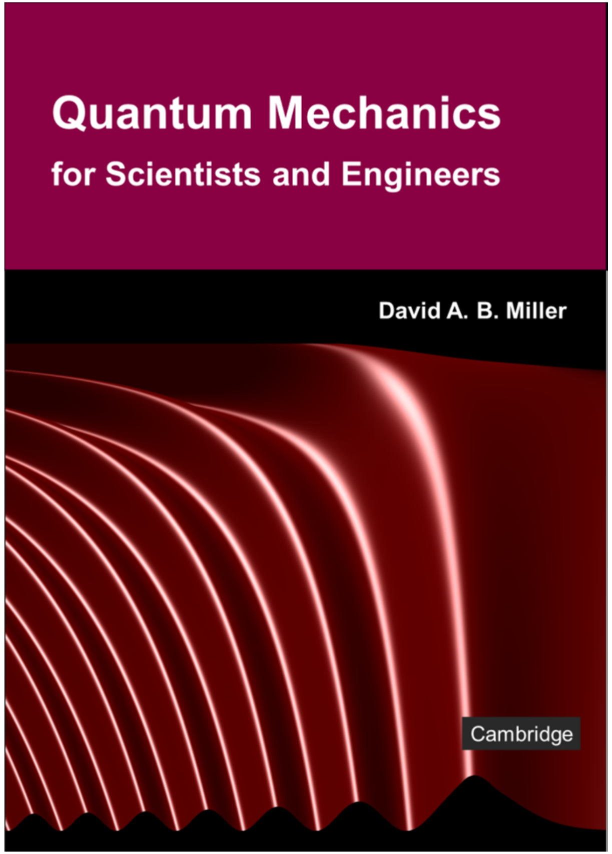
6.3 Operators and quantum mechanics

Slides: Video 6.3.1 Hermitian operators in quantum mechanics

Text reference: Quantum Mechanics for Scientists and Engineers

Section 5.1



Operators and quantum mechanics

Hermitian operators in quantum mechanics

Quantum mechanics for scientists and engineers

David Miller

Commutation of Hermitian operators

For Hermitian operators $\hat{A}$ and $\hat{B}$ representing physical variables

- it is very important to know if they commute
  - i.e., is $\hat{A}\hat{B} = \hat{B}\hat{A}$?

Remember that

- because these linear operators obey the same algebra as matrices
  - in general operators do not commute

Commutator

For quantum mechanics, we formally define an entity

$$\boxed{\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}}$$

This entity is called the commutator

An equivalent statement to saying $\hat{A}\hat{B} = \hat{B}\hat{A}$

is then $\left[\hat{A}, \hat{B}\right] = 0$

Strictly, this should be written $\left[\hat{A}, \hat{B}\right] = 0\hat{I}$

where $\hat{I}$ is the identity operator

but this is usually omitted

Commutation of operators

If the operators do not commute

then $\left[\hat{A},\hat{B}\right]=0$ does not hold

and in general we can choose to write

$$\left[\hat{A},\hat{B}\right]=i\hat{C}$$

where $\hat{C}$ is sometimes referred to as

the remainder of commutation or

the commutation rest

Commuting operators and sets of eigenfunctions

Operators that commute share the same set of eigenfunctions

and

operators that share the same set of eigenfunctions commute

We will now prove both of these statements

Commuting operators and sets of eigenfunctions

Suppose that operators $\hat{A}$ and $\hat{B}$ commute

and suppose the $|\psi_n\rangle$ are the eigenfunctions of $\hat{A}$

with eigenvalues A_i

Then $\hat{A}\hat{B}|\psi_i\rangle = \hat{B}\hat{A}|\psi_i\rangle = \hat{B}A_i|\psi_i\rangle = A_i\hat{B}|\psi_i\rangle$

i.e., $\hat{A}\left[\hat{B}|\psi_i\rangle\right] = A_i\left[\hat{B}|\psi_i\rangle\right]$

But this means that the vector $\hat{B}|\psi_i\rangle$

is also the eigenvector $|\psi_i\rangle$ or is proportional to it

i.e., for some number B_i

$$\hat{B}|\psi_i\rangle = B_i|\psi_i\rangle$$

Commuting operators and sets of eigenfunctions

This kind of relation $\hat{B}|\psi_i\rangle = B_i|\psi_i\rangle$

holds for all the eigenfunctions $|\psi_i\rangle$

so these eigenfunctions

are also the eigenfunctions of the operator $\hat{B}$

with associated eigenvalues B_i

Hence we have proved the first statement that

operators that commute share the same set of eigenfunctions

Note that the eigenvalues A_i and B_i are not in general equal to one another

Commuting operators and sets of eigenfunctions

Now we consider the statement

operators that share the same set of eigenfunctions commute

Suppose that the Hermitian operators $\hat{A}$ and $\hat{B}$

share the same complete set $|\psi_n\rangle$ of eigenfunctions

with associated sets of eigenvalues A_n and B_n respectively

Then

$$\hat{A}\hat{B}|\psi_i\rangle = \hat{A}B_i|\psi_i\rangle = A_iB_i|\psi_i\rangle$$

and similarly

$$\hat{B}\hat{A}|\psi_i\rangle = \hat{B}A_i|\psi_i\rangle = B_iA_i|\psi_i\rangle$$

Commuting operators and sets of eigenfunctions

Hence, for any function $|f\rangle$

which can always be expanded in this complete set of functions $|\psi_n\rangle$ i.e., $|f\rangle = \sum_i c_i |\psi_i\rangle$

we have

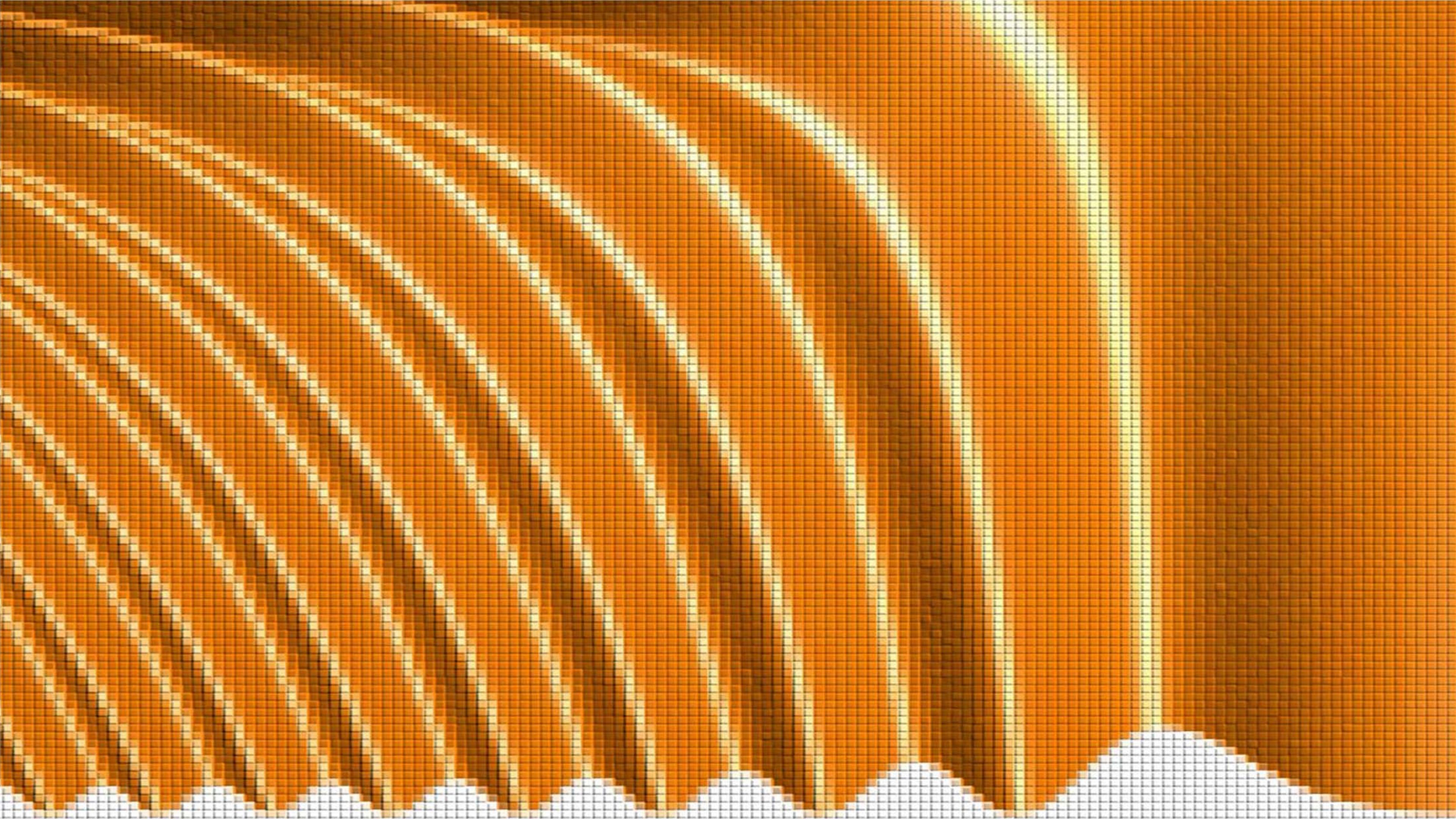
$$\hat{A}\hat{B}|f\rangle = \sum_i c_i A_i B_i |\psi_i\rangle = \sum_i c_i B_i A_i |\psi_i\rangle = \hat{B}\hat{A}|f\rangle$$

Since we have proved this for an arbitrary function

we have proved that the operators commute

hence proving the statement

operators that share the same set of eigenfunctions commute

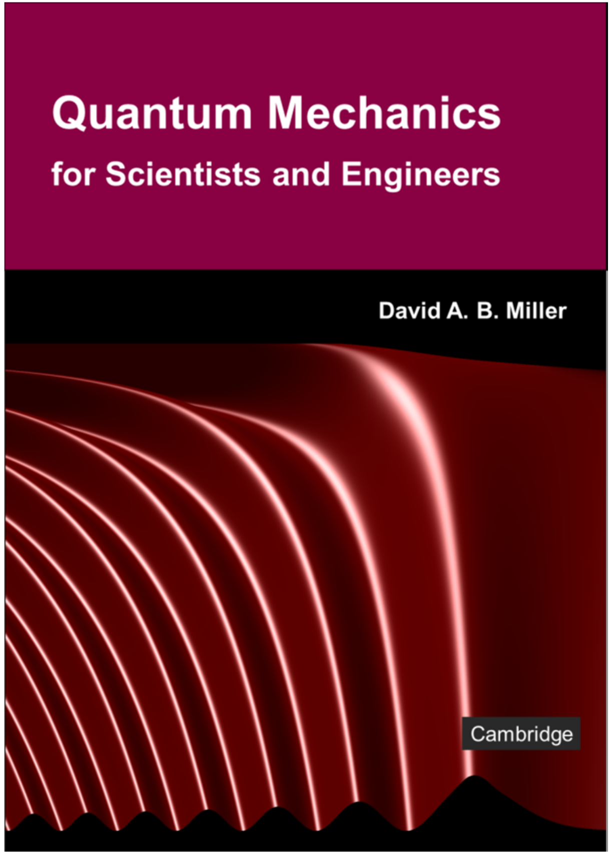


6.3 Operators and quantum mechanics

Slides: Video 6.3.3 General form of the uncertainty principle

Text reference: Quantum Mechanics for Scientists and Engineers

Section 5.2 (up to "Position-momentum uncertainty principle")



Operators and quantum mechanics

General form of the uncertainty principle

Quantum mechanics for scientists and engineers

David Miller

General form of the uncertainty principle

First, we need to set up the concepts of the mean and variance of an expectation value

Using $\bar{A}$ to denote the mean value of a quantity A

we have, in the bra-ket notation

for a measurable quantity associated with the Hermitian operator $\hat{A}$

when the state of the system is $|f\rangle$

$$\bar{A} \equiv \langle A \rangle = \langle f | \hat{A} | f \rangle$$

General form of the uncertainty principle

Let us define a new operator $\Delta\hat{A}$

associated with the difference between the measured value of A and its average value

$$\Delta\hat{A} = \hat{A} - \overline{A}$$

Strictly, we should write $\Delta\hat{A} = \hat{A} - \overline{A}\hat{I}$

but we take such an identity operator to be understood

Note that this operator is also Hermitian

General form of the uncertainty principle

Variance in statistics is the "mean square" deviation from the average

To examine the variance of the quantity A

we examine the expectation value of the operator $(\Delta\hat{A})^2$

Expanding the arbitrary function $|f\rangle$

on the basis of the eigenfunctions $|\psi_i\rangle$ of $\hat{A}$

i.e., $|f\rangle = \sum_i c_i |\psi_i\rangle$

we can formally evaluate the expectation value of $(\Delta\hat{A})^2$ when the system is in state $|f\rangle$

General form of the uncertainty principle

We have

$$\left\langle (\Delta\hat{A})^2 \right\rangle = \langle f \,|(\Delta\hat{A})^2|\, f \rangle = \left(\sum_i c_i^* \langle \psi_i | \right) \left(\hat{A} - \bar{A} \right)^2 \left(\sum_j c_j |\psi_j\rangle \right)$$

$$= \left(\sum_i c_i^* \langle \psi_i | \right) \left(\hat{A} - \bar{A} \right) \left(\sum_j c_j \left(A_j - \bar{A} \right) |\psi_j\rangle \right)$$

$$= \left(\sum_i c_i^* \langle \psi_i | \right) \left(\sum_j c_j \left(A_j - \bar{A} \right)^2 |\psi_j\rangle \right) = \sum_i |c_i|^2 \left(A_i - \bar{A} \right)^2$$

General form of the uncertainty principle

Because the $|c_i|^2$ are the probabilities that the system is found, on measurement, to be in the state $|\psi_i\rangle$

and $\left(A_i - \bar{A}\right)^2$ for that state simply represents

the squared deviation of the value of the quantity A

from its average value

then by definition

$$\overline{(\Delta A)^2} \equiv \left\langle \left(\Delta\hat{A}\right)^2 \right\rangle = \left\langle \left(\hat{A} - \bar{A}\right)^2 \right\rangle = \left\langle f \middle| \left(\hat{A} - \bar{A}\right)^2 \middle| f \right\rangle$$

is the mean squared deviation for the quantity A

on repeatedly measuring the system prepared in state $|f\rangle$

General form of the uncertainty principle

In statistical language

the quantity $\overline{(\Delta A)^2}$ is called the variance

and the square root of the variance

which we can write as $\Delta A \equiv \sqrt{\overline{(\Delta A)^2}}$

is the standard deviation

In statistics

the standard deviation gives a

well-defined measure of

the width of a distribution

General form of the uncertainty principle

We can also consider some other quantity B

associated with the Hermitian operator $\hat{B}$

$$\overline{B} = \langle B \rangle = \langle f | \hat{B} | f \rangle$$

and, with similar definitions

$$\overline{(\Delta B)^2} \equiv \left\langle \left(\Delta \hat{B}\right)^2 \right\rangle = \left\langle \left(\hat{B} - \overline{B}\right)^2 \right\rangle = \langle f | \left(\hat{B} - \overline{B}\right)^2 | f \rangle$$

So we have ways of calculating the uncertainty in the measurements of the quantities A and B

when the system is in a state $|f\rangle$

to use in a general proof of the uncertainty principle

General form of the uncertainty principle

Suppose two Hermitian operators $\hat{A}$ and $\hat{B}$ do not commute

and have a commutation rest $\hat{C}$

as defined above in $\left[\hat{A}, \hat{B}\right] = i\hat{C}$

Consider, for some arbitrary real number α , the number

$$G(\alpha) = \left\langle \left(\alpha\Delta\hat{A} - i\Delta\hat{B}\right) f \middle| \left(\alpha\Delta\hat{A} - i\Delta\hat{B}\right) f \right\rangle \geq 0$$

By $\left|\left(\alpha\Delta\hat{A} - i\Delta\hat{B}\right) f\right\rangle$ we mean the vector $\left(\alpha\Delta\hat{A} - i\Delta\hat{B}\right)\left| f \right\rangle$

written this way to emphasize it is simply a vector

so it must have an inner product with itself

that is greater than or equal to zero

General form of the uncertainty principle

So

$$G(\alpha) = \langle f | \left(\alpha\Delta\hat{A} - i\Delta\hat{B}\right)^{\dagger} \left(\alpha\Delta\hat{A} - i\Delta\hat{B}\right) | f \rangle \ (\geq 0)$$

$$= \langle f | \left(\alpha\Delta\hat{A}^{\dagger} + i\Delta\hat{B}^{\dagger}\right)\left(\alpha\Delta\hat{A} - i\Delta\hat{B}\right) | f \rangle$$

By Hermiticity

$$= \langle f | \left(\alpha\Delta\hat{A} + i\Delta\hat{B}\right)\left(\alpha\Delta\hat{A} - i\Delta\hat{B}\right) | f \rangle$$

$$= \langle f | \alpha^2 \left(\Delta\hat{A}\right)^2 + \left(\Delta\hat{B}\right)^2 - i\alpha\left(\Delta\hat{A}\Delta\hat{B} - \Delta\hat{B}\Delta\hat{A}\right) | f \rangle$$

$$= \langle f | \alpha^2 \left(\Delta\hat{A}\right)^2 + \left(\Delta\hat{B}\right)^2 - i\alpha\left[\Delta\hat{A}, \Delta\hat{B}\right] | f \rangle$$

$$= \langle f | \alpha^2 \left(\Delta\hat{A}\right)^2 + \left(\Delta\hat{B}\right)^2 + \alpha\hat{C} | f \rangle$$

General form of the uncertainty principle

So

$$G(\alpha) = \langle f | \alpha^2 \left(\Delta\hat{A}\right)^2 + \left(\Delta\hat{B}\right)^2 + \alpha\hat{C} | f \rangle \quad (\geq 0)$$

$$= \alpha^2 \overline{(\Delta A)^2} + \overline{(\Delta B)^2} + \alpha\bar{C}$$

where $\bar{C} \equiv \langle C \rangle = \langle f | \hat{C} | f \rangle$

By a simple (though not obvious) rearrangement

$$G(\alpha) = \overline{(\Delta A)^2}\left[\alpha + \frac{\bar{C}}{2\overline{(\Delta A)^2}}\right]^2 + \overline{(\Delta B)^2} - \frac{\left(\bar{C}\right)^2}{4\overline{(\Delta A)^2}} \geq 0$$

General form of the uncertainty principle

But
$$G(\alpha) = \overline{(\Delta A)^2}\left[\alpha + \frac{\bar{C}}{2\overline{\overline{(\Delta A)^2}}}\right]^2 + \overline{(\Delta B)^2} - \frac{(\bar{C})^2}{4\overline{\overline{(\Delta A)^2}}} \geq 0$$

must be true for arbitrary α

so it is true for $\alpha = -\frac{\bar{C}}{2\overline{\overline{(\Delta A)^2}}}$

which sets the first term equal to zero

so $\overline{(\Delta A)^2}\,\overline{(\Delta B)^2} \geq \frac{(\bar{C})^2}{4}$ or $\Delta A \Delta B \geq \frac{|\bar{C}|}{2}$

General form of the uncertainty principle

So, for two operators $\hat{A}$ and $\hat{B}$

corresponding to measurable quantities A and B

for which $\left[\hat{A},\hat{B}\right]=i\hat{C}$

in some state $|f\rangle$ for which $\bar{C}\equiv\langle C\rangle=\langle f|\hat{C}|f\rangle$

we have the uncertainty principle

$$\boxed{\Delta A\Delta B\geq\frac{\left|\bar{C}\right|}{2}}$$

where ΔA an ΔB are the standard deviations of the values of A and B we would measure

General form of the uncertainty principle

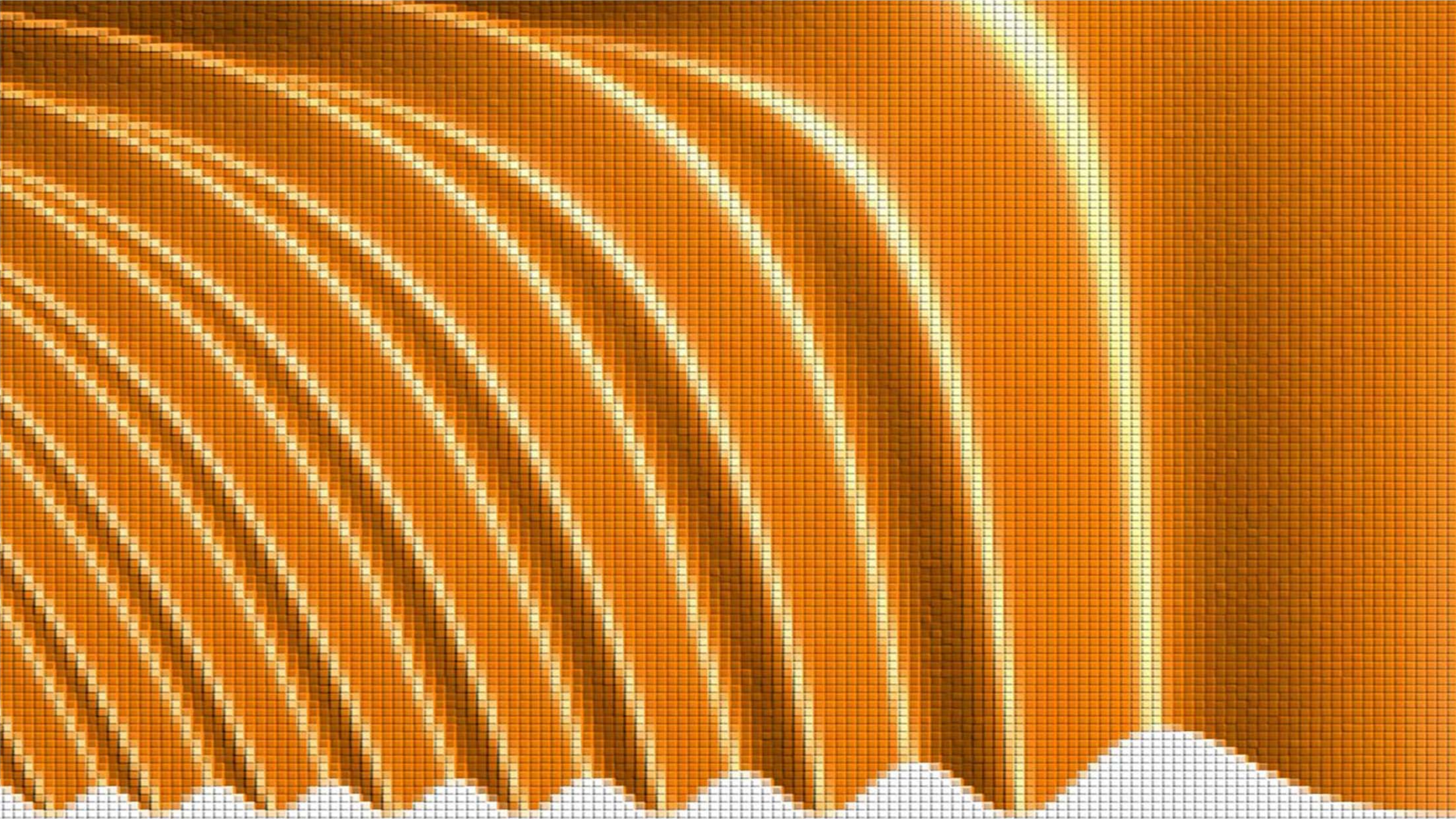
Only if the operators $\hat{A}$ and $\hat{B}$ commute

i.e., $\left[\hat{A},\hat{B}\right]=0$ (or, strictly, $\left[\hat{A},\hat{B}\right]=0\hat{I}$)

or if they do not commute, i.e., $\left[\hat{A},\hat{B}\right]=i\hat{C}$

but we are in a state $\left|f\right\rangle$ for which $\left\langle f\middle|\hat{C}\middle|f\right\rangle=0$

is it possible for both A and B simultaneously to have exact measurable values

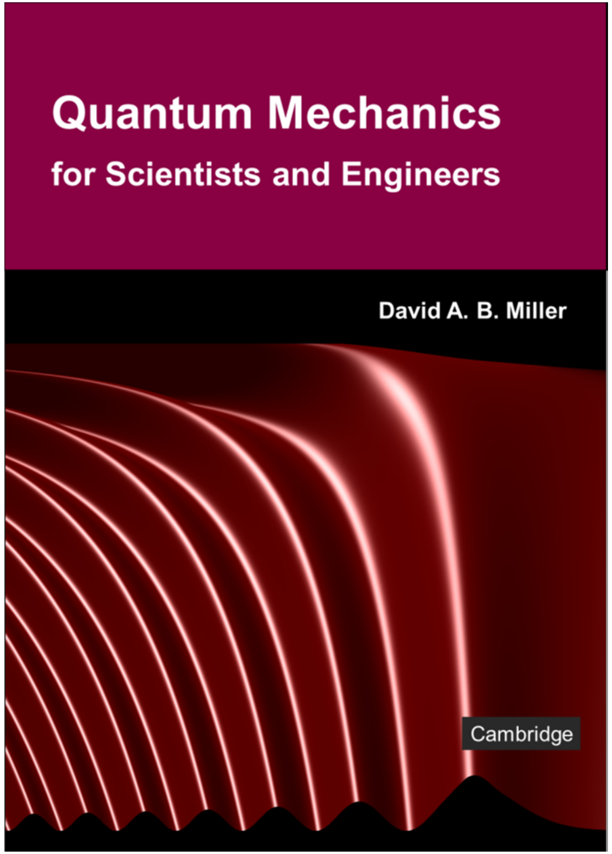


6.3 Operators and quantum mechanics

Slides: Video 6.3.5 Specific uncertainty principles

Text reference: Quantum Mechanics for Scientists and Engineers

Section 5.2 (starting from "Position-momentum uncertainty principle")



Operators and quantum mechanics

Specific uncertainty principles

Quantum mechanics for scientists and engineers

David Miller

Position-momentum uncertainty principle

We now formally derive the position-momentum relation

Consider the commutator of $\hat{p}_x$ and x

(We treat the function x as the operator for position)

To be sure we are taking derivatives correctly

we have the commutator operate on an arbitrary function

$$[\hat{p}_x, x]|f\rangle = -i\hbar\left(\frac{d}{dx}x - x\frac{d}{dx}\right)|f\rangle = -i\hbar\left\{\frac{d}{dx}\left(x|f\rangle\right) - x\frac{d}{dx}|f\rangle\right\}$$

$$= -i\hbar\left\{|f\rangle + x\frac{d}{dx}|f\rangle - x\frac{d}{dx}|f\rangle\right\} = -i\hbar|f\rangle$$

Position-momentum uncertainty principle

In $[\hat{p}_x, x]|f\rangle = -i\hbar|f\rangle$

since $|f\rangle$ is arbitrary

we can write $[\hat{p}_x, x] = -i\hbar$

and the commutation rest operator $\hat{C}$

is simply the number $\hat{C} = -\hbar$

Hence $\bar{C} = -\hbar$

and so, from $\Delta A \Delta B \geq |\bar{C}|/2$

we have $\Delta p_x \Delta x \geq \dfrac{\hbar}{2}$

Energy-time uncertainty principle

The energy operator is the Hamiltonian $\hat{H}$

and from Schrödinger's equation $\hat{H}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$

so we use $\hat{H} \equiv i\hbar\partial/\partial t$

If we take the time operator to be just t

then using essentially identical algebra as used for the momentum-position uncertainty principle

$$\left[\hat{H},t\right] = i\hbar\left(\frac{\partial}{\partial t}t - t\frac{\partial}{\partial t}\right) = i\hbar$$

so, similarly we have

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Frequency-time uncertainty principle

We can relate this result mathematically to

the frequency-time uncertainty principle

that occurs in Fourier analysis

Noting that $E = \hbar\omega$ in quantum mechanics

we have

$$\Delta\omega\Delta t \geq \frac{1}{2}$$