

Quantum Theory

lecture 1: Fundamental concepts

from wave mechanics to matrix mechanics

- position and momentum representation S-1.6,1.7
- states and operators (bra-ket notation) S-1.2,1.3
- unitary transformations S-1.5, 2.1
- Heisenberg equations of motion, Ehrenfest theorem S-2.2
- Hellmann-Feynman theorem
- uncertainty relation S-1.4

S = Sakurai, 2nd edition

position & momentum representation

position operator: $\hat{q}\psi(q) = q\psi(q)$

eigenstate $\delta(q - q_0)$ at eigenvalue q_0

$$\hat{q}\delta(q - q_0) = q\delta(q - q_0) = q_0\delta(q - q_0)$$

momentum operator: $\hat{p}\psi(q) = -i\hbar\frac{\partial}{\partial q}\psi(q)$

eigenstate $\psi_p(q) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipq/\hbar}$ because $\hat{p}\psi_p(q) = p\psi_p(q)$

normalization: $\int dq \psi_{p'}^*(q)\psi_p(q) = \delta(p - p')$

$$\text{recall: } \int_{-\infty}^{\infty} dx e^{ikx} = 2\pi\delta(k)$$

$$\phi(p) = \int dq \psi_p^*(q)\psi(q) = \frac{1}{\sqrt{2\pi\hbar}} \int dq e^{-ipq/\hbar} \psi(q)$$

momentum representation: $\hat{p}\phi(p) = p\phi(p)$, $\hat{q}\phi(p) = i\hbar\frac{\partial}{\partial p}\phi(p)$

states & operators (bra-ket notation)

state: $|\psi\rangle$ (ket = column vector) and $\langle\psi|$ (bra = row vector)

scalar product: $\langle\chi|\phi\rangle = \langle\phi|\chi\rangle^*$

orthonormal set: $\langle\phi_n|\phi_m\rangle = \delta_{nm}$

$$\text{completeness: } |\psi\rangle = \sum_n |\phi_n\rangle\langle\phi_n|\psi\rangle \Rightarrow \sum_n |\phi_n\rangle\langle\phi_n| = \hat{1}$$

“resolution of the identity”

operator: $\langle\chi|A\phi\rangle = \langle\chi|A|\phi\rangle$, $\langle A\chi|\phi\rangle = \langle\chi|A^\dagger|\phi\rangle$

Hermitian conjugate or adjoint operator: $(A^\dagger)_{nm} = A_{mn}^*$

self-adjoint (Hermitian): $A^\dagger = A$ (real eigenvalues, observable)

from q to p representation: $\psi(q) = \langle q|\psi\rangle$, $\phi(p) = \langle p|\psi\rangle$

$$\langle p|\psi\rangle = \int dq \langle p|q\rangle\langle q|\psi\rangle \Rightarrow \langle p|q\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipq/\hbar}$$

unitary transformations

$$\langle \hat{U}\phi | \hat{U}\chi \rangle = \langle \phi | \chi \rangle \Rightarrow \hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{1}$$

or $U^{-1} = U^\dagger$ **unitary operator**

example: $\hat{U} = e^{i\hat{A}}$ with \hat{A} Hermitian

eigenvalues on the unit circle in the complex plane

$\phi' = \hat{U}\phi, \chi' = \hat{U}\chi$ is a change of basis for the states, what is the corresponding basis change for the operators?

$$\langle \phi | \hat{O} | \chi \rangle = \langle \phi' | \hat{U} \hat{O} \hat{U}^\dagger | \chi' \rangle \Rightarrow \hat{O}' = \hat{U} \hat{O} \hat{U}^\dagger$$

check that commutator $[\hat{q}, \hat{p}] = i\hbar$ is unchanged upon unitary transformation

Heisenberg equation

solution of Schrödinger equation is a unitary transformation

$$i\hbar \frac{\partial}{\partial t} \psi(t) = \hat{H} \psi(t) \Rightarrow \psi(t) = e^{-i\hat{H}t/\hbar} \psi(0)$$

Schrödinger picture: time dependence in states

Heisenberg picture: time dependence in operators

$$\langle \phi(t) | \hat{O} | \chi(t) \rangle = \langle \phi | \hat{O}(t) | \chi \rangle$$

with $|\psi\rangle \equiv |\psi(0)\rangle$ and $\hat{O}(t) = e^{i\hat{H}t/\hbar} \hat{O} e^{-i\hat{H}t/\hbar}$

$$i\hbar \frac{d}{dt} \hat{O} = \hat{O} \hat{H} - \hat{H} \hat{O} = [\hat{O}, \hat{H}]$$

Heisenberg equation of motion

Ehrenfest theorem (1927):

$$m \frac{d}{dt} \langle x \rangle = \langle p \rangle, \quad \frac{d}{dt} \langle p \rangle = -\langle V'(x) \rangle, \quad \text{for } H = p^2/2m + V(x).$$

$$[x, F(p)] = i\hbar F', \quad [p, G(x)] = -i\hbar G'$$

Hellmann-Feynman theorem

$$\frac{d}{d\lambda} E(\lambda) = \left\langle \psi(\lambda) \left| \frac{dH(\lambda)}{d\lambda} \right| \psi(\lambda) \right\rangle.$$

for $H(\lambda)\psi(\lambda) = E(\lambda)\psi(\lambda)$

the derivative $d\psi/d\lambda$ does not contribute because of normalization,

$$\langle \psi' | H | \psi \rangle + \langle \psi | H | \psi' \rangle = E \frac{d}{d\lambda} \langle \psi | \psi \rangle = 0.$$

uncertainty relation

see exercise 1.4

$$\Delta A = A - \langle A \rangle, \quad \Delta B = B - \langle B \rangle : \quad \langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} |\langle [A, B] \rangle|^2.$$

proof from Cauchy-Schwarz inequality:

$$|\langle \alpha | \alpha \rangle| |\langle \beta | \beta \rangle| \geq |\langle \alpha | \beta \rangle|^2 \Rightarrow \langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq |\langle \Delta A \Delta B \rangle|^2.$$

$$\Delta A \Delta B = \frac{1}{2} [\Delta A, \Delta B] + \frac{1}{2} \{ \Delta A, \Delta B \} = \text{real} + \text{imaginary}$$

$$\Rightarrow |\langle \Delta A \Delta B \rangle|^2 = \frac{1}{4} |\langle [\Delta A, \Delta B] \rangle|^2 + \frac{1}{4} |\langle \{ \Delta A, \Delta B \} \rangle|^2 \geq \frac{1}{4} |\langle [\Delta A, \Delta B] \rangle|^2.$$