Pure state quantum statistical mechanics

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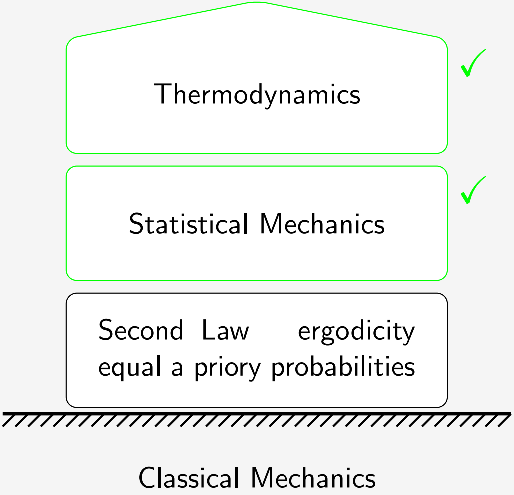
New foundation for Statistical Mechanics



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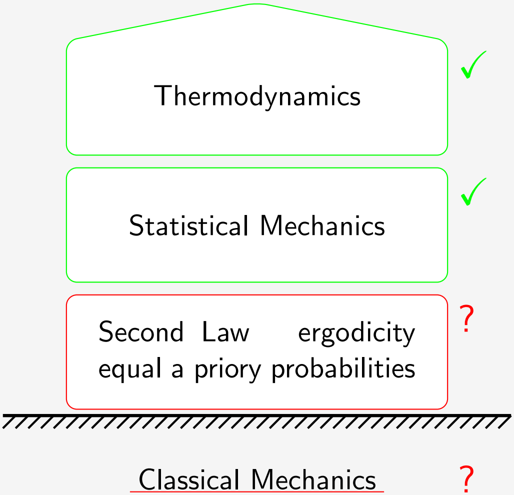

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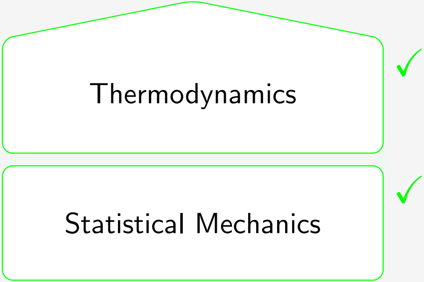

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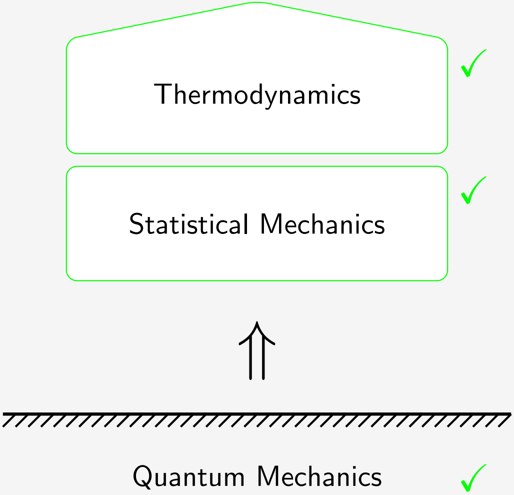

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Why do electrons hop between energy eigenstates?

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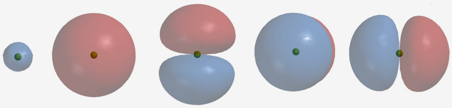
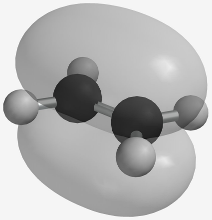
quantum mechanical orbitals





coherent superpositions

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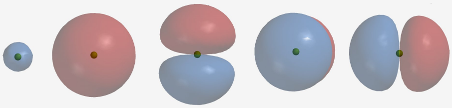
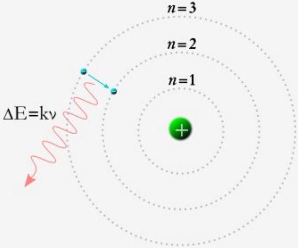
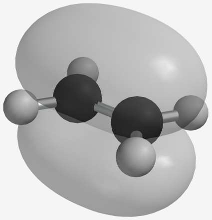


discrete energy levels





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hopping

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Setup and notation

Notation and some technicalities

- Operational distinguishability (trace distance)

$$\mathcal{D}(\rho,\sigma) = \frac{1}{2}\|\rho - \sigma\|_1 = \max_{0 \leq A \leq \mathbb{1}} \mathrm{Tr}[A\,\rho] - \mathrm{Tr}[A\,\sigma]$$

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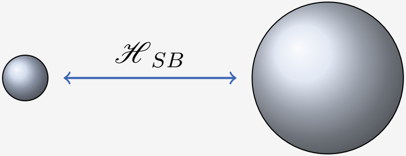
$$\overset{\text{(Assumption 1)}}{=} \frac{1}{\sum_k |\langle\psi_0|E_k\rangle|^4} \sim \text{\# energy eigenstates in } \psi_0$$

Setup

System, $\mathcal{H}_S, \mathscr{H}_S$ Bath, $\mathcal{H}_B, \mathscr{H}_B$



$$\rho_t^S = \mathrm{Tr}_B[\psi_t] \qquad \rho_t^B = \mathrm{Tr}_S[\psi_t]$$

$$\frac{d\psi_t}{dt} = \mathrm{i}\,[\psi_t, \mathscr{H}]$$

A very weak assumption on the Hamiltonian

$$\mathscr{H} = \mathscr{H}_S \otimes \mathbb{1} + \mathbb{1} \otimes \mathscr{H}_B + \mathscr{H}_{SB}$$

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Assumption 1

A Hamiltonian has non–degenerate energy gaps iff:

$$E_k - E_l = E_m - E_n$$

$$\Longrightarrow k = l \wedge m = n \text{ or } k = m \wedge l = n$$

Subsystem equilibration

Measure concentration in Hilbert space

Theorem 1

For random $\psi_0 \in \mathcal{P}_1(\mathcal{H})$ *with* $d = \dim(\mathcal{H})$

$$\Pr\left\{ d^{\text{eff}}(\omega) < \frac{d}{4} \right\} \leq 2\,\mathrm{e}^{-c\sqrt{d}}$$

$$d^{\text{eff}}(\omega) = \frac{1}{\operatorname{Tr}[\omega^2]} = \frac{1}{\sum_k |\langle\psi_0|E_k\rangle|^4} \sim \#\text{ energy eigenstates in } \psi_0$$

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$\Longrightarrow$ If d is large then $d^{\text{eff}}(\omega)$ is large.

[3]

Equilibration

Theorem 2

For every $\psi_0 \in \mathcal{P}_1(\mathcal{H})$

$$\langle \mathcal{D}(\rho_t^S, \omega^S) \rangle_t \leq \frac{1}{2} \sqrt{\frac{d_S^2}{d^{\mathrm{eff}}(\omega)}}$$

where

$$\rho_t^S = \mathrm{Tr}_B\, \psi_t \qquad \omega^S = \langle \rho_t^S \rangle_t \qquad \omega = \langle \psi_t \rangle_t$$

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$\Longrightarrow$ If $d^{\text{eff}}(\omega) \gg d_S^2$ then ρ_t^S equilibrates.

[3]

Speed of the fluctuations around equilibrium

$$v_S(t) = \lim_{\delta t \to 0} \frac{\mathcal{D}(\rho_t^S, \rho_{t+\delta t}^S)}{\delta t} = \frac{1}{2} \left\| \frac{d\rho_t^S}{dt} \right\|_1$$

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For every $\psi_0 \in \mathcal{P}_1(\mathcal{H})$

$$\langle v_S(t) \rangle_t \leq \| \mathscr{H}_S \otimes \mathbb{1} + \mathscr{H}_{SB} \|_\infty \sqrt{\frac{d_S^3}{d^{\mathrm{eff}}(\omega)}}$$

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$\Longrightarrow$ If $d^{\mathrm{eff}}(\omega) \gg d_S^3$ then ρ_t^S is slow.

[4]

Summary

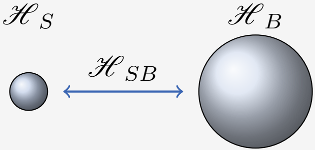
Typical states of large quantum systems

- have a high average effective dimension,
- their subsystems equilibrate
- and fluctuate slowly around the equilibrium state.

Decoherence under weak interaction

Approach 1: Effective dynamics

standard QM:



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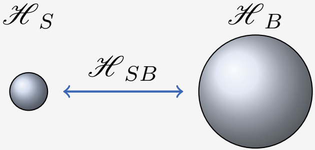

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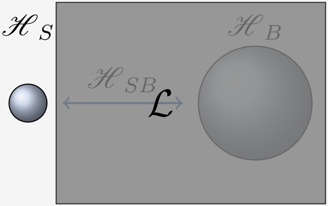

$$\frac{d\rho_t^S}{dt} = \mathrm{i}\,[\rho_t^S, \mathscr{H}_S] + \mathrm{i}\ \mathcal{L}(\rho_t^S)$$

Approach 2: Decoherence à la Zurek

- Special Hamiltonian with pointer sates $|p\rangle$:

$$\mathscr{H} = \sum_p |p\rangle\langle p| \otimes \mathscr{H}^{(p)}$$

- Initial product state $\psi_0 = \rho_0^S \otimes \psi_0^B$

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Einselection

Off-diagonal elements in the pointer basis are suppressed:

$$\langle p|\rho_t^S|p'\rangle = \langle p|\rho_0^S|p'\rangle \underbrace{\langle \psi_0^B|U_t^{(p')^\dagger} U_t^{(p)}|\psi_0^B\rangle}_{\leq 1}$$

[5]

Comparison

Pros and cons

	unitary evolution	general mechanism
effective dynamics	X	✓
einselection	✓	X

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Can we find a more general mechanism based on standard Quantum Mechanics?

Yes we can!

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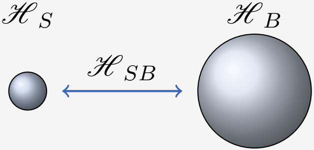
$$\| \mathscr{H}_{SB} \|_\infty \ll \| \mathscr{H}_S \|_\infty,$$



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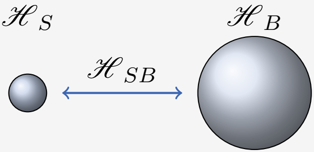

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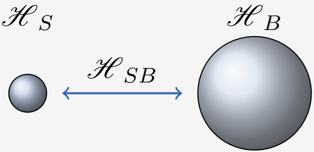

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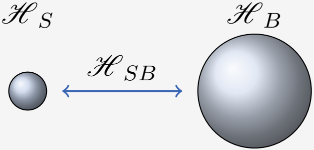

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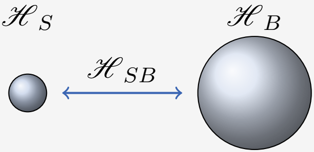

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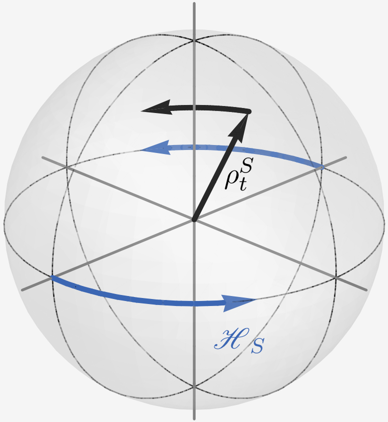

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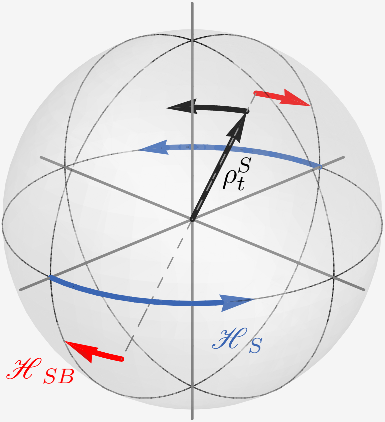

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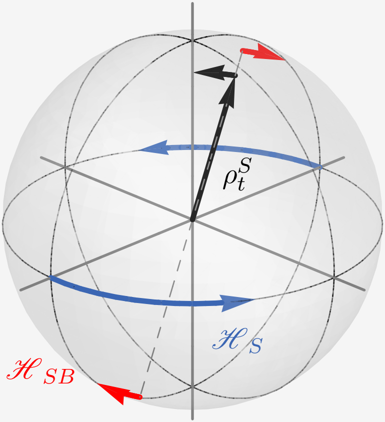

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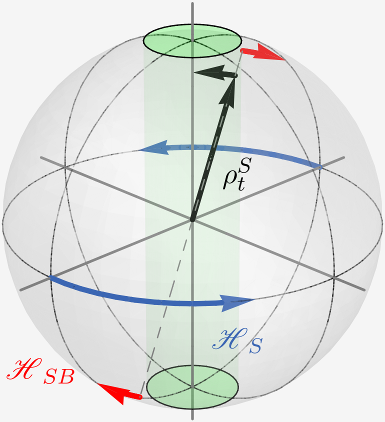

Decoherence through weak interaction

Theorem 4

All reduced states ρ_t^S *satisfy*

$$\max_{k\neq l} 2\,|E_k^S - E_l^S|\,|\rho_{kl}^S| \leq 2\,\|\,\mathscr{H}_{SB}\,\|_\infty + \left\|\frac{d\rho_t^S}{dt}\right\|_1,$$

where $\rho_{kl}^S = \langle E_k^S|\rho_t^S|E_l^S\rangle$.

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and moreover

$$\max_{\{(k,l)\}} \sum_{(k,l)} 2 \, |E_k^S - E_l^S| \, |\rho_{kl}^S| \leq 2 \, \| \mathscr{H}_{SB} \|_\infty + \left\| \frac{d\rho_t^S}{dt} \right\|_1 ,$$

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where $\rho_{kl}^S = \langle E_k^S|\rho_t^S|E_l^S\rangle$.

$\Longrightarrow$ If $\mathscr{H}_{SB}$ is weak and ρ_t^S is slow its off-diagonal elements are small.

[6]

Consequences for small and large systems

$$\max_{\{(k,l)\}} \sum_{(k,l)} 2\,|E_k^S - E_l^S|\,|\rho_{kl}^S| \leq 2\,\|\,\mathscr{H}_{SB}\,\|_\infty + \left\|\frac{d\rho_t^S}{dt}\right\|_1$$

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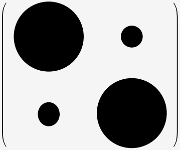

Decoherence in the $\mathscr{H}_S$ eigenbasis

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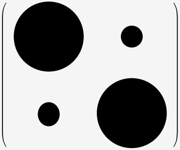

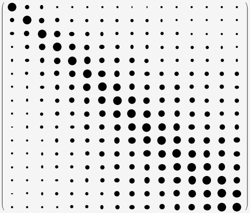

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No Schrödinger's cat states

Take-home message

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- have a high average effective dimension,
- their subsystems equilibrate
- and fluctuate slowly around the equilibrium state,
- and given the interaction is weak they are close to diagonal in the local energy eigenbasis.

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Thank you for your attention!

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