6 Operators and observables

Bring solutions along to the class at 10am on 9/11/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time. Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

6.0 Videos

Please watch this week's videos: V6.1, V6.2, V6.3, V6.4.

All videos are available on the youtube channel Introductory Quantum Mechanics (link available at felixflicker.com/teaching, or on Learning Central).

6.1 The Heisenberg picture

In the Heisenberg picture states $|\psi\rangle$ are time-independent, but operators are time dependent:

$$\hat{A}_H(t) = \exp\left(i\hat{H}t/\hbar\right)\hat{A}_S \exp\left(-i\hat{H}t/\hbar\right). \tag{118}$$

Here $\hat{A}_H(t)$ is a time-dependent operator in the Heisenberg picture and $\hat{A}_S$ is a time-independent operator in the Schrödinger picture (*e.g.* $\hat{x}$). Similarly, in the Schrödinger picture states are time dependent:

$$|\psi_S(t)\rangle = \exp\left(-i\hat{H}t/\hbar\right)|\psi_S(0)\rangle = \exp\left(-i\hat{H}t/\hbar\right)|\psi_H\rangle \tag{119}$$

where $|\psi_S(t)\rangle$ is a time-dependent state in the Schrödinger picture and $|\psi_H\rangle$ is a time-independent state in the Heisenberg picture, and an arbitrary choice of global phase has been made to set the two states equal at $t = 0$.

6.1.1

Two matrices or operators $\hat{A}$ and $\hat{B}$ are equivalent iff

$$\langle\varphi|\hat{A}|\psi\rangle = \langle\varphi|\hat{B}|\psi\rangle \quad \forall|\varphi\rangle, |\psi\rangle. \tag{120}$$

Show that

$$\langle\varphi_H|\hat{A}_H(t)|\psi_H\rangle = \langle\varphi_S(t)|\hat{A}_S|\psi_S(t)\rangle \tag{121}$$

and hence the two pictures are equivalent.

6.1.2

(a) Using the TDSE explain why the differential operator $i\hbar\partial_t$ must commute with the Hamiltonian $\hat{H}$:

$$\left[i\hbar\partial_t, \hat{H}\right] = 0. \tag{122}$$

(b) Why must

$$\left[\hat{H}, f\left(\hat{H}\right)\right] = 0 \tag{123}$$

for any function f?

6.1.3

Hence derive the Heisenberg equation of motion:

$$i\hbar\frac{\mathrm{d}\hat{A}_H(t)}{\mathrm{d}t} = \left[\hat{A}_H(t), \hat{H}\right]. \tag{124}$$

6.1.4

Use this result to prove Ehrenfest's theorem:

$$i\hbar\frac{\mathrm{d}\langle\hat{A}\rangle}{\mathrm{d}t} = \langle\left[\hat{A}, \hat{H}\right]\rangle. \tag{125}$$

6.1.5

Prove Ehrenfest's theorem another way, by taking the partial time derivative of the expectation value of a time-independent operator in the Schrödinger picture:

$$\langle\varphi_S(t)|\hat{A}_S|\psi_S(t)\rangle. \tag{126}$$

6.1.6

In fact operators in the Schrödinger picture can have their own time dependences; for example, we might be interested in a potential which varies with time. Such cases are beyond the syllabus for this course. Show that if $\hat{A}_S(t)$ has a time dependence the Heisenberg equation of motion reads

$$i\hbar\frac{\mathrm{d}\hat{A}_H(t)}{\mathrm{d}t} = \left[\hat{A}_H(t), \hat{H}\right] + i\hbar\exp\left(-i\hat{H}t/\hbar\right)\left(\frac{\partial\hat{A}_S(t)}{\partial t}\right)\exp\left(i\hat{H}t/\hbar\right). \tag{127}$$

6.2 The Heisenberg Uncertainty Principle

6.2.1

State the (generalised) Heisenberg uncertainty principle, explaining the various terms in the expression.

6.2.2

The *canonical commutation relation* (an experimentally-derived result which you should memorise!) states that

$$[\hat{x}, \hat{p}] = i\hbar\hat{\mathbb{I}} \tag{128}$$

where $\hat{\mathbb{I}}$ is the identity operator, for which any state is an eigenstate with with eigenvalue 1. Use this to find the Heisenberg uncertainty relation between the position and momentum of a particle.

6.2.3

Using the commutation relation between spin operators:

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z \tag{129}$$

find the uncertainty relation between the x- and y- components of the intrinsic angular momentum.

6.2.4

Give a physical explanation for the mathematical results you just derived.

6.3 The correspondence principle

The correspondence principle is the idea that classical mechanics should be returned as the $\hbar \to 0$ limit of quantum mechanics ($\hbar$ is constant, but if it could vary, setting it to zero would result in a classical universe). Part of this is the idea that quantum results should approximate classical results at large quantum numbers. Ehrenfest's theorem is often used as evidence in support of this idea.

6.3.1

Prove the general matrix result

$$[AB, C] = A[B, C] + [A, C]B. \tag{130}$$

6.3.2

Using the canonical commutation relation show that

$$\left[\hat{x}^2, \hat{p}\right] = 2i\hbar\hat{x}. \tag{131}$$

6.3.3

Another way to show the same result is by 'pulling through' the $\hat{p}$ operator, which is a very useful trick. Noting that

$$\hat{p}\hat{x} = \hat{x}\hat{p} - [\hat{x}, \hat{p}] \tag{132}$$

by the definition of the commutator, you can pull the $\hat{p}$ operator through the $\hat{x}$ operator, switching their order, at the cost of subtracting the commutator.

a) Show that

$$\hat{p}\hat{x}^2 = (\hat{x}\hat{p} - [\hat{x}, \hat{p}])\,\hat{x} \tag{133}$$

and therefore

$$\hat{p}\hat{x}^2 = \hat{x}\hat{p}\hat{x} - i\hbar\hat{x}. \tag{134}$$

b) Repeating the same technique, show that

$$\hat{p}\hat{x}^2 = \hat{x}^2\hat{p} - 2i\hbar\hat{x}. \tag{135}$$

c) Therefore deduce that

$$\left[\hat{x}^2, \hat{p}\right] = 2i\hbar\hat{x}. \tag{136}$$

6.3.4

This technique of pulling through the operator can be used to prove a more general result.

a) Show that

$$\hat{p}\hat{x}^n = \hat{x}\hat{p}\hat{x}^{n-1} - i\hbar\hat{x}^{n-1} \tag{137}$$

b) Noting that the first term on the right-hand side contains $\hat{p}\hat{x}^{n-1}$, and that you have already worked this out in (a) (replacing n with $n-1$), show that

$$\hat{p}\hat{x}^n = \hat{x}^2\hat{p}\hat{x}^{n-2} - 2i\hbar\hat{x}^{n-1}. \tag{138}$$

c) Therefore explain why

$$\hat{p}\hat{x}^n = \hat{x}^n\hat{p} - ni\hbar\,\hat{}^{\hat{n}-1}\hat{x} \tag{139}$$

and deduce that

$$[\hat{x}^n, \hat{p}] = ni\hbar\,\hat{x}^{n-1}. \tag{140}$$

d) # How might you denote the result of

$$\frac{1}{i\hbar}\left[f\left(\hat{x}\right), \hat{p}\right]? \tag{141}$$

6.3.5

Using Ehrenfest's theorem, show that

$$\frac{\mathrm{d}\left\langle \hat{x} \right\rangle}{\mathrm{d}t} = \frac{\left\langle \hat{p} \right\rangle}{m}. \tag{142}$$

This suggests that the expectation values of quantum operators obey the classical equation $\dot{x} = p/m$, even if quantum operators do not.

6.3.6

a) Using Ehrenfest's theorem, and defining $V\left(\hat{x}\right)$ by its Taylor series, show that

$$\frac{\mathrm{d}\left\langle \hat{p} \right\rangle}{\mathrm{d}t} = -\left\langle V'\left(\hat{x}\right)\right\rangle \tag{143}$$

where $f'\left(x\right) = \partial f\left(x\right)/\partial x$.

b) Which classical equation of motion does this resemble?

c) Combined with the previous result it is tempting to say that the expectation values of quantum operators obey classical equations of motion. What feature of this second equation makes such a statement inaccurate?

d) Find a condition on the expectation values of the power of the position operator for which the statement is accurate.

e) Show that this condition is obeyed in the case of a quadratic potential.

6.4 Joint eigenvectors

In this question we will prove that if two matrices commute they have a joint set of eigenvectors.

6.4.1

Consider two matrices A and B which have all the same eigenvectors but potentially different eigenvalues:

$$A|v_n\rangle = a_n|v_n\rangle \tag{144}$$

$$B|v_n\rangle = b_n|v_n\rangle. \tag{145}$$

Assuming that neither A nor B has a zero eigenvalue, show that

$$[A, B] = 0. \tag{146}$$

6.4.2

Now we'll prove the converse. Define the eigenvectors of A to be

$$A|a_n\rangle = a_n|a_n\rangle. \tag{147}$$

Show that if

$$[A, B] = 0 \tag{148}$$

then $|a_n\rangle$ must also be an eigenvector of B.

6.4.3

Explain why these results show that if two quantum mechanical observables can be known simultaneously their operators must commute, and vice versa.

6.5 Quantum numbers

6.5.1

Explain what is meant by a quantum number.

6.5.2

Using Ehrenfest's theorem, explain why, for an observable to be a quantum number, the corresponding operator must commute with the Hamiltonian.

6.5.3

Hence explain why energy is always a good quantum number.

6.5.4

Explain why it is always possible to have simultaneous knowledge of a quantum number and of the energy of the system.

6.6 # Energy-time uncertainty

The energy-time uncertainty relation cannot be made precise like other uncertainty relations, because there is no time operator in quantum mechanics. This question explores one approach to making a precise statement of the energy-time uncertainty due to Mandelstam and Tamm.

6.6.1

List some reasons we expect there to be some kind of uncertainty relation between energy and time.

6.6.2

Use Ehrenfest's theorem and the generalised Heisenberg uncertainty equation to show that

$$\sigma_{\hat{H}} \left(\frac{\sigma_{\hat{A}}}{\left| \frac{\mathrm{d}\langle A \rangle}{\mathrm{d}t} \right|} \right) \geq \frac{\hbar}{2} \tag{149}$$

where $\sigma_{\hat{A}}$ is the uncertainty in $\hat{A}$, defined in the usual way as the standard deviation, $\hat{H}$ is the Hamiltonian, and $\hat{A}$ is an arbitrary operator.

6.6.3

Suggest an interpretation of the formula you have just found.