5. Density operators, quantum statistics, & measurement

5.1 Density operators & Quantum Stat. mech

So far: discussed "pure" quantum states – definite states in Hilbert space $\mathcal{H}$.

Sometimes there is classical uncertainty

"Mixture" of states – collection of quantum states combined with classical probabilities. [Each state can be pure quantum state given by quantum superposition of states w/ part. values wrt a given observable.]

Ex: roll dice in a box.

Classical mixture not a fundamental physical phenomenon – just a measure of our lack of knowledge.

Density matrix:

If system is in state $|\alpha^i\rangle$ with classical probability w_i, ($\sum w_i = 1$)

then ensemble-averaged value of $\langle A \rangle$ is:

$$[A] = \sum_i w_i \langle \alpha^i | A | \alpha^i \rangle = \mathrm{Tr}\, \rho A$$

where $\rho = \sum_i w_i |\alpha^i\rangle\langle\alpha^i|$ density operator

(density matrix: $\langle a' | \rho | a'' \rangle$ in fixed basis)

Ex: roll 6-sided die. 6 different states $|1\rangle, |2\rangle, \ldots, |6\rangle$

$w_i = 1/6 \quad \forall i$

$$\rho = \frac{1}{6}\begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}$$ totally classical mixture of states.

Pure state of spin-1/2 particle

$$|+\rangle \;\longrightarrow\; \rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$|S_x;\pm\rangle = \frac{1}{\sqrt{2}}\left(\sqrt{+} \pm \sqrt{-}\right) \;\longrightarrow\; \rho = \frac{1}{2}\begin{pmatrix} 1 & \pm 1 \\ \pm 1 & 1 \end{pmatrix}$$

Mixed states:

$$\begin{matrix} w_+ = 1/2 \\ w_- = 1/2 \end{matrix} \;\longrightarrow\; \rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

$$\begin{matrix} w = 1/2 : \frac{\alpha}{\sqrt{2}}(|+\rangle + |-\rangle) \\ w = 1/2 : \frac{\beta}{\sqrt{2}}(|+\rangle - |-\rangle) \end{matrix} \;\longrightarrow\; \rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

$(|\alpha| = |\beta| = 1)$ phases

<u>same</u> density matrices.

[point: different defs of mixture give same ρ]

Properties of ρ:

- ρ Hermitian (from definition)
- $\operatorname{Tr} \rho = [1] = 1$

ρ describes a <u>pure state</u> if $\rho^2 = \rho$ (projector)

$$\rho^2 = \rho \iff \rho = \begin{pmatrix} 1 & & & \\ & 0 & 0 & \\ & 0 & 0 & \\ & & & 0 \end{pmatrix} \text{ in some basis}$$

$(\rho = |\alpha\rangle\langle\alpha|$ for some $|\alpha\rangle)$

$$\iff \operatorname{Tr} \rho^2 = 1.$$

Difference between pure & mixed states:

Pure: some measurements are 100% determined, define state

Mixed: any measurement in relevant class gives uncertain result

Ex: spin-1/2 particle: pure state gives $|\hat{n};+\rangle$ always for some axis $\hat{n}$.
mixed $\rightarrow$ uncertain value for <u>any</u> orientation of expt (spins from oven)

Time evolution of density operator

If $\rho(t_0) = \sum w_i |\alpha^i\rangle\langle\alpha^i|$

$$\rho(t) = \sum w_i \, U(t,t_0) |\alpha^i\rangle\langle\alpha^i| U^\dagger(t,t_0)$$

$$\Rightarrow \quad i\hbar \frac{\partial \rho(t)}{\partial t} = \sum w_i \left(H|\alpha^i;t\rangle\langle\alpha^i;t| - |\alpha^i;t\rangle\langle\alpha^i;t| H \right)$$

$$= -[\rho, H].$$

{Analogue: $\partial \rho_{class}/\partial t = -\{\rho_{class}, H\}$: Liouville}

Continuum generalization: same idea using countable bases

$$\rho = \sum w_i |\alpha^i\rangle\langle\alpha^i|$$

$$\Rightarrow \langle x|\rho|x'\rangle = \sum w_i \, \phi_i(x)\, \phi_i^*(x')$$

Quantum Statistical Mechanics

Define entropy of quantum system?

Classically: entropy $\sim \ln$ (Volume in phase space)

$\longrightarrow$ measures # of degrees of uncertainty about state

For pure quantum states — expect $\emptyset$ entropy (no uncertainty)

(even though some observables $\to$ uncertain results)
idea is that this info is not part of system (Hidden variables)

For totally random mixture of N states $\quad w_i = \frac{1}{N} \quad i = 1, \ldots, N$

$$\rho = \frac{1}{N}\begin{pmatrix} 1 & & \\ & 1 & \\ & & \ddots & \\ & & & 1 \end{pmatrix} \qquad \text{expect} \quad \sigma = \ln N$$

(information theoretic entropy)

Quantum entropy:

If diagonalize ρ. $\rho = \begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_N \end{pmatrix}$

Information entropy $\sigma = -\sum_i w_i \ln w_i$

measures # of degrees of freedom unknown.

Take as definition

$$\boxed{\sigma = -\mathrm{Tr}\, \rho \ln \rho}$$

Entropy of density operator ρ.

Classical entropy related to σ by

$$S = k_B \sigma.$$

Quantum definition measures <u>finite #</u> of DOF, not phase space volume.

<u>Thermodynamic equilibrium</u>

Maximize $\sigma = -\sum w_i \ln w_i$

subject to $\sum w_i E_i = [H] = U$ fixed (canonical ensemble)
and $\sum w_i = 1$.

Use Lagrange multipliers

$$\partial_i \sigma = \beta E_i + \delta$$
$$= -\ln w_i - 1$$

$$\Rightarrow \quad w_i = e^{-\beta E_i - \delta - 1} = \frac{e^{-\beta E_i}}{\text{const.}}$$

so $$\boxed{w_i = e^{-\beta E_i} \Big/ \sum_j e^{-\beta E_j}},$$

Defines thermodynamic equilibrium for fixed $U = [H]$.

Partition function: $Z = \sum e^{-\beta E_i}$ $\qquad \beta = \frac{1}{k_B T}$

so $$w_i = e^{-\beta E_i} / Z$$

so $$[H] = U = \frac{\sum E_i e^{-\beta E_i}}{Z} = -\frac{\partial}{\partial \beta} \ln Z$$

Quantum stat. mech. is fundamental starting point for classical stat. mech., thermodynamics. [All follows from this picture.]

5.2 Quantum measurement, EPR paradox, & Bell's inequalities. a la GHZ

Recall problem 3-24 (problem 1, PS 11)

2 spin-1/2 particles in $J=0$ state

$$|\alpha_0\rangle = \frac{1}{\sqrt{2}}\Big(|+-\rangle - |-+\rangle\Big) = \frac{1}{\sqrt{2}}\Big(|+_x -_x\rangle - |-_x +_x\rangle\Big)$$

(same state in $|S_x; \pm\rangle$ basis since $J=0$ is rotation invariant)

Send particles in opposite directions to 2 distant observers

O_1 measures $S_z^{(1)}$ O_2 measures $S_z^{(2)}$.

O_1, O_2 get opposite spins (50% $\uparrow\downarrow$, 50% $\downarrow\uparrow$)

If instead

O_1 measures $S_x^{(1)}$ O_2 measures $S_x^{(2)}$

same result (50% $\uparrow\downarrow$, 50% $\downarrow\uparrow$)

Imagine O_1 does measurement first (in rest frame)

$$\left.\begin{array}{llll} \text{If } O_1 \text{ measures} & S_z = +\hbar/2, & |\alpha_0\rangle \to & |\alpha\rangle = |+-\rangle \\ \text{"} \quad \text{"} \quad \text{"} & S_z = -\hbar/2, & |\alpha_0\rangle \to & |\alpha\rangle = |-+\rangle \\ & S_x = +\hbar/2, & & |\alpha\rangle = |+_x -_x\rangle \\ & S_x = -\hbar/2 & & |\alpha\rangle = |-_x +_x\rangle \end{array}\right\} \text{state on which B does measurement.}$$

seems disturbing — O_1's measurement affects state at O_2 — even if spacelike separat
(Both O_1's choice of what to measure & result of measurement)
change $|\alpha\rangle$.

Einstein, Podolsky & Rosen (EPR) paradox:

[Should not be any "spooky" action at a distance.]

Action of O_1 should not affect state of system @ O_2 outside light-cone.

Philosophy or physics?

"Hidden variable" theories: QM is not complete description of system.

Perhaps hidden variables can make QM deterministic, avoid apparent nonlocality of measurement?

Bell: proved that local hidden variable theories make <u>quantitatively</u> different predictions from QM

Found testable inequalities for measurement correlations.

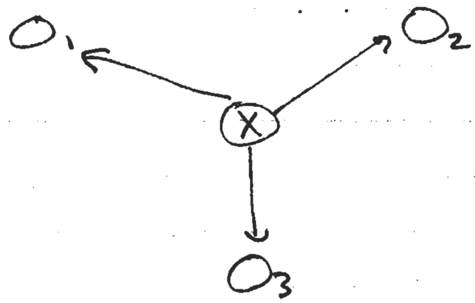
Conceptually simpler analog of Bell ineq:

GHZ (Greenberger, Horne, Zeilinger: Ann. J. Phys. 58 (1990) 1131;
Mermin Physics Today June 1990 p. 9
Coleman: "QM in your face" seminar 1994)

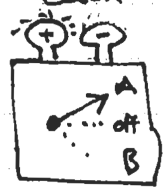
GHZ:

Consider central station ⓧ

Sends packets to 3 observing stations O_1 O_2 O_3



Observers O_1, O_2, O_3 each have black boxes



Can measure A or B. Results: +1 or -1.

O_1, O_2, O_3 perform experiment on many ~~packets~~:
Each independently chooses A or B, measures.

[could be measuring anything: chem comp, DNA of org, q spins, nothing at all]

Example measurements:

$$
\begin{array}{lll}
A_1 = +1 & A_2 = -1 & B_3 = +1 \\
A_1 = -1 & B_2 = +1 & B_3 = -1 \\
B_1 = +1 & B_2 = +1 & A_3 = +1 \\
 & \vdots &
\end{array}
$$

Pattern: whenever 2 measure B, one measures A,
product is +1

$$\left.\begin{aligned} A_1 B_2 B_3 &= +1 \\ B_1 A_2 B_3 &= +1 \\ B_1 B_2 A_3 &= +1 \end{aligned}\right\} \text{ always.}$$

<u>If</u> classical picture of information is correct (local HVT), results must be decided from comb. of data in obs. stations and from X.

Classical logic $\Rightarrow$ If all measure A,

$$A_1 A_2 A_3 = (A_1 B_2 B_3)(B_1 A_2 B_3)(B_1 B_2 A_3) = +1.$$

Consider 3-spin system with

$$|\alpha_0\rangle = \frac{1}{\sqrt{2}}\left(|+++\rangle - |---\rangle\right)$$

$$A^{(i)} = \sigma_x^{(i)} \qquad B^{(i)} = \sigma_y^{(i)}$$

Can check

$$A_1 B_2 B_3 |\alpha_0\rangle = |\alpha_0\rangle, \quad \text{same for } 1 \to 2 \to 3, \ldots$$

(each matrix flips spin, B factors $\rightarrow (\pm i)^2 = -1$)

<u>BUT</u>

$$A_1 A_2 A_3 |\alpha_0\rangle = -|\alpha_0\rangle \; !$$

So: if all observers measure A, get

$$A_1 A_2 A_3 = -1 \qquad \underline{\text{always}}$$

Classical logic $\Rightarrow$ $A_1 A_2 A_3 = +1$
Quantum mechanics $\Rightarrow$ $A_1 A_2 A_3 = -1$.

Experiments testing Bell inequalities validate quantum mechanics
dispr(ove) local hidden variable theories.

Note: This does not mean information can be
transmitted faster than light (time travel)

Back to $J=0$ 2 spin system. $\frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$

If O_1 measures S_z,

state at B: $\left.\begin{array}{l} 50\% \;\; |+\rangle \\ 50\% \;\; |-\rangle \end{array}\right\}$ classical mixture.

$$\Rightarrow \rho_B = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \quad \text{density matrix}$$

If O_1 measures S_x

state at B: 50% $|S_x;+\rangle$
50% $|S_x;-\rangle$

$$\rho_B = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \quad \underline{\text{same}} \text{ density matrix.}$$

So B can't tell difference, due to <u>classical</u> mixture of states.

Seems strange?

Possible resolution:

1) Nonlocal hidden variable theories (?) [Hard to see how causality works]

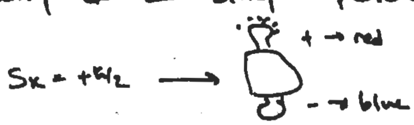
2) Experiments of O_1, O_2, O_3 cannot really be chosen randomly — decision about what to measure encoded in info defining observers
[com. produced when obs. agree to do expt]
[No free choice]

3) Accept non-local collapse of wavefunction in Hamiltonian formalism

4) "Copenhagen" interpretation: Universe branches every time a measurement occurs — all possibilities realized

5) There <u>is no collapse</u> (Coleman)

Q: why do I only experience one result?



A: define "definiteness" operator D

apparatus: $|+, M_0\rangle \longrightarrow |+, M_+\rangle$ $\quad D|M_+\rangle = M_+$
$|-, M_0\rangle \longrightarrow |-, M_-\rangle$ $\quad D|M_-\rangle = M_-$

therefore $D|\psi\rangle = |\psi\rangle$ when $\psi = \frac{1}{\sqrt{2}}(|+, M_+\rangle + |-, M_-\rangle)$ (!)

6) Use path integrals, only correlations relevant, no realist interpretati

7) Something wierder underlies QM.

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7 (incl. me)