DAY-4

LECTURE 13 09:30-11:00

QUANTUM THERMODYNAMICS

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FOCUS :- Thermalization in Quantum Systems (Not Thermal Machines)

Ref:- Popescu, Short, Winter Nat Phys (2006)

Put a system in a Heat Bath → maximum entropy state = Thermal State

$$\rho_{th} = \frac{e^{-\beta H}}{Tr(e^{-\beta H})}$$

Q:- How does the Quantum System get Thermalized ?

In open system dynamics $\xrightarrow[\text{Bath}]{\text{Heat}} \frac{d\rho}{dt} = i[H,\rho] + \underbrace{\mathcal{L}[\rho]}_{\text{Lindbladian}} \xrightarrow[\text{time}]{\text{In } t\to\infty} \rho_{th}$

(Markovian Dynamics)

Q:- If $\mathcal{H}_S \otimes \mathcal{H}_E$ is total Hilbert Space but $\exists$ constraints such that effectively the Hilbert Space $\mathcal{H}_R \subseteq \mathcal{H}_S \otimes \mathcal{H}_E$. Now if I take equal a-priory probable state $= \mathcal{E}_R = \frac{\mathbb{1}_R}{d_R}$ in $\mathcal{H}_R$.

Concentrate on state of the system.

$Tr_E\, \mathcal{E}_R = \Omega_S$ → The State to which the system equilibriates.

Start with an arbitray pure state $|\phi\rangle_{SE}$ s.t. $\rho_S = Tr_E |\phi\rangle\langle\phi|$

Target :- if $D(\rho_S, \Omega_S) \leq \epsilon$ → Thermalization (Trace Distance) i.e. $\text{Prob}\left[\|\rho-\Omega_s\|_1 > \eta\right] < \eta'$ → Very improbable to go far apart from equilibrium state

(condition → effective dimension $d_{eff}^{\text{environment}} \gg d_{\text{system}}$)

If H is two-level → $\rho_{th} = \begin{bmatrix} p & 0 \\ 0 & \tilde{p} \end{bmatrix}$ Where $p = \dfrac{e^{-\beta E_0}}{e^{-\beta E_1} + e^{-\beta E_0}}$ & $\tilde{p} = 1-p$

$\rho \xrightarrow{\mathcal{N}} \rho_{th} \Rightarrow \rho_{th} = \frac{1}{2}(\mathbb{1} + \underbrace{\vec{n}_{th}}_{} \cdot \vec{\sigma})$

Pin map → Every map gets pinned to one target state

Q:- Can you give me a Hamiltonian Which takes ($t \to \infty$ limit) → ??

Append some ancilla to the system.

for a finite dimensional ancilla → β itself changes → Not compatible with Classical Thermo dynamics

Proof of $\text{Prob}\left[\|\rho-\Omega_s\|_1 > \eta\right] < \eta'$

Theorem:- For a randomly chosen state $|\phi\rangle \in \mathcal{H}_R$ & $\epsilon > 0$ The distance $\|\text{Tr}_E(|\phi\rangle\langle\phi|) - \Omega_s\|_1$

$\text{Prob}\left[\|\rho-\Omega_s\|_1 > \eta\right] < \eta'$ Where $\eta = \varepsilon + \sqrt{\dfrac{d_S}{d_{eff}^{env.}}}$, $\eta' = 2e^{-c d_R \varepsilon^2}$

Proof:- Probabilitic Theoretic Result → Levy's Lemma → Given a fn $f: S^d \to \mathbb{R}$ & a point $\phi \in S^d$ chosen with uniform probability, then $\text{Prob}\,|f(\phi) - \langle f\rangle| \leq e^{-\frac{2c(d+1)\varepsilon^2}{\eta^2}}$ Where $\eta = \sup_\phi |\vec{\nabla}.f|$ & $C = \frac{1}{18\pi^3}$

(Ref:- Millman) $\left[\langle f\rangle = \int_{\phi \in S^d} f(\phi)\, d\phi\right]$

Here $|\phi\rangle \in \mathcal{H}_R$ → Any pure state representible here interms of $2d_R - 1$ dimensional Hypersphere S^{2d_R-1}

Now define $f(\phi) = \|\text{Tr}_E |\phi\rangle\langle\phi| - \Omega_s\|_1$ (Trace 1-norm)

Now using levy's Lemma requires finding out Lipschutz Constant $\eta = 2$.. (HW)

Now we get $\text{Prob}\left[\big|\|\rho_s - \Omega_s\|_1 - \langle\|\rho_s - \Omega_s\|_1\rangle\big| \geq \varepsilon\right] \leq 2\exp\left(\frac{\quad}{\eta}\right)$

$\Rightarrow \text{Prob}\left[\|\rho_s - \Omega_s\|_1\right] \geq \langle\|\rho_s - \Omega_s\|_1\rangle + \varepsilon] \leqslant 2\exp\left(-C d_R \varepsilon^2\right)$

The average $\langle\|\rho_s - \Omega_s\|_1\rangle \leq \sqrt{d_s}\,\underbrace{\langle\|\rho_s - \Omega_s\|_2\rangle}$

$$\sqrt{d_s}\int_{\varphi \in S^{2d_R-1}} d\varphi\, \|\text{Tr}_R|\varphi\rangle\langle\varphi| - \Omega_s\|_2 \xrightarrow[\text{calculation}]{\text{After some}} \leq \sqrt{d_s}\sqrt{\int d\varphi\, \|\text{Tr}_R|\varphi\rangle\langle\varphi| - \Omega_s\|_2^2}$$

but $\langle\rho_s\rangle = \int_{\varphi \in S^{2d_R-1}} d\varphi\, \text{Tr}_E|\varphi\rangle\langle\varphi| = \Omega_s$

finally $\leq \sqrt{d_s}\cdot\sqrt{\langle\text{Tr}\,\rho_s^2\rangle - \text{Tr}\,\Omega_s^2}$

What is $\langle\text{Tr}\,\rho_s^2\rangle$? This is $\leqslant \text{Tr}\langle\rho\rangle^2 + \text{Tr}\langle\rho_E\rangle^2$
$= \text{Tr}(\Omega_s)^2 + \text{Tr}\langle\rho_E\rangle^2$

But $\langle\rho_E\rangle = \Omega_E \therefore \langle\text{Tr}\,\rho_s^2\rangle \leqslant \text{Tr}(\Omega_s)^2 + \text{Tr}(\Omega_E)^2$

Now $d_{eff} = \dfrac{1}{\text{Tr}(\Omega_E)^2} \rightarrow$ Then $\langle\|\rho_s - \Omega_s\|_1\rangle \leq \sqrt{\dfrac{d_s}{d_E^{eff}}}$

Thus $\rightarrow \text{Tr}\left(\|\rho_s - \Omega_s\|_1 \geqslant \varepsilon + \sqrt{\dfrac{d_s}{d_E^{eff}}}\right)$ has prob $\leqslant 2\exp\left[-C d_R \varepsilon^2\right]$
$\therefore$ (Proved)

Sanity Check

$\mathcal{H}_R = \mathcal{H}_S \otimes \mathcal{H}_E \rightarrow d_{eff} = \dfrac{1}{\text{Tr}_E\,\Omega^2} = d_E \longrightarrow$ expected

Now $\sqrt{\dfrac{d_s}{d_E^{eff}}} \leq \sqrt{\dfrac{d_s}{d_R}}$ $\quad \Omega_E = \sum_k \lambda_k |\varphi_k\rangle\langle\varphi_k| \rightarrow$ Spectral Decomposition

Proof :- 2 line (HW)

i.e. avg $\langle\|\rho_s - \Omega_s\|_1\rangle$ is small if $d_{eff} \gg d_s$

Levy's Lemma + This $\longrightarrow$ Thermalization }

Implications of This Theorem

Reconciling with standard Stat Mech

Assume Energy of the system E is given $\longrightarrow$ Temp β given

$H_{tot} = H_s \otimes \mathbb{1} + \mathbb{1} \otimes H_R + \underbrace{H_{int}}_{\text{Weak enough interaction}}$ & assume dense energy spectrum

$\Omega_S^{(\varepsilon)} = \mathrm{Tr}_{\varepsilon}\, \mathcal{E}_R \overset{\text{can}}{\underset{\text{be shown}}{=\!=}} \dfrac{e^{-\beta H_S}}{\mathrm{Tr}(e^{-\beta H_S})}$ $\longrightarrow$ All Previous Results valid for This also

Thermal Canonical Equilibriation Principle → Start from arbitrary state subject to these constraints - Thermalizes

Models with spins :- N spins ...... Show that these bounds can be sharpened

(no interaction) in external $\vec{B}$ field → Next Lecture

LECTURE 16 16:30 - 18:00

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In Last Lecture $\rightarrow$ start with any state ρ_s $\rightarrow$ end up with a very high prob very near the thermal state subject to d_{eff} (env.) $\gg d$ system.

Can We do Better? (Better values of η and η'?)

YES $\Rightarrow$ FOR SPECIFIC MODELS

Thm:- (Modification of Morning Thm) [Statement Only]

Assume $\exists$ some bounded +ve operator X_R on $\mathcal{H}_R$ satisfying $0 \leq X_R \leq \mathbb{1}_R$ [POVM Elements] such that with $\tilde{\mathcal{E}}_R = X_R^{1/2} \mathcal{E}_R X_R^{1/2}$, we have

$$Tr(\tilde{\mathcal{E}}_R) = Tr(\mathcal{E}_R X_R) \geqslant 1 - \delta$$

High Chance on equiprobable states $\mathcal{E}_R$ to get this measurement outcome

For a randomly chosen state $|\phi\rangle \in \mathcal{H}_R$ & $\varepsilon > 0$

$$Prob\left[\| \rho_S - \Omega_S \|_1 \geqslant \tilde{\eta} \right] \leqslant \tilde{\eta}'$$

Where $\tilde{\eta} = \varepsilon + \sqrt{\frac{d_s}{d_{eff}}} + 4\sqrt{\delta}$

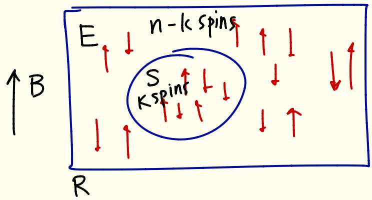
and $\tilde{\eta}' = 2 \exp\left[-c\, d_R\, \varepsilon^2\right]$

$$\tilde{\Omega}_E = Tr_S(\tilde{\mathcal{E}}_R)$$

$$\tilde{d}^{eff}_E = \frac{1}{Tr\, \tilde{\Omega}_E^2}$$

Example :-

SPIN SYSTEM



$R \equiv np$ spins in $\uparrow$
$\equiv n(1-p)$ spins in $\downarrow$ } say

$d_S = 2^k$; $d_E = 2^{n-k}$ $\Rightarrow$ What can I say about d_R ?

$$d_R = \binom{n}{np} = \frac{n!}{(np)!\,nq!}$$

$$\geq \frac{2^{nH(p)}}{n+1} \quad [H(p) = 2 \text{ point Shannon Entropy}] \quad (\text{for large } n)$$

Now using Thm 1 (Maning) $\longrightarrow$

$$\text{Prob}\left[\|\rho_S - \Omega_S\|_1 \geq \eta\right] \leq \eta'$$

Where $\eta = \varepsilon + \sqrt{\frac{d_S}{d_{eff}}}$, $\eta' = \exp\left[-c\, d_R\, \varepsilon^2\right]$

$$\sqrt{\frac{d_S}{d_E^{eff}}} \leq \sqrt{\frac{d_S^2}{d_R}} \leq d_S \frac{\sqrt{n+1}}{2^{\frac{nH(p)}{2}}} = \frac{2}{\sqrt{n+1}}\, 2^{-(nH(p)-2k)/2} \quad \text{and} \quad \varepsilon = d_R^{-\frac{1}{3}} \leq \frac{(n+1)^{1/3}}{2^{\frac{nH(p)}{3}}}$$

$\lll 1$ for $n \to \infty$

$$\therefore \text{Prob}\left[\|\rho_S - \Omega_S\|_1 \geq d_R^{-\frac{1}{3}} + \sqrt{\frac{2^k}{d_{eff}}}\right] \leq 2e^{-c\, d_R^{1/3}}$$

Putting this expression $\rightarrow$ (for n = very large) $\Rightarrow$ $\|\rho_S - \Omega_S\|_1 \longrightarrow 0$ in the large n limit.

[Valid subject to $n \gg k$]

Moral :- For arbitrary pure state $\in \mathcal{H}_R \longrightarrow$ it WILL Thermalize ... (For This Specific System)

Popescu, Short, Winter $\longrightarrow$ arXiv version $\rightarrow$ 2005

so; $\underbrace{d_{eff} \ll d_{env}}$ but so long as $d_{eff} \gg d_S \rightarrow$ Thermalization is safe. ☺

THERMAL MACHINES

What happens if we go from Classical $\rightarrow$ Quantum Engines

Popescu et al PRL (2010) — Smallest Possible Refrigerator

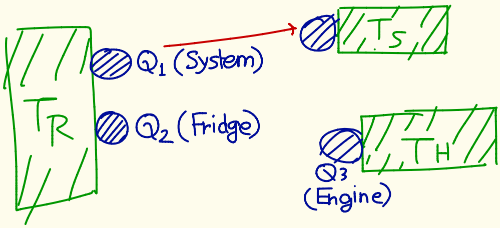
Claim :-
1) It can be done
2) Even Better $\rightarrow$ it can go to $T \rightarrow 0$ limit

Q :- Smallest Hilbert Space dimension in which I can construct a refrigerator ?

- Two Qubit Model
- Qubit Qutrit with n-n interaction
- Single Qutrit system

POPESCU, LINDEN } 3 models

Today :- Only the two-qubit model



T_R = room temp
T_H = Bath temp (Hot)
} $T_R < T_H$

Free Hamiltonian $H_0 = E_1 \underbrace{|1\rangle\langle 1|} + E_2 \underbrace{|2\rangle\langle 2|}$

(Assume $E_1 < E_2$)

$|i\rangle\langle i|$ = excited state of i-th qubit ($i = 1, 2$)

Ground State Energy for both qubits $= 0$ .. (assume)

$\therefore$ Thermal State of First Qubit $= \tau_1 = \dfrac{e^{-\beta E_1 |1\rangle\langle 1|}}{Tr\left[e^{-\beta E_1 |1\rangle\langle 1|}\right]}$

$= r_1 |0\rangle\langle 0| + (1-r_1)|1\rangle\langle 1| \quad \left\{ r_1 = \dfrac{1}{1+e^{-\beta E_1}};\ r_2 = \dfrac{e^{-\beta E_1}}{1+e^{-\beta E_1}} \right\}$

Similarly for the second qubit τ_2

$\therefore$ Joint State $\rightarrow \tau_1 \otimes \tau_2$ $\quad \therefore$ When Refrigeration occurs $\rightarrow$ The system achieves some steady state temp T_1^S & the new τ_f of the first qubit $= r_1^s |0\rangle\langle 0| + (1-r_1^s)|1\rangle\langle 1|$

Clearly here $r_1^s > r_1$ $\quad [\because \rho_f^1 < \rho_{init}^1]$

$$\therefore \tau_1 \otimes \tau_2 = \begin{bmatrix} r_1 r_2 & & & 0 \\ & r_1 \tilde{r}_2 & & \\ & & \tilde{r}_1 r_2 & \\ 0 & & & \tilde{r}_1 \tilde{r}_2 \end{bmatrix} \quad \tilde{r}_i = 1 - r_i \ (i = 1, 2)$$

Now if $E_1 < E_2$ implies $\underline{r_1 > r_2}$ }

$\therefore$ Here coefft of $|01\rangle$ has higher energy than $|10\rangle$ $\xrightarrow{\text{Swap}}$ .... $\equiv$ Cooling

Caveat :- Applying this unitary Swap is not free $\longrightarrow$ Idea :- Use free Energy

Add a third qubit which is at contact with a high temp bath ($E_3 = E_2 - E_1$)

Joint State of the system $\tau_1 \otimes \tau_2 \otimes \tau_3$

$$= \begin{bmatrix} r_1 r_2 r_3 & & & & 0 \\ & r_1 r_2 \tilde{r}_3 & & & \\ & & \ddots & & \\ & 0 & & \ddots & \\ & & & & \tilde{r}_1 \tilde{r}_2 \tilde{r}_3 \end{bmatrix}$$

Check:- Verify that coefft of $|010\rangle$ = coefft of $|101\rangle$

$[r_1 \tilde{r}_2 r_3 = \tilde{r}_1 r_2 \tilde{r}_3]$

Now can I cool ? (Not forbidden now !)

Won't be using SWAP, rather will use an interaction

$H_{int} = g\left(|010\rangle\langle 101| + |101\rangle\langle 010|\right)$; Assume $E_i \gg g \rightarrow$ Will not change eigenvalues & eigenvectors significantly.

What happens to free coherence constraints ? → Study!

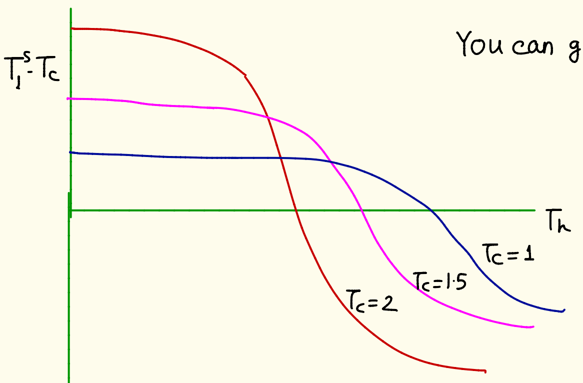
Phenomenological model:-

With probability $p_i \rightarrow$ the i-th qubit goes back to original state
per unit time

Now I wan't a dynamics for this

Master Equation:- $\dfrac{\partial \rho}{\partial t} = -i\left[H_0 + H_{int}, \rho\right] + \sum_{i=1}^{3} p_i \underbrace{\left(\tau_i \otimes Tr_i \rho - \rho\right)}_{\text{Lindblad term}}$

Approach:- Look at the steady state solution & corresponding steady state temperature
↓
Doable analytically, but boring hard calculation → done numerically.



You can go $T \to 0$ → Efficiency $\simeq$ Carnot Efficiency