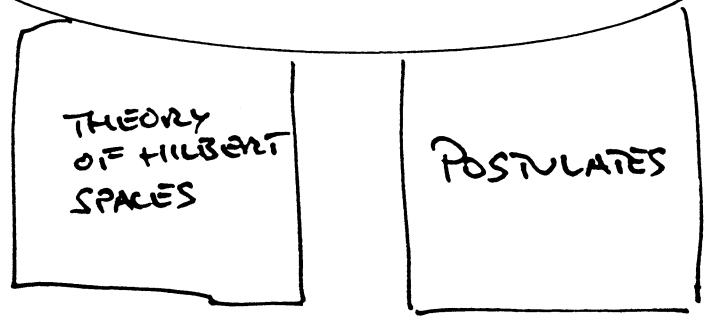


# QUANTUM MECHANICS



HOW TO THINK  
ABOUT PHYSICAL  
SYSTEMS AND  
MEASUREMENTS

- I. ....  
II. ....  
III. ....

TIME  
EVOLUTION

$$\text{IV. } i\hbar |\dot{\psi}\rangle = \hat{H}|\psi\rangle$$

(non-relativistic)

# THE POSTULATES OF QUANTUM MECHANICS

I - III



Particle in a state  $|\psi(t)\rangle$



*four-step program ( $\leftarrow$  postulates I - III)*

step 1: construct  $\Omega = \omega(x \rightarrow X, p \rightarrow P)$

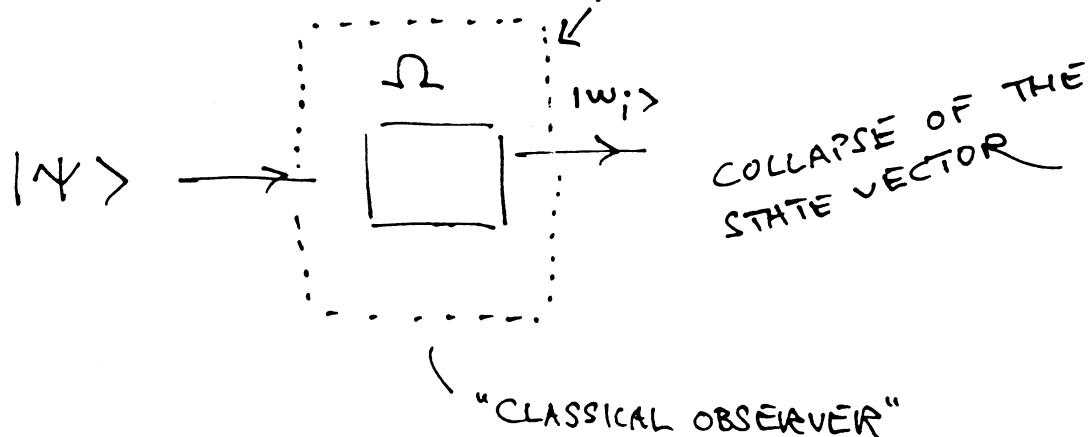
step 2: find the eigenkets  $|\omega_i\rangle$  and eigenvalues  $\omega_i$  of  $\Omega$

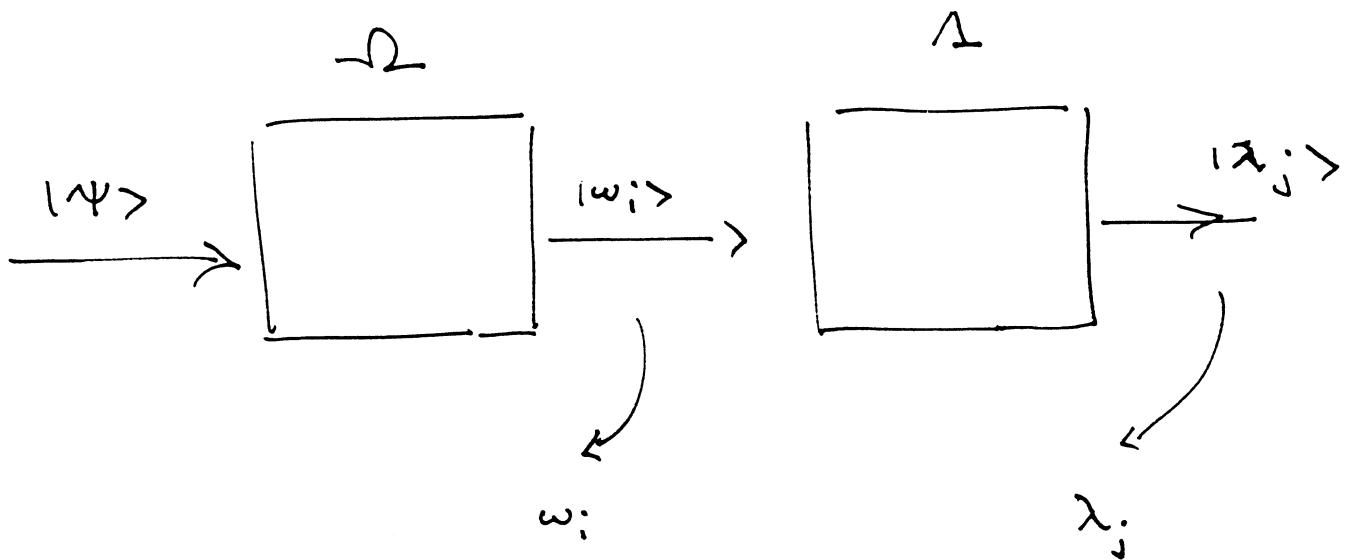
step 3: expand  $|\psi\rangle$  in this basis :

$$|\psi\rangle = \sum_{i=1}^n |\omega_i\rangle \langle \omega_i | \psi \rangle$$

step 4: the probability  $P(\omega_i)$  of measuring  $\omega_i$  :

$$\begin{aligned} P(\omega_i) &\sim |\langle \omega_i | \psi \rangle|^2 = \langle \psi | \omega_i \rangle \langle \omega_i | \psi \rangle \\ &= \langle \psi | \Pi_{\omega_i} | \psi \rangle \end{aligned}$$





$$[\hat{P}, \hat{A}] \neq 0$$



INCOMPATIBLE OBSERVABLES CANNOT BE MEASURED SIMULTANEOUSLY!



HEISENBERG UNCERTAINTY RELATION

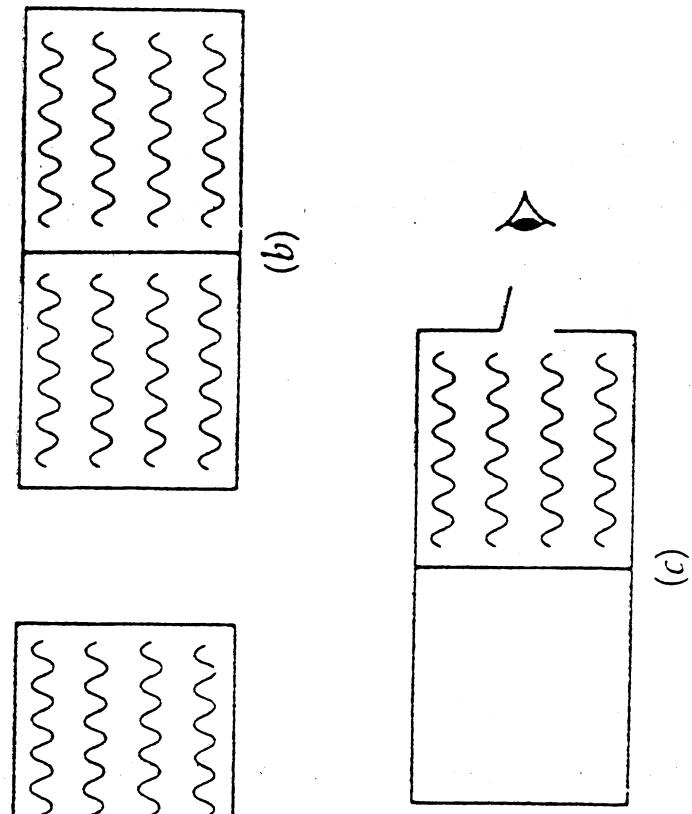
$$[\hat{P}, \hat{A}] = i\hbar$$

$$(\Delta \hat{P})^2 (\Delta \hat{A})^2 \geq \frac{1}{4} \langle \psi | \{\hat{P}, \hat{A}\} | \psi \rangle^2 + \frac{1}{4} \langle \psi | \hat{A}^2 | \psi \rangle^2$$

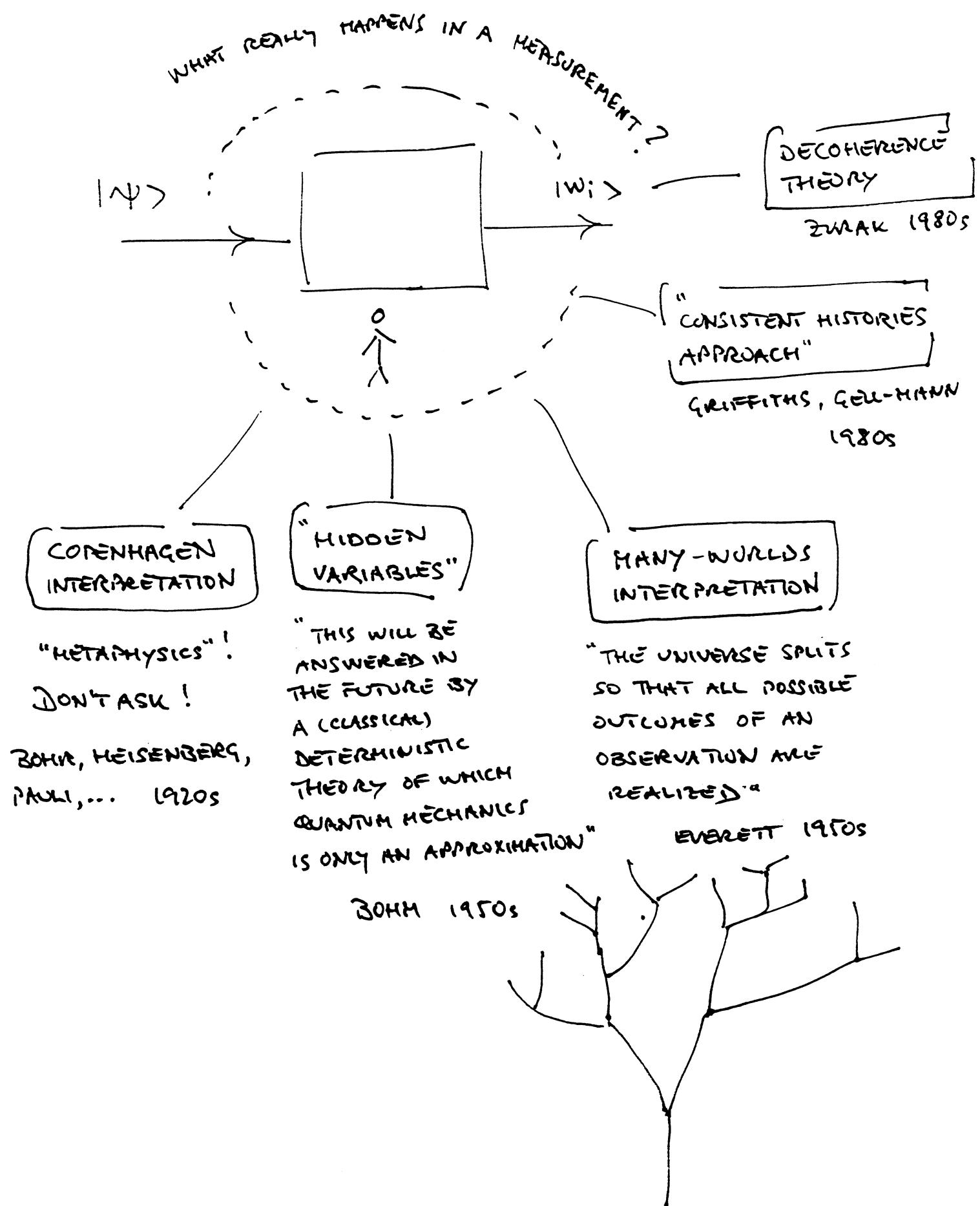
$\hat{P}, \hat{A}$  CANONICALLY CONJUGATE  $\Rightarrow \hat{A} = \frac{i}{\hbar} \hat{P}$

$$\Rightarrow (\Delta \hat{P})(\Delta \hat{A}) \geq \frac{\hbar}{2}$$

*Collapse of a quantum wave.* (a) When a single quantum particle is confined to a box its associated wave is spread uniformly throughout the interior. (b) A screen is inserted, dividing the box into two isolated chambers. (c) An observation reveals the particle to be in the right-hand chamber. Abruptly the wave in the other chamber, which represents the probability of finding the particle there, vanishes.



# THE MEASUREMENT PROBLEM



## THE FOURTH POSTULATE

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

SCHRÖDINGER EQUATION

HAMILTONIAN

ANSWERS THE QUESTION

"GIVEN  $|\psi(0)\rangle$ , WHAT IS  $|\psi(t)\rangle$ ?"

## EXAMPLES OF HAMILTONIANS

### HARMONIC OSCILLATOR

$$\tilde{H} = \frac{\vec{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 \xrightarrow{p \rightarrow \vec{P}, x \rightarrow X} H = \frac{\vec{P}^2}{2m} + \frac{1}{2}m\omega^2 X^2$$

### PARTICLE IN AN E.M. FIELD

$$\tilde{H} = \frac{|\vec{p} - (\frac{q}{c}) \vec{A}(\vec{r}, t)|^2}{2m} + q\phi(\vec{r}, t)$$

$$\downarrow p \rightarrow \vec{P}, x \rightarrow X, y \rightarrow Y, z \rightarrow Z \\ \text{SYMMETRIZE!}$$

$$H = \frac{1}{2m} \left( \vec{P}^2 - \frac{q}{c} (\vec{P} \cdot \vec{A} + \vec{A} \cdot \vec{P}) + \left(\frac{q}{c}\right)^2 \vec{A}^2 \right)$$

$$+ q\phi(X, Y, Z) \quad \vec{A} = \vec{A}(X, Y, Z)$$

# How does it work?

ASSUME H TIME-INDEPENDENT (COMMON!)

GIVEN  $|\psi(0)\rangle$ , WHAT IS  $|\psi(t)\rangle$  ?

SOLVE  $\{ i\hbar |\dot{\psi}\rangle = H |\psi\rangle \} ! \star$

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle$$

↑ "TIME-EVOLUTION OPERATOR"  
= "PROPAGATOR"

$U(t)$  ?

SOLVE  $\star$  !

blackboard

$$U(t) = \sum_E |E\rangle \langle E| e^{-iEt/\hbar} \stackrel{H|\psi}{\downarrow} = e^{-iHt/\hbar}$$

- WHAT IF THE SPECTRUM OF  $H$  IS DEGENERATE ?

BRING IN A COMPATIBLE OBSERVABLE  $A$  !

$$A|\tilde{\epsilon}, \lambda\rangle = \lambda|\tilde{\epsilon}, \lambda\rangle$$

$$U(t) = \sum_{\lambda} \sum_{\tilde{\epsilon}} |\tilde{\epsilon}, \lambda\rangle \langle \tilde{\epsilon}, \lambda| e^{-i\tilde{\epsilon}t/\hbar}$$

- WHAT IF THE SPECTRUM IS CONTINUOUS ?

$$U(t) = \int d\tilde{\epsilon} |\tilde{\epsilon}\rangle \langle \tilde{\epsilon}| e^{-i\tilde{\epsilon}t/\hbar}$$

$|\tilde{\epsilon}(t)\rangle = |\tilde{\epsilon}\rangle e^{-i\tilde{\epsilon}t/\hbar}$  ARE CALLED "STATIONARY STATES"  
SINCE ANY OBSERVABLE IS TIME-INDEPENDENT IN SUCH A STATE

$$P(\omega, t) = |\langle \omega | \tilde{\epsilon}(t) \rangle|^2 = |\langle \omega | \tilde{\epsilon} \rangle e^{-i\tilde{\epsilon}t/\hbar}|^2 = |\langle \omega | \tilde{\epsilon} \rangle|^2 = P(\omega, 0)$$

- WHAT IF  $H$  IS TIME-DEPENDENT ?

LATER .... SEE SAKURAI p 72f & chapter 5



HOW TO SOLVE THE TIME-INDEPENDENT  
SCHRODINGER EQ.

$$H|\psi\rangle = E|\psi\rangle \quad ?$$

blackboard



$H$  IS A GENERATOR OF TIME TRANSLATIONS

$$U(t) = e^{-iHt/\hbar} \approx 1 - \frac{i}{\hbar} H t + \cancel{O(t^2)}$$

$t = \Delta t \ll 1$

$H$  HERMITIAN  $\rightarrow$   $U$  UNITARY



TIME EVOLUTION = "ROTATION" IN  
HILBERT SPACE



HEISENBERG PICTURE.

blackboard

## FREE PARTICLE IN 1D

$$i\hbar |\dot{\psi}\rangle = \hat{H}|\psi\rangle = \frac{\hat{p}^2}{2m}|\psi\rangle \quad \leftarrow \text{time dependent!}$$

STATIONARY STATES  $|\psi\rangle = |E\rangle e^{-iEt/\hbar}$

↓

$$\hat{H}|E\rangle = \frac{\hat{p}^2}{2m}|E\rangle = E|E\rangle$$

$$\hat{P}|p\rangle = p|p\rangle \Rightarrow \frac{\hat{p}^2}{2m}|p\rangle = E|p\rangle$$

$$\Rightarrow \left( \frac{p^2}{2m} - E \right) |p\rangle = 0$$

↓  $|p\rangle \neq |0\rangle$

$$p = \pm \sqrt{2mE}$$

$$\begin{cases} |E_+ + \rangle = |p = \sqrt{2mE} \rangle \\ |E_- - \rangle = |p = -\sqrt{2mE} \rangle \end{cases} \rightarrow |p\rangle$$

$$|E\rangle = \alpha |p = \sqrt{2mE} \rangle + \beta |p = -\sqrt{2mE} \rangle$$

IS ALSO AN EIGENSTATE

## PROPAGATOR

$$U(t) = \int_{-\infty}^{\infty} |p\rangle \langle p| e^{-iE(p)t/\hbar} dp = \int_{-\infty}^{\infty} |p\rangle \langle p| e^{-ip^2t/2m\hbar} dp$$

$$\langle x | U(t) | x' \rangle = U(x, t; x') = \int_{-\infty}^{\infty} \langle x | p \rangle \langle p | x' \rangle e^{-ip^2t/2m\hbar} dp$$

$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{ip(x-x')/\hbar} e^{-ip^2t/2m\hbar} dp$$

GAUSSIAN  
INTEGRAL

$$= \left( \frac{m}{2\pi\hbar it} \right)^{1/2} e^{im(x-x')^2/2it\hbar}$$

\*

$$\psi(x, t) = \int U(x, t; x') \psi(x', 0) dx' \quad **$$

## SPECIAL CASES

(1)

$$\psi(x') = \delta(x' - x'_0) \Rightarrow \psi(x, t) = U(x, t; x'_0)$$

start off with the particle localized at  $x'_0$



THE PROPAGATOR (IN THE  $|x\rangle$  BASIS) IS THE AMPLITUDE THAT A PARTICLE STARTING OUT AT  $(x'_0, t' = 0)$  ENDS UP AT  $(x, t)$

"TRANSITION  
AMPLITUDE"

$$② \quad \psi(x') = e^{\frac{i p_0 x' / \hbar}{\Delta}} \frac{e^{-x'^2 / 2\Delta^2}}{(n\Delta^2)^{1/4}}$$

$\uparrow$  correction!

wave packet at  $t' = 0$

$$\langle X \rangle = 0$$

$$\Delta X = \Delta / \sqrt{2}$$

$$\langle P \rangle = p_0$$

$$\Delta P = \hbar / \sqrt{2} \Delta$$

Sakurai p. 57 f

(\*) & (\*\*)



$$\psi(x, t) = \left[ \sqrt{n} \left( \Delta + \frac{i \hbar t}{m \Delta} \right) \right]^{-1/2} \exp \left\{ \frac{-(x - p_0 t / m)^2}{2\Delta^2 (1 + i \hbar t / m \Delta^2)} \right\} \\ \times \exp \left\{ \frac{i p_0}{\hbar} \left( x - \frac{p_0 t}{2m} \right) \right\}$$



$$1) \quad \langle X \rangle = \frac{p_0 t}{m} = \frac{\langle P \rangle t}{m}$$

"THE CLASSICAL EQUATIONS  
OBEDIED BY DYNAMICAL VARIABLES  
HAVE COUNTERPARTS IN Q.M.  
AS RELATIONS AMONG EXPECTATION  
VALUES"

Cf. Ehrenfest's theorem

$$2) \quad \Delta X = \left( \langle (X - \langle X \rangle)^2 \rangle \right)^{1/2} = \frac{\Delta}{\sqrt{2}} \left( 1 + \frac{\hbar^2 t^2}{m^2 \Delta^4} \right)^{1/2}$$

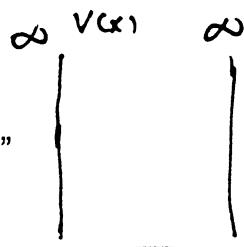
$\curvearrowleft$   
increasing uncertainty  
in position

That's basically all there is to quantum mechanics...

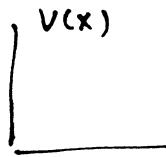
the rest are applications!

### SIMPLE PROBLEMS IN 1D

FREE PARTICLE

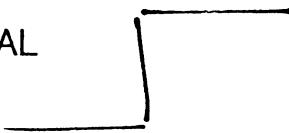


"PARTICLE IN A BOX"



POTENTIAL WELL

$V(x)$



SINGLE STEP POTENTIAL



POTENTIAL BARRIER

and variations on this theme....

### A SPECIAL PROBLEM

THE HARMONIC OSCILLATOR

"...the most important problem in quantum physics"

J. Schwinger

**ALL OTHER PROBLEMS**  
(October - December!)

# The harmonic oscillator

## Why bother?

Any system fluctuating by small amounts near a configuration of stable equilibrium may be described by an oscillator or a system of decoupled harmonic oscillators..... and the problem can be solved exactly!

Classical Hamiltonian  $\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$

↓ HAMILTON'S EQUATIONS

$$\dot{x} = \frac{\partial \mathcal{H}}{\partial p} = \frac{p}{m}, \quad \dot{p} = -\frac{\partial \mathcal{H}}{\partial x} = -m\omega^2x$$

equations of motion

$$\ddot{x} + \omega^2x = 0$$

↓

$$x(t) = A \cos \omega t + B \sin \omega t = x_0 \cos(\omega t + \phi)$$

## Quantum

$$i\hbar \frac{d}{dt} |\psi\rangle = \hat{H} |\psi\rangle, \quad \hat{H} = \mathcal{H}(x \rightarrow X, p \rightarrow P)$$
$$= \frac{P^2}{2m} + \frac{1}{2}m\omega^2X^2$$

As always: the complete dynamics is coded by the propagator  $U(t)$  which can be expressed in terms of the eigenvectors and eigenvalues of  $H$ . Find these!

## RECIPE :

START IN THE ENERGY BASIS (EIGENBASIS TO H)

$$U(t) = \sum_E |E\rangle \langle E| e^{-iEt/\hbar}$$

$$\underbrace{\left( \frac{P^2}{2m} + \frac{1}{2} m\omega^2 X^2 \right)}_H |E\rangle = E |E\rangle$$

PROJECT ONTO THE X-BASIS :  $X \rightarrow x$ ,  $P \rightarrow -i\hbar \frac{d}{dx}$ ,  $|E\rangle \rightarrow \Psi_E(x)$

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \right) \Psi_E(x) = E \Psi_E(x)$$

TIME-INDEPENDENT EQUATION  
SCALAR PRODUCT

FIND ALL SOLUTIONS TO THIS EQUATION THAT  
LIE IN THE (PHYSICAL) HILBERT SPACE (OF FUNCTIONS  
NORMALIZABLE TO UNITY OR THE DIRAC DELTA FUNCTION)

↓ *a long and winding road...*

$$E_n = (n + \frac{1}{2})\hbar\omega, n = 0, 1, 2, \dots$$

$$\Psi_n(x) = \left( \frac{m\omega}{\pi\hbar^2 2^n (n!)^2} \right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) H_n\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right]$$

Hermite polynomials

$$U(x, t; x', t') = \sum_{n=0}^{\infty} A_n^2 \exp\left(-\frac{m\omega}{2\hbar} x'^2\right) H_n(x) \exp\left(-\frac{m\omega}{2\hbar} x'^2\right)$$

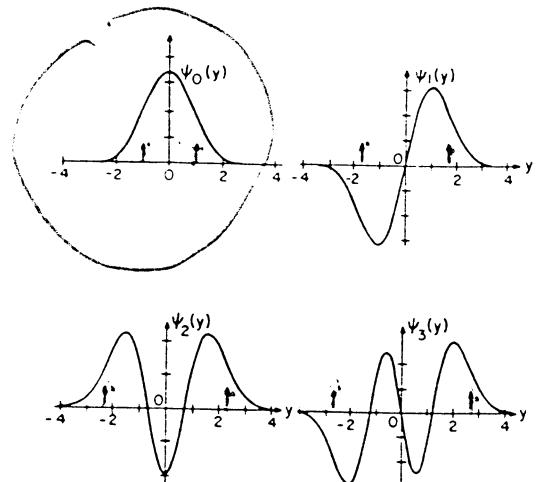
$$x + H_n(x') \exp\left[-i(n + \frac{1}{2})\omega(t - t')\right]$$

## Some observations:

- 1) Quantization from the requirement of a (physical) Hilbert space
- 2) Equally spaced energy levels → think of "quanta" (fictitious particles) of energy  $\hbar\omega$   
 $E_n = (n + \frac{1}{2})\hbar\omega, n = \dots, -1, 0, 1, \dots$   
 (cf Einstein, 1907)

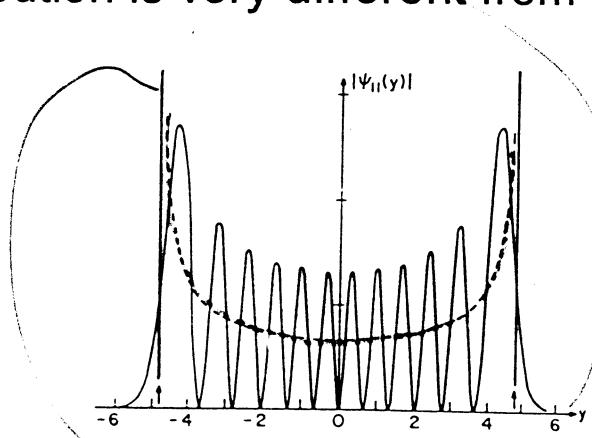
- 3) Zero point energy  $\hbar\omega/2$

- 4) Eigenfunctions are even or odd



- 5) Excursions beyond the classical turning point possible!

- 6) The probability distribution is very different from the classical case



However, at large  $n$  (cf. Bohr's "correspondence principle") the quantum distribution wiggles so rapidly (on a scale set by the classical amplitude) that only its mean can be detected, and this agrees with the classical case.

A smarter way to handle the harmonic oscillator....

Could we work directly in the energy basis without knowing ahead of time the operators X and P in this basis?

Dirac (1928): "Yes, use the fact that the canonical commutation relation  $[X, P] = i\hbar$  is basis independent!"



(BLACK BOARD)