QUANTUM MECHANICS, FALL 2000

First five weeks (1/3 of the course):

We've covered most of chapters 1& 2 in Sakurai

= *THE BASICS OF QUANTUM MECHANICS*, except:

Stern-Gerlach (self study!)

The uncertainty relation (self study!)

Potentials and gauge transformations
(this week's reading assignment
+ discussion later in the course)

Next...

The theory of angular momentum
(Sakurai, chapter 3)

basic ingredient in most of quantum physics....

from

the foundation of *quantum field theory...*

(*Spin-Statistics Theorem for General Spin*)

For a general irreducible spinor field the "wrong" connection of spin with statistics

$$[\varphi_\alpha(x), \varphi_\alpha{}^*(y)]_+ = 0 \quad \varphi \text{ of integer spin}$$

$$[\varphi_\alpha(x), \varphi_\alpha{}^*(y)]_- = 0 \quad \varphi \text{ of half-odd integer spin}$$

$$\text{for } (x-y)^2 < 0 \qquad (4\text{–}48)$$

implies $\varphi_\alpha(x)\Psi_0 = 0$. In a field theory in which all fields either commute or anti-commute this implies $\varphi_\alpha = \varphi_\alpha{}^* = 0$.

...to

solid state architectures for quantum computers

spins inside

QUANTUM PRO

PROCESSOR

Selected Lecture Notes
Quantum Mechanics
FKA 081, fall 2000
Henrik Johannesson

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THEORY OF ANGULAR MOMENTUM

"WARM UP"

TRANSLATIONS IN SPACE

Translations in Q.M.

Classically $x \to x + \varepsilon$, $p \to p$ $\Longrightarrow$ Ehrenfest — $T(\varepsilon)$ —
$$\boxed{\begin{array}{l} \langle x \rangle \to \langle x \rangle + \varepsilon \\ \langle p \rangle \to \langle p \rangle \end{array}}$$

$$T(\varepsilon) | \psi \rangle = | \psi_\varepsilon \rangle$$

$$\langle x | \psi_\varepsilon \rangle = \langle x | T_\varepsilon | \psi \rangle = \psi(x - \varepsilon) \equiv \tilde{\psi}(x)$$

$$\Updownarrow$$

$$\tilde{\psi}(x + \varepsilon) = \psi(x)$$

IMPORTANT!

The translation operator takes the number $\psi(x)$ assigned to the point x and reassigns it to the translated point $x' = x + \varepsilon$

TRANSLATIONAL INVARIANCE

$$\langle \psi | H | \psi \rangle = \langle \psi_\varepsilon | H | \psi_\varepsilon \rangle = \langle \psi | T^+(\varepsilon) H T(\varepsilon) | \psi \rangle$$

$T(\varepsilon) = \mathbb{1} - \frac{i\varepsilon}{\hbar} P \longrightarrow$
$$= \langle \psi | (1 + \tfrac{i\varepsilon}{\hbar} P) H (1 - \tfrac{i\varepsilon}{\hbar} P) | \psi \rangle$$
$$= \langle \psi | H | \psi \rangle + \tfrac{i\varepsilon}{\hbar} \langle \psi | [P, H] | \psi \rangle$$

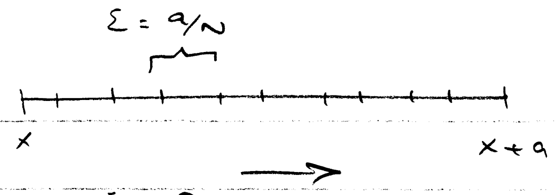
Ehrenfest

$$\Rightarrow \langle [P, H] \rangle = 0 \quad \Rightarrow \langle \dot{P} \rangle = 0$$

$$\Updownarrow$$

MOMENTUM CONSERVATION

Finite translations



$$T(\varepsilon) = T(a/N) = 1 - \frac{ia}{\hbar N}\hat{P}$$

$$\Rightarrow T(a) = \lim_{N\to\infty}\left[T(a/N)\right]^N = e^{-ia\hat{P}/\hbar}$$

use $e^{-ax} = \lim_{N\to\infty}\left(1 - \frac{ax}{N}\right)^N$

(Ok since $\hat{P}$ commutes with itself!)

TIME TRANSLATIONS

$$T(\varepsilon) = 1\!\!1 - \frac{i\varepsilon}{\hbar}H$$ ← Hamiltonian = generator of infinitesimal time translations

TIME TRANSLATIONAL INVARIANCE

$$\Downarrow$$

$$\langle \dot{H} \rangle = 0$$

ENERGY CONSERVATION

Rotations in space

1D $\longrightarrow$ 2D , 3D

$$\begin{cases} P_x \to -i\hbar\, \partial_x \\ P_y \to -i\hbar\, \partial_y \end{cases}$$ in a coordinate basis $|x,y\rangle$
$= |x\rangle \otimes |y\rangle$

eigenket of X, Y

Vector operator $\vec{P} = P_x \hat{x} + \underbrace{P_y}_{\text{along } \hat{y}} \hat{y}$

P_x translates along $\hat{x}$

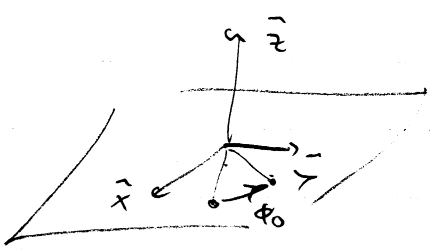
$P_{\hat{n}} = \hat{n} \cdot \vec{P}$ GENERATOR OF TRANSLATIONS ALONG $\hat{n}$.

Classical state specified by coordinates (x,y) and momenta (P_x, P_y).

ROTATION IN 2D:

$$\begin{pmatrix} x \\ y \end{pmatrix} \to \begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix} = \begin{pmatrix} \cos\phi_0 & -\sin\phi_0 \\ \sin\phi_0 & \cos\phi_0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\begin{pmatrix} P_x \\ P_y \end{pmatrix} \to \begin{pmatrix} \tilde{P}_x \\ \tilde{P}_y \end{pmatrix} = \underbrace{\begin{pmatrix} \cos\phi_0 & -\sin\phi_0 \\ \sin\phi_0 & \cos\phi_0 \end{pmatrix}}_{R(\phi_0 \hat{z})} \begin{pmatrix} P_x \\ P_y \end{pmatrix}$$



What is the operator that implements this rotation on the corresponding QUANTUM STATE $\in$ Hilbert space?

SAKURAI

Let's call that operator $U[R(\phi_0 \hat{z})] \equiv \mathcal{D}_z(\phi_0)$.
It has the property

$$|\psi\rangle \xrightarrow[U[R(\phi_0\hat{z})]]{} |\psi_R\rangle = U[R(\phi_0\hat{z})]\,|\psi\rangle$$

EHRENFEST

"The expectation values of X, Y, P_x and P_y satisfy the same equations as the corresponding classical variables"

$$\begin{pmatrix} \langle X\rangle_R \\ \langle Y\rangle_R \end{pmatrix} = \begin{pmatrix} \cos\phi_0 & -\sin\phi_0 \\ \sin\phi_0 & \cos\phi_0 \end{pmatrix} \begin{pmatrix} \langle X\rangle \\ \langle Y\rangle \end{pmatrix}$$

$$\langle \Gamma\rangle_R \equiv \langle\psi_R|\Gamma|\psi_R\rangle$$

$$\begin{pmatrix} \langle P_x\rangle_R \\ \langle P_y\rangle_R \end{pmatrix} = \begin{pmatrix} & -\text{''}- & \end{pmatrix} \begin{pmatrix} \langle P_x\rangle \\ \langle P_y\rangle \end{pmatrix}$$

$$\langle\Gamma\rangle \equiv \langle\psi|\Gamma|\psi\rangle$$

$$\Gamma = X, Y, P_x, P_y$$

$\Downarrow$ in the coordinate basis (eigenbasis of the X and Y operators)

$$U[R(\phi_0\hat{z})]\,|x,y\rangle = |\cos\phi_0\, x - \sin\phi_0\, y,\ \sin\phi_0\, x + \cos\phi_0\, y\rangle \quad ✡$$

This gives us a hint of how to explicitly construct $U[R]$!

Consider first $\phi_0 = \varepsilon \ll 1$. Guided by the structure of the infinitesimal space- and time translation operators, let's try

$$U[R(\varepsilon\hat{z})] = \mathbb{1} - \frac{i\varepsilon}{\hbar} L_z$$

what is L_z?

~~A~~ to $\mathcal{O}(\varepsilon)$:

$$U[R(\varepsilon\hat{z})]\,|xy\rangle = |x - y\varepsilon,\ x\varepsilon + y\rangle$$

$$\Rightarrow \langle xy|\,\mathbb{1} - \tfrac{i\varepsilon}{\hbar}L_z\,|\psi\rangle := \psi(x + y\varepsilon,\ y - x\varepsilon)$$

REQUIRED!

(use that $\langle xy|\,\mathbb{1} - \frac{i\varepsilon}{\hbar}L_z = \left[(\mathbb{1} + \frac{i\varepsilon}{\hbar}L_z)|xy\rangle\right]^+$ if $L_z^+ = L_z$

$\rightarrow = (|x+y\varepsilon,\ y - x\varepsilon\rangle)^+ = \langle x+y\varepsilon,\ y-x\varepsilon|$)

to $\mathcal{O}(\varepsilon)$

$$\Rightarrow \cancel{\psi(x,y)} - \frac{i\varepsilon}{\hbar}\langle xy|L_z|\psi\rangle = \cancel{\psi(x,y)} + \frac{\partial\psi}{\partial x}(y\varepsilon) + \frac{\partial\psi}{\partial y}(-x\varepsilon)$$

$$\Rightarrow \langle xy|L_z|\psi\rangle = \left\{x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right)\right\}\psi(x,y)$$

$$\Downarrow$$

$$L_z \xrightarrow[\{|xy\rangle\}\text{ basis}]{} x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right) = XP_y - YP_x$$

This we recognize as the "operator form" of the z-component of the angular momentum. Why didn't we just define

$$\vec{L} = \vec{r}\times\vec{p} \xrightarrow[\text{QUANTUM}]{} \vec{L} = \vec{R}\times\vec{P}, \quad \vec{R} = (X, Y, Z)$$

$$\vec{P} = (P_x, P_y, P_z) = -i\hbar\nabla$$

?

Wait and see...

FINITE ROTATIONS ?

$$U[R(\phi_0 \hat{z})] = \lim_{N\to\infty}\left(\mathbb{1} - \frac{i}{\hbar}\frac{\phi_0}{N} L_z\right)^N = \exp(-i\phi_0 L_z/\hbar)$$

As any analytic function of an operator, this is defined by its Taylor expansion. Gets messy since $x(-i\hbar\frac{\partial}{\partial y})$ and $y(-i\hbar\frac{\partial}{\partial x})$ don't commute ...

Simpler in POLAR COORDINATES

$$L_z \xrightarrow[\{|\rho\,\phi\rangle\}]{} -i\hbar\frac{\partial}{\partial\phi} \Rightarrow \exp(-i\phi_0 L_z/\hbar) \longrightarrow \exp\left(-\phi_0\frac{\partial}{\partial\phi}\right)$$

Now it's obvious that L_z rotates the state by an angle ϕ about the $\hat{z}$-axis:

$$\exp\left(-\phi_0\frac{\partial}{\partial\phi}\right)\psi(\rho,\phi) \underset{\text{Taylor expand for small } \phi_0}{=} \psi(\rho,\phi-\phi_0)$$

ROTATIONAL INVARIANCE

$$\langle\psi_R|H|\psi_R\rangle = \langle\psi|H|\psi\rangle$$

$$\Downarrow\ R = R(\varepsilon\hat{z})$$

$$[L_z, H] = 0 \Rightarrow \text{(L_z AND H COMPATIBLE (}\Rightarrow\text{ COMMON EIGENBASIS))}$$

Ehrenfest

$$\langle\dot{L}_z\rangle = 0$$

Aside:

Note about VECTOR OPERATORS

$$\vec{\Omega} = \Omega_x \hat{x} + \Omega_y \hat{y}$$

transforms as a vector in $V^2(R)$

operators in Hilbert space (= vector space)

VECTOR OPERATOR IF

rotation matrix elements

$$U^\dagger[R]\,\Omega_i\,U[R] = \sum_j R_{ij}\,\Omega_j \qquad i = x, y$$

Ex. $\vec{\Omega} = \vec{R} = (X, Y)$, $\vec{P} = (P_x, P_y)$. CHECK!

EIGENVALUE PROBLEM OF L_z

We have seen that in a rotationally invariant problem, H and L_z share a common eigenbasis. What does that mean? Let's first check out L_z!

$$L_z|\ell_z\rangle = \ell_z|\ell_z\rangle$$

$\Downarrow$ $\{|\rho\phi\rangle\}$ basis

$$-i\hbar\frac{\partial \psi_{\ell_z}(\rho,\phi)}{\partial\phi} = \ell_z\psi_{\ell_z}(\rho,\phi), \quad \psi_{\ell_z}(\rho,\phi) \equiv \langle\rho\phi|\ell_z\rangle$$

$\Downarrow$

$$\psi_{\ell_z}(\rho,\phi) = R(\rho)\,e^{i\ell_z\phi/\hbar}$$

ℓ_z SHOULD BE REAL (EIGENVALUE OF AN OBSERVABLE!)

ARBITRARY NORMALIZABLE FUNCTION

HERMITICITY CONDITION ON L_z

$\Rightarrow$

$$\Rightarrow \langle \psi_1 | L_z | \psi_2 \rangle = \langle \psi_2 | L_z | \psi_1 \rangle^*$$

COORDINATE BASIS $\Rightarrow$

$$\int_0^\infty \rho\, d\rho \int_0^{2\pi} d\phi\, \psi_1^* \left(-i\hbar \frac{\partial}{\partial\phi}\right) \psi_2 = \left[\int_0^\infty \rho\, d\rho \int_0^{2\pi} d\phi\, \psi_2^* \left(-i\hbar \frac{\partial}{\partial\phi}\right) \psi_1 \right]^* \qquad (\square)$$

$$\Bigg[\text{LHS} = \langle \psi_1 | L_z | \psi_2 \rangle \overset{\text{"COMPLETENESS"}}{=} \iint dx\, dy\, dx'\, dy'\, \langle \psi_1 | xy \rangle \langle xy | \overbrace{XP_y - YP_x}^{L_z} | x'y' \rangle \langle x'y' | \psi_2 \rangle$$

$$= \iint dx\, dy\, dx'\, dy'\, \langle \psi_1 | xy \rangle \underbrace{\left(-i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}\right)\right)} \delta(x-x')\, \delta(y-y') \langle x'y' | \psi_2 \rangle$$

representation of L_z in the $|xy\rangle$ basis

$$= \iint dx\, dy\, \psi_1^*(x,y)\, L_z\, \psi_2(x,y)$$

$$= \{ x,y \to \rho,\phi \} = \int_0^\infty \rho\, d\rho \int_0^{2\pi} d\phi\, \psi_1^*(\rho,\phi) \left(-i\hbar \frac{\partial}{\partial\phi}\right) \psi_2(\rho,\phi)$$

SAME FOR THE RHS. Make sure that you understand this. It's important! In particular, note that

$$\langle xy | \underset{\substack{\uparrow \\ X \text{ Hermitian}}}{X} P_y | x'y' \rangle = x \langle xy | P_y | x'y' \rangle$$

$$= x \overbrace{\langle x | \otimes \underbrace{\langle y | P_y | y' \rangle}_{-i\hbar \frac{\partial}{\partial y} \delta(y-y')} \otimes | x' \rangle}^{\delta(x-x')} = x \left(-i\hbar \frac{\partial}{\partial y'}\right) \delta(x-x')\, \delta(y-y')$$

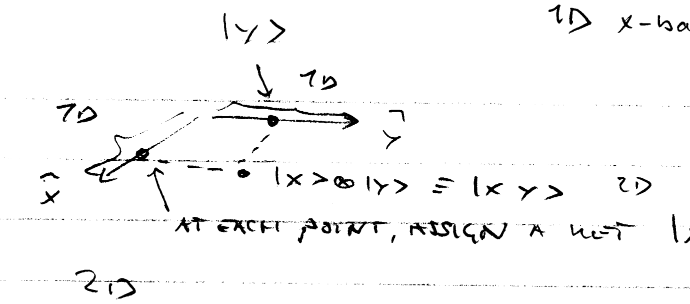
$|xy\rangle$ is a common eigenket to X and Y

label — eigenvalues y

labels — eigenvalues x

and can be written as $|x\rangle \otimes |y\rangle$

1D x-basis   1D y-basis



$\Bigg]$

Integrate (II) by parts $\Rightarrow \psi(\rho, 0) = \psi(\rho, 2\pi)$

$$\Rightarrow R(\rho) = R(\rho)\, e^{i l_z 2\pi/\hbar} \Rightarrow l_z = m\hbar$$

$m = 0, \pm 1, \pm 2, \ldots$

"MAGNETIC QUANTUM NUMBERS"

$\Downarrow$

ψ single valued function of ϕ

QUANTIZATION FROM THE HERMITICITY CONDITION

IMPORTANT

$$\psi(\rho, \phi) = R(\rho)\, e^{im\phi}$$

HUGE DEGENERACY SINCE $R(\rho)$ ARBITRARY !

Bring in a compatible observable to remove the degeneracy !

Choose the Hamiltonian H ?

Simple for ROTATIONALLY INVARIANT PROBLEMS ! (NO ANGULAR DEPENDENCE IN H)

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(\rho, \cancel{\phi}) \Rightarrow [H, L_z] = 0$$

Eigenvalue problem for H (= "time-independent Schrödinger equation")

$$H\psi_{E,m} = E\psi_{E,m}$$

POLAR COORDINATES

$\psi_{E,m}$ common eigenfunction to H and L_z

$m \to \mu$

$$\left\{ -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) + V(\rho) \right\} \psi_{E,m}(\rho,\phi) = E\,\psi_{E,m}(\rho,\phi) \quad *$$

But we know the form of $\psi_{E,m}$!

$$\psi_{E,m} = R_{E,m}(\rho)\,\Phi_m(\phi), \quad \text{where } \Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

Feed this into (*)!

$R_{E,m}(\rho) = \sqrt{2\pi}\, R(\rho)$ in our old notation

$$\left\{ -\frac{\hbar^2}{2\mu}\left(\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} - \frac{m^2}{\rho^2}\right) + V(\rho) \right\} R_{E,m}(\rho) = E\,R_{E,m}(\rho)$$

① **Note**: the angular momentum generates a negative (centrifugal) potential

② $\Phi_m(\phi)$ provides the angular part of any rotationally invariant Hamiltonian in 2D

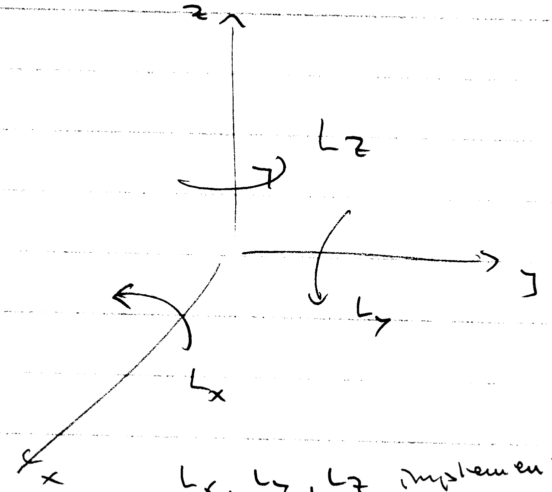
TO SOLVE THE EQUATION, WE NEED TO KNOW $V(\rho)$.
YOU'LL DO SOME EXAMPLES IN THE WEEKS TO COME!

WHAT ABOUT 3D?

$$L_z = XP_y - YP_x$$

$$L_y = ZP_x - XP_z$$

$$L_x = YP_z - ZP_y$$



L_x, L_y, L_z implement the rotations in Hilbert space

$$\Downarrow$$

$$[L_i, L_j] = i\hbar\varepsilon_{ijk} L_k$$

$i,j,k = x, y$ or z

ANGULAR MOMENTUM COMMUTATION RELATIONS

"SU(2) ALGEBRA"

$$\varepsilon_{ijk} = \begin{cases} 0 & \text{if } i=j \text{ or } i=k \text{ or } j=k \\ 1 & \text{if } (ijk) \text{ a cyclic permutation of } (x,y,z) \\ -1 & \text{otherwise} \end{cases}$$

$$\vec{L} = (L_x, L_y, L_z) = L_x\hat{x} + L_y\hat{y} + L_z\hat{z}$$

$$|\vec{L}|^2 = L^2 = L_x^2 + L_y^2 + L_z^2$$

$$\Downarrow$$

$$[L^2, L_i] = 0 \qquad i = x, y, z$$

ROTATIONAL INVARIANCE IN 3D

$$\langle \psi_R | H | \psi_R \rangle = \langle \psi | H | \psi \rangle$$

$$\Downarrow$$

$$U^\dagger[R] \, H \, U[R] = H$$

$$\Downarrow$$

$$[H, L_i] = 0 \qquad i = x, y, z$$

$$\Downarrow$$

$$\left[H, L^2 \right] = 0$$

$$\Downarrow$$

H, L_z, L^2 COMPATIBLE

SPECIFY A UNIQUE BASIS