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: $\int dq\, \psi^*_{p'}(q)\psi_p(q) = \delta(p - p')$

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

momentum representation:

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

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

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

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

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

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

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

proof from Cauchy-Schwarz inequality:

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

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

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