10/09/15

Lecture 17 - Entropy & The Schrödinger Equation

1. Entropy
2. Schrödinger's Equation
3. Time Evolution of Density Matrices

1. Entropy of Density Matrices

Density matrices take "pure states"
↓change to↓
mixed states (which have classical probabilities)

- For the Bloch Sphere:
  Surface of the sphere ($\vec{a}^2=1$)
  = pure states
  interior of the sphere = mixed states
- For density matrices:
  ρ is Hermitian — i.e., we can diagonalize it
  $= \sum_j p_j |\psi_j\rangle\langle\psi_j|$
  $Tr(\rho)=1 \iff \sum_j p_j = 1$
  State is a "Pure State" IFF $p_j=1$ for some j (all other values of $j=0$)
  ↳ $\rho = |\psi\rangle\langle\psi|$
  For mixed states: $p_j<1$
  → $p_j^2 < p_j$
  → $Tr(\rho^2) = \sum_j p_j^2 < 1$

But how mixed are these states?
Use entropy to quantify the amount of mixing!

- Entropy from classical stat mech:
  $S(E) = k_B \ln(\Omega(E))$
  ↳ Ω = # of configurations
  → quantifies how random a system is, ln(# of states)
  for a classical system, $j=1\ldots p$, have probabilities p_j
  * Entropy is "extensive" (entropy of system)
  N copies of the system $\longleftrightarrow$ N·S
  $N\to\infty$, $\Omega = \dfrac{N!}{\prod_j \underbrace{(Np_j)}_{n_j}}$ — combinatorics

-Entropy of Density Matrices-

$$S = \frac{1}{N} \ln\left[\frac{N!}{\prod_j (Np_j)!}\right]$$

Use Stirling's approximation: $\ln(N!) \sim N\ln(N) - N \ldots$

$$S \sim -k_B \sum_j p_j \ln(p_j)$$

└ set Boltzmann const. = 1

$$S = -\sum_j p_j \ln(p_j)$$

$$= -\mathrm{Tr}\left(\sum_j p_j \ln(p_j) |\psi_j\rangle\langle\psi_j|\right)$$

↑ Remember: a function on the eigenkets is just a function on the eigenvalues × the eigenkets

$$= -\mathrm{Tr}(\rho \ln(\rho))$$

↑ the von Neumann entropy ~ thermodynamic entropy

HW6.P1

(but not infinitely so!

$S \geq 0 \rightarrow$ minimal $S = 0$

only occurs for $p_j = 1$ for some j

└ a.k.a. a pure state! $\rho = |\psi\rangle\langle\psi|$

$\rightarrow$ maximal S @ $p_j = \frac{1}{P}$

$S_{max} = \ln(P)$ (ψ_j's are different configurations

$$\rho_{max} = \sum_j \frac{1}{P} |\psi_j\rangle\langle\psi_j|$$

$$= \frac{1}{P} \underbrace{\sum_j |\psi_j\rangle\langle\psi_j|}_{\mathbb{1}} = \frac{\mathbb{1}}{P}$$

$\Rightarrow$ the maximally mixed state! (unique)

(max randomness -- Bloch sphere $\vec{a} = 0$)

mms @ origin → for 2×2 system

Connection to Entanglement

Using the "reduced density matrix"

States A&B $\rightarrow$ $\underbrace{|\Psi\rangle}_{\text{a pure state}}$, which has a reduced DM ρ_A

$\rightarrow$ Entanglement entropy $= -\mathrm{Tr}(\rho_A \ln(\rho_A))$

$= S_{ent}$

$S_{ent} = 0$ for product states
↳ $|\Psi\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle$

Theorem: (property of density matrices)
$S_{ent}(A) = S_{ent}(B)$
$\leq \ln(D_A) \quad \leq \ln(D_B)$
→ Using this, we can check that $\rho_A = |\Psi_A\rangle\langle\Psi_A|$
if $\dim\{\mathcal{H}_A\} = D_A$, $\dim\{\mathcal{H}_B\} = D_B$
then the entanglement entropy of the maximally entangled state is $S_{ent,max} = \min\{\ln(D_A), \ln(D_B)\}$
* The EPR (Einstein-Podolsky-Rosen) state was a maximally entangled state; the "poster child entangled state"

2. Schrödinger's Equation

Hamiltonian as the generator of time translation
$|\alpha\rangle = |\alpha; t = t_0\rangle$
↳ arbitrary state; explicit time-dependence
→ $t = t_1$
$|\alpha; t = t_1\rangle$ The superposition principle tells us that if we have two states
$C_\alpha |\alpha; t = t_0\rangle + C_{\alpha'} |\alpha'; t = t_0\rangle$
then after some time t those states will be
$C_\alpha |\alpha; t = t_1\rangle + C_{\alpha'} |\alpha'; t = t_1\rangle$
↳ time translation must be linear! (if it's a superposition, it stays a superposition, etc.)

$|\alpha; t = t_1\rangle = U(t_0, t_1) |\alpha; t = t_0\rangle$
unitary time-evolution operator

Because it is linear, $t_0 \to t_1 \to t_2$ must $= t_0 \to t_2$
$U(t_0, t_2) = U(t_1, t_2) U(t_0, t_1)$ (I)
$U(t_0, t_0) = \mathbb{1}$ (II)
Also, if $|\alpha; t = t_0\rangle$ is normalized, so is $|\alpha; t = t_1\rangle$
⟹ $U(t_0, t_1)$ is unitary
↳ unitarity allows us to say
$U(t_0, t_1) U^\dagger(t_0, t_1) = \mathbb{1}$

$U^\dagger(t_0,t_1) = U(t_1,t_0)$ -- time can be represented in reverse here! (but is time reversal invariant per symmetry requirements)

Consider $t_1 = t_0 + \Delta t$ $(\Delta t \to 0)$
└ infinitesimal shift

→ Taylor expand ↴

$$U(t_0, t_0+\Delta t) \approx \mathbb{1} - \frac{i\Delta t}{\hbar}\mathcal{H}(t_0) + \dots$$

from (II) ↑ ; └ definition of Hamiltonian

Using equation (I):

$$U(t_0, t_1+\Delta t) = U(t_1, t_1+\Delta t)\,U(t_0,t_1)$$
$$= \left[\mathbb{1} - \frac{i\Delta t}{\hbar}\mathcal{H}(t_1)\right]U(t_0,t_1)$$

$$\lim_{\Delta t\to 0}\frac{U(t_0,t_1+\Delta t) - U(t_0,t_1)}{\Delta t} = \frac{-i}{\hbar}\mathcal{H}(t_1)\,U(t_0,t_1)$$

$$\Rightarrow \partial_{t_1} U(t_0,t_1) = -i/\hbar\,\mathcal{H}(t_1)\,U(t_0,t_1)$$

└ Schrödinger equation for the unitary time evolution operator

define: $\mathcal{H}(t) \equiv i\hbar(\partial_t U)U^\dagger$

$$|\alpha; t=t_1\rangle = U(t_0,t_1)\,|\alpha; t=t_0\rangle$$

$$\Rightarrow i\hbar\partial_{t_1}|\alpha; t=t_1\rangle = \mathcal{H}(t_1)\,|\alpha; t=t_1\rangle$$

└ general time-dependent Schrödinger equation recovered

Working with the Schrödinger Equation

Case 1: $\mathcal{H}(t) = \mathcal{H}$ (independent of t)

Guess/Check

$$U(t_0,t_1) = \exp(-i/\hbar\,\mathcal{H}(t_1-t_0))$$

└ only valid for $\mathcal{H}$ time-independent

$$= \sum_n \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!}(t_1-t_0)^n\mathcal{H}^n$$

$i\hbar\partial_{t_1}U = \dots = \mathcal{H}U(t_0,t_1)$ ✓

↑ "some stuff happens with the factorial, etc., and then the answer falls out!"

→

Case 2: $[\mathcal{H}(t), \mathcal{H}(t')] = 0$

↳ $\mathcal{H}$ is time-dependent but commutes at different times

"trick":

$$U(t_0,t_1) = (U^\dagger(t_0,t_0+\Delta t)U^\dagger(t_0+\Delta t, t_0+2\Delta t)\cdots U^\dagger(t_1-\Delta t,t_1))^\dagger$$
$$= e^{-i\mathcal{H}(t_1)\Delta t/\hbar} \cdots e^{-i\Delta t/\hbar \mathcal{H}(t_0+\Delta t)} e^{-i\mathcal{H}(t_0)\Delta t/\hbar}$$

→ use Campbell-Baker-Hausdorff ↘

for $[A,B]=0$, $e^A e^B = e^{A+B}$, then

$$U(t_0,t_1) = e^{-i\Delta t/\hbar \sum_{n=0}^{N} \mathcal{H}(t_0+n\Delta t)}$$

$$\xrightarrow{\Delta t\to 0} e^{-i/\hbar \int_{t_0}^{t_1} \mathcal{H}(\tau)d\tau} = U(t_0,t_1)$$

e.g. $\vec{B}(t) = \underbrace{\lambda(t)\hat{z}}$

field direction flips with t

Case 3: The general case

$\partial_{t_1} U(t_0,t_1) = -i/\hbar \mathcal{H}(t_1)U(t_0,t_1)$

- solve iteratively

gives $U^{(0)}(t_0,t_1) = \mathbb{1}$

$U(t_0,t_1) = -i/\hbar \int_{t_0}^{t_1} d\tau\, \mathcal{H}(\tau)U(t,\tau) + \mathbb{1}$

$U^{(1)}(t_0,t_1) = \mathbb{1} - i/\hbar \int_{t_0}^{t_1} d\tau_1 \mathcal{H}(\tau_1)$

$\vdots$

$$U(t_0,t_1) = \mathbb{1} - i/\hbar \int_{t_0}^{t_1} d\tau_1 \mathcal{H}(\tau_1) + (-i/\hbar)^2 \int_{t_0}^{t} d\tau_1 \int_{t_0}^{\tau_1} d\tau_2 \mathcal{H}(\tau_2)\mathcal{H}(\tau_1) \cdots$$

↳ this is known as the Dyson Series

Back to Case 1: time-independent $\mathcal{H}(t) = \mathcal{H}$

$$U(t_0,t_1) = e^{-i/\hbar \mathcal{H}(t_1-t_0)}$$

↖ closed-form time evolution operator

$\mathcal{H}$ → hermitian
A → observable(s)
} $[\mathcal{H},A]=0$

$|a\rangle$, $A|a\rangle = a|a\rangle$

$\mathcal{H}|a\rangle = E_a|a\rangle$

because they commute, A and $\mathcal{H}$ are simultaneously diagonizable

→ Diagonalize $\mathcal{H}$ →

→

$U(t_0,t_1)|a\rangle = e^{-i/\hbar(t_1-t_0)\hat{H}}|a\rangle$ ($t_1-t_0 = \tilde{t}$)

$= \text{power series} \ldots = \exp(-i\tilde{t}/\hbar E_a)|a\rangle$

$|a;t=t_1\rangle = e^{\frac{-i(t_1-t_0)}{\hbar}E_a}|a;t=t_0\rangle$

such that $\langle a;t=t_1|B|a;t=t_1\rangle = \langle a;t=t_0|B|a;t=t_0\rangle$ (phases cancel)

↑ some observable

⟹ This is our Stationary State

$|\alpha;t=t_1\rangle = \sum_a C_a|a;t=t_1\rangle$

↳ the coefficient of expanding α in the a-basis

$C_a = \langle a;t=t_0|\alpha;t=t_0\rangle$

Starting @ $t=t_0$, we can now calculate any state @ $t=t_1$ (for the time-independent Schrödinger equation)

$\rightarrow = \sum_a \underbrace{C_a e^{-i(t_1-t_0)E_a/\hbar}}_{C_a(t=t_1)} \underbrace{|a;t=t_0\rangle}_{|a\rangle}$

so if we want to calculate the expectation values of B with respect to these eigenstates:

$\langle\alpha;t=t_1|B|a;t=t_1\rangle$

$= \sum_{aa'} \underbrace{C_a^*(t_1)C_{a'}(t_1)}\langle a|B|a'\rangle$

$= C_a^* C_{a'} \underbrace{e^{+i(t_1-t_0)E_a/\hbar} e^{-i(t_1-t_0)E_{a'}/\hbar}}$

$= e^{-i/\hbar(t_1-t_0)(E_{a'}-E_a)}$

↳ a bunch of oscillations

3. Time Evolution of Density Matrices

Schrödinger's equation tells how pure states evolve in time, but what about mixed states?

$\rho(t=t_0) = \sum_j p_j|\psi_j(t=t_0)\rangle\langle\psi_j(t=t_0)|$

$\downarrow U(t_0,t_1)\downarrow$

$\rho(t=t_1) = \sum_j p_j|\psi_j(t=t_1)\rangle\langle\psi_j(t=t_1)|$

(under unitary evolution, the states are unchanged)

$$= \sum_j p_j U(t_0,t_1)|\psi_j(t=t_0)\rangle\langle\psi_j(t=t_0)|U^\dagger(t_0,t_1)$$

$$= U(t_0,t_1)\rho(t=t_0)U^\dagger(t_0,t_1)$$

$\dagger$ picks up the complex conjugate

$$\partial_{t_1}\rho(t=t_1) = -i/\hbar\,\mathcal{H}(t_1)\underbrace{U(t_0,t_1)\rho(t=t_0)U^\dagger(t_0,t_1)}_{=\rho(t=t_1)}$$

$$+ U(t_0,t_1)\rho(t=t_0)U^\dagger(t_0,t_1)(i/\hbar)\mathcal{H}(t_1)$$

$$\Rightarrow i\hbar\partial_t\rho = [\mathcal{H}(t_1), \rho(t=t_1)]$$

→ Bloch Sphere – rotation of $\vec{a}(t)$