Under what conditions do quantum systems thermalize?

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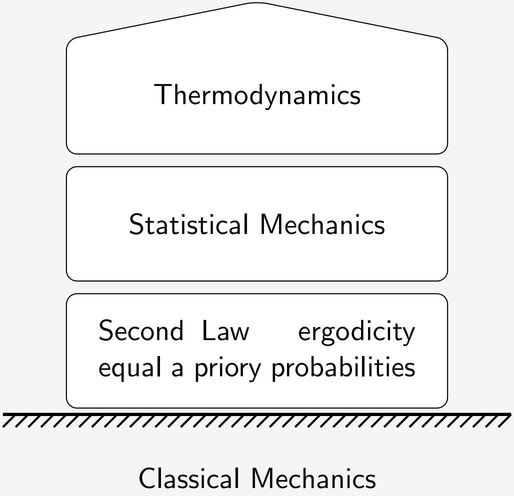
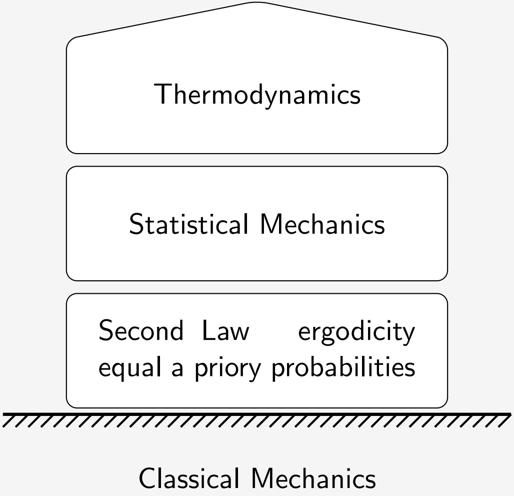
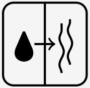
Motivation

New foundation for statistical mechanics



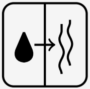
New foundation for statistical mechanics



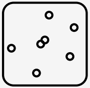


New foundation for statistical mechanics

Thermodynamics



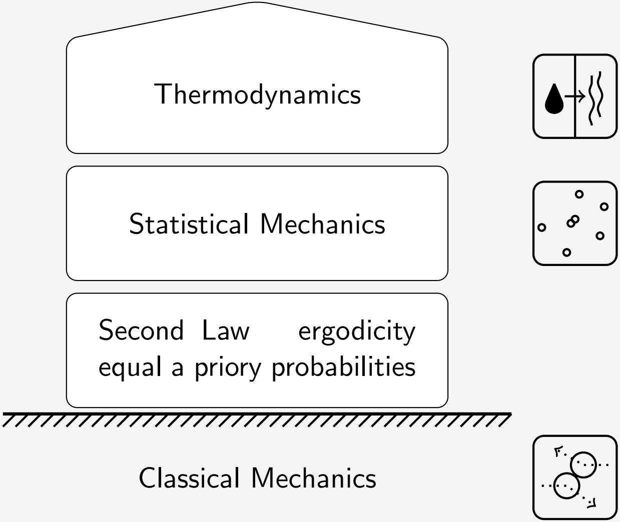
Statistical Mechanics



Second Law ergodicity
equal a priory probabilities

Classical Mechanics

New foundation for statistical mechanics



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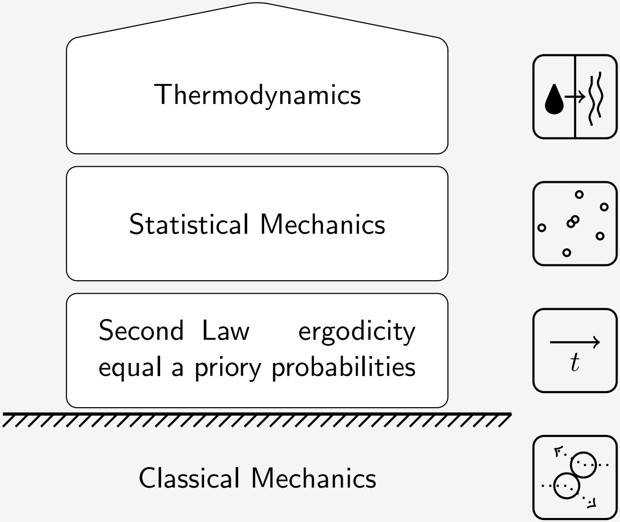

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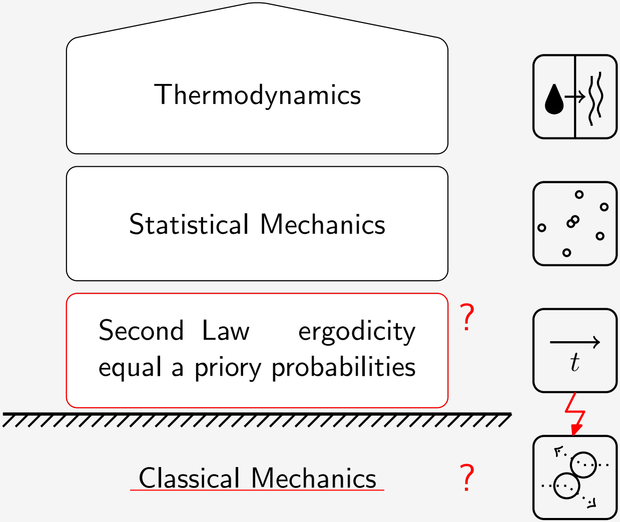

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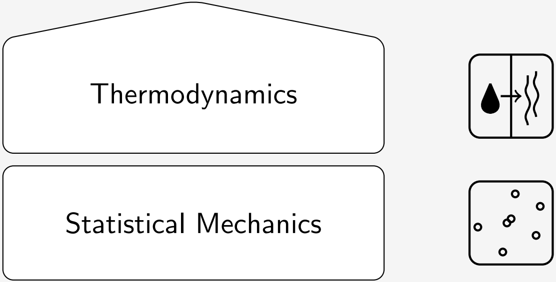
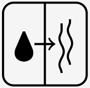
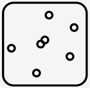


New foundation for statistical mechanics

Thermodynamics



Statistical Mechanics



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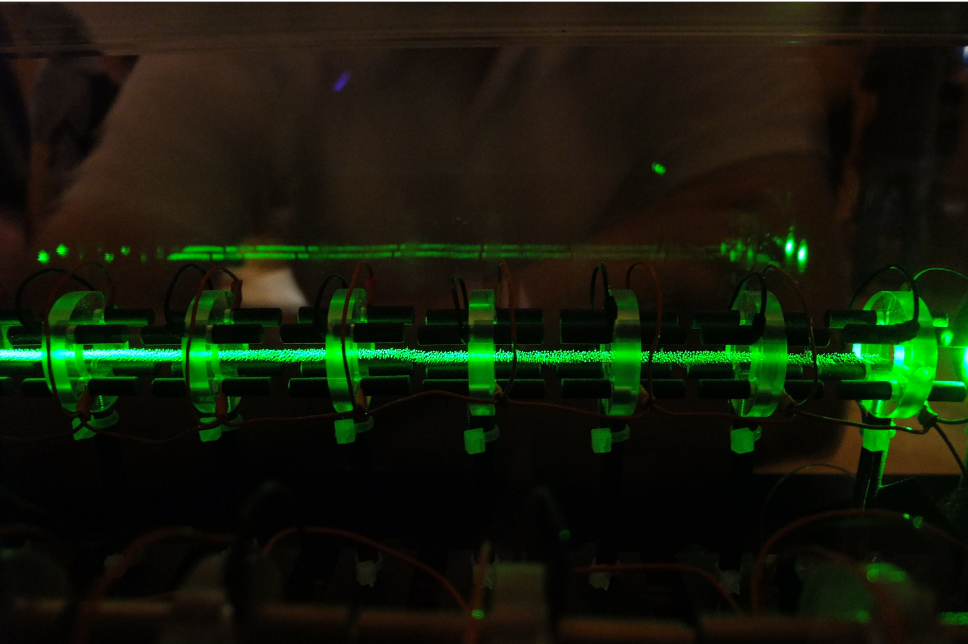
Quantum Mechanics

Ultra cold quantum gases



Setup

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

$$d_S = \dim(\mathcal{H}_S)$$

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

$$d_B \gg d_S$$

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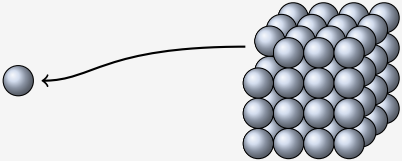

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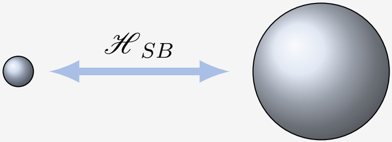

$$\mathscr{H} = \mathscr{H}_S \otimes \mathbb{1} + \mathbb{1} \otimes \mathscr{H}_B + \mathscr{H}_{SB}$$

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

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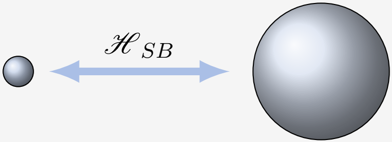

$$\psi_t^S = \mathrm{Tr}_B[\psi_t]$$

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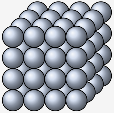
Understanding thermalization



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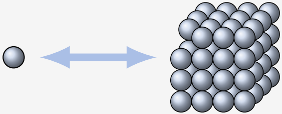

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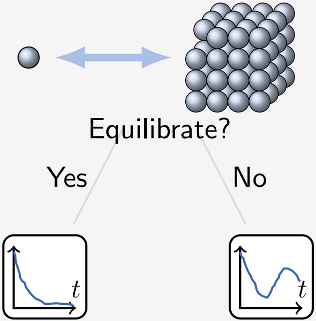

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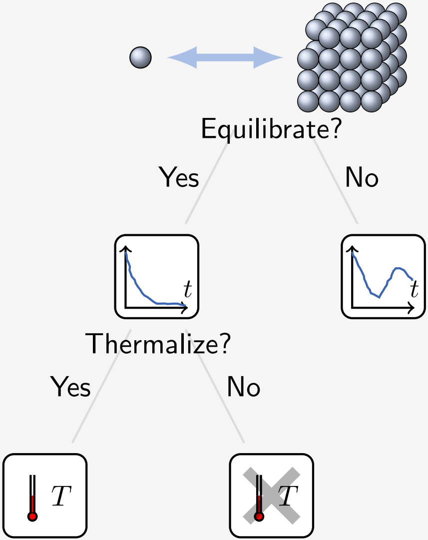

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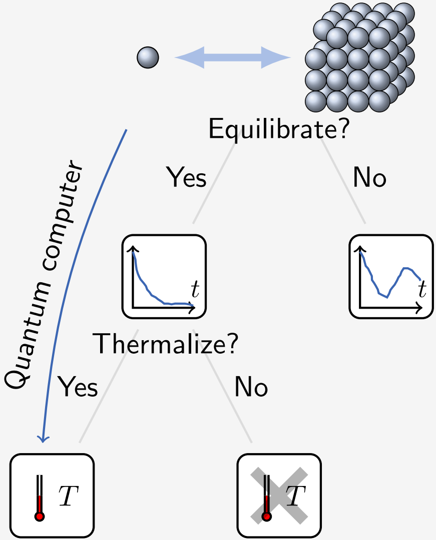


Equilibration

Equilibration

Theorem 1 (Equilibration [1])

If $\mathscr{H}$ has non-degenerate energy gaps, then for every $\psi_0 = |\psi_0\rangle\langle\psi_0|$ there exists a ω^S such that:

$$\overline{\mathcal{D}(\psi_t^S, \omega^S)} \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d^{\mathrm{eff}}}}.$$

[1] N. Linden, S. Popescu, A. J. Short, and A. Winter, PRE 79 (2009) no. 6, 061103

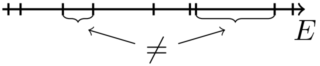
Equilibration

Non-degenerate energy gaps

$\mathscr{H}$ has non–degenerate energy gaps iff:

$$E_k - E_l = E_m - E_n$$

$$\implies k = l \wedge m = n \quad \vee \quad k = m \wedge l = n$$



Intuition: Sufficient for $\mathscr{H}$ to be fully interactive

$$\mathscr{H} \neq \mathscr{H}_1 \otimes \mathbb{1} + \mathbb{1} \otimes \mathscr{H}_2$$

Theorem

If $\mathscr{H}$ has

there exis

$\langle\psi_0|$

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Effective dimension

$$d^{\text{eff}} = \frac{1}{\sum_k |\langle E_k|\psi_0\rangle|^4}.$$

Intuition: Dimension of supporting energy subspace

[1] N. Linden, S. Popescu, A. J. Short, and A. Winter, PRE 79 (2009) no. 6, 061103

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$$\overline{\mathcal{D}(\psi_t^S, \omega^S)} \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d^{\mathrm{eff}}}}.$$

$\Longrightarrow$ If $d^{\mathrm{eff}} \gg d_S^2$ then ψ_t^S equilibrates.

[1] N. Linden, S. Popescu, A. J. Short, and A. Winter, PRE 79 (2009) no. 6, 061103

Maximum entropy principle

Theorem 2 (Maximum entropy principle [2])

If $\mathrm{Tr}[A\,\psi_t]$ equilibrates, it equilibrates towards its time average

$$\overline{\mathrm{Tr}[A\,\psi_t]} = \mathrm{Tr}[A\,\overline{\psi_t}] = \mathrm{Tr}[A\,\omega],$$

and

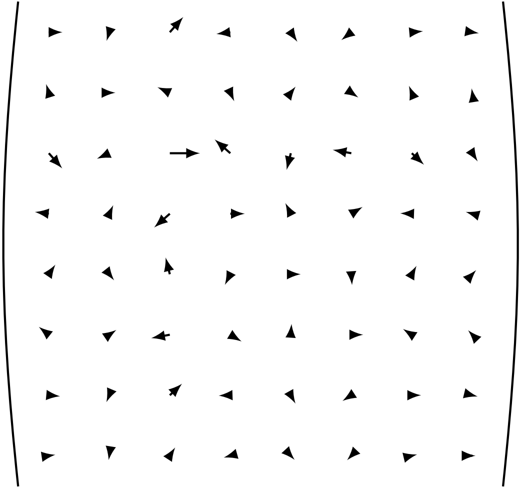
$$\omega = \sum_k \pi_k \psi_0 \pi_k$$

(with π_k the energy eigen projectors) is the dephased state that maximizes the von Neumann entropy, given all conserved quantities.

[2] C. Gogolin, M. P. Mueller, and J. Eisert, PRL 106 (2011) 040401

Maximum entropy principle

Time averaging

$\psi_0 =$ 

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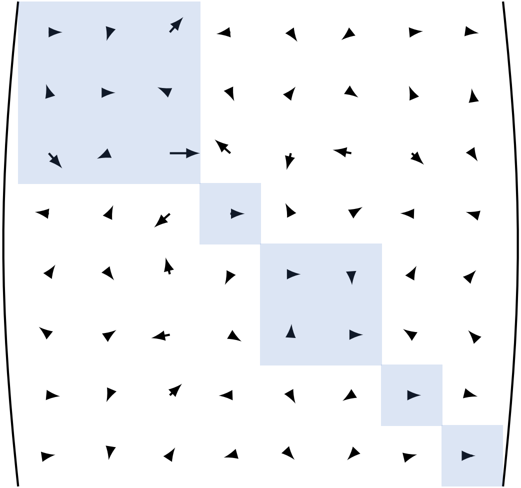

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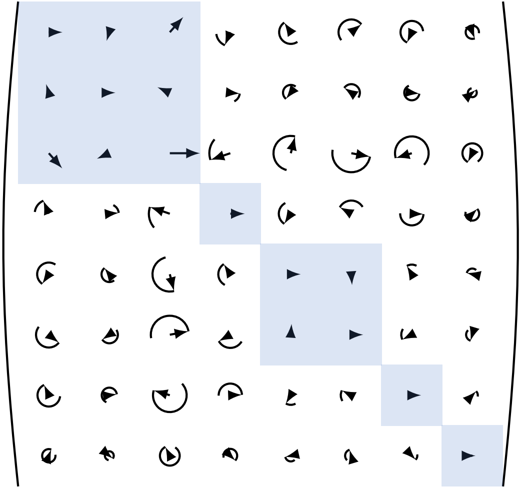

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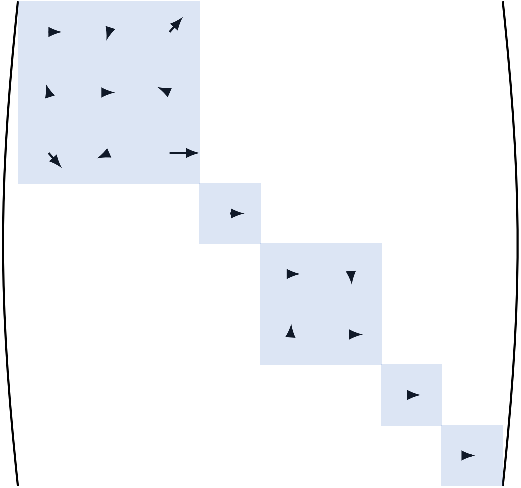
$\omega =$ 

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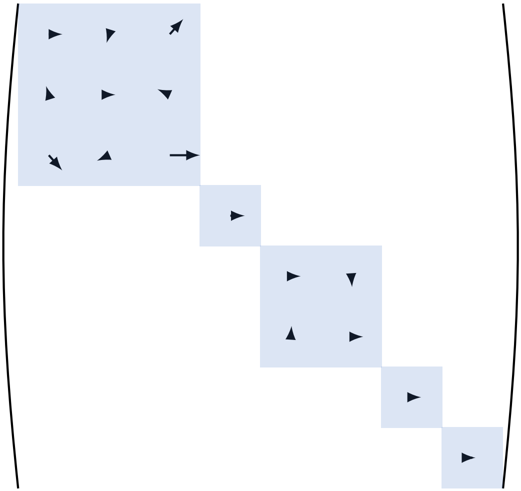

$\psi_0 \to \omega$ is a pinching $\Rightarrow \omega$ maximizes entropy.

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(with π_k the energy eigen projectors) is the dephased state that maximizes the von Neumann entropy, given all conserved quantities.

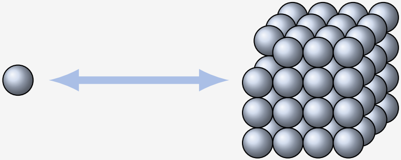
$\Rightarrow$ Maximum entropy principle from pure quantum dynamics.

Proves a conjecture from the condensed matter literature from 2007.

[2] C. Gogolin, M. P. Mueller, and J. Eisert, PRL 106 (2011) 040401

Thermalization and realistic weak coupling

Thermalization is a complicated process



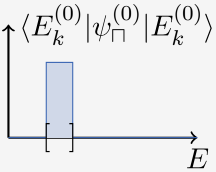
Thermalization implies:

1. Equilibration [1]
2. Subsystem initial state independence [2]
3. Weak bath state dependence [3]
4. Diagonal form of the subsystem equilibrium state [4]
5. Gibbs state $\omega^S = \mathrm{Tr}_B[\omega] \approx \mathrm{e}^{-\beta\,\mathscr{H}_S}$ [3]

[1] N. Linden, S. Popescu, A. J. Short, and A. Winter, PRE 79 (2009) no. 6, 061103
[2] C. Gogolin, M. P. Mueller, and J. Eisert, PRL 106 (2011) 040401
[3] A. Riera, C. Gogolin, and J. Eisert, 1102.2389
[4] C. Gogolin, PRE 81 (2010) no. 5, 051127

Level counting with no coupling

$$\| \mathscr{H}_{SB} \|_\infty = 0$$



[5] S. Goldstein, PRL 96 (2006) no. 5, 050403

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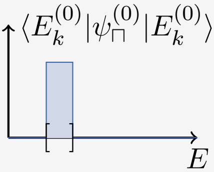

Well known fact [5]:

no coupling

\# bath states in $[E - E_k^S, E - E_k^S + \Delta]$

$$\omega_\sqcap^{S(0)} \propto \sum_k \Omega_\Delta^B(E - E_k^S) \, |E_k^S\rangle\langle E_k^S|$$

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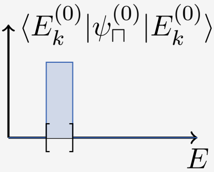

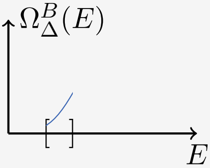

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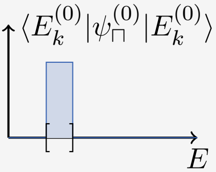

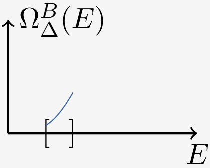

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exponentially dense spectrum

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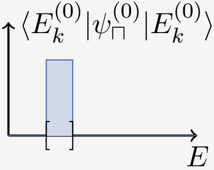

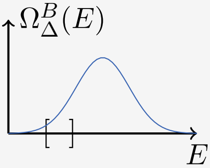

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Perturbative coupling $\| \mathscr{H}_{SB} \|_\infty < \mathrm{gaps}(\mathscr{H}_0) \ldots$

- ...is unrealistic as the spectrum of $\mathscr{H}_0$ becomes exponentially dense.

[2] C. Gogolin, M. P. Mueller, and J. Eisert, PRL 106 (2011) 040401

Perturbative coupling $\| \mathscr{H}_{SB} \|_\infty < \text{gaps}(\mathscr{H}_0)$ ...

- ... is unrealistic as the spectrum of $\mathscr{H}_0$ becomes exponentially dense.
- ... provably prevents thermalization because

perturbative coupling

$\Downarrow$ [2]

effective entanglement in the eigenbasis $R(\psi_0)$ is small

$\Downarrow$ [2]

absence of initial state independence.

$$\mathcal{D}(\omega^{S(1)}, \omega^{S(2)}) \geq \mathcal{D}(\psi_0^{S(1)}, \psi_0^{S(2)}) - R(\psi_0^{S(1)}) - R(\psi_0^{S(2)})$$

[2] C. Gogolin, M. P. Mueller, and J. Eisert, PRL 106 (2011) 040401

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Effective entanglement in the eigenbasis

$$R(\psi_0) = \sum_k |\langle E_k|\psi_0\rangle|^2 \, \mathcal{D}(\mathrm{Tr}_B \, |E_k\rangle\langle E_k|, \psi_0^S)$$

Measures how entangled the eigenbasis feels for the given initial state.

all

$$\mathcal{D}(\omega^{S(1)}, \omega^{S(2)}) \geq \mathcal{D}(\psi_0^{S(1)}, \psi_0^{S(2)}) - R(\psi_0^{S(1)}) - R(\psi_0^{S(2)})$$

[2] C. Gogolin, M. P. Mueller, and J. Eisert, PRL 106 (2011) 040401

Perturbative coupling $\| \mathscr{H}_{SB} \|_\infty < \mathrm{gaps}(\mathscr{H}_0)$ ...

- ... is [...]ally dense.
- ... pr[...]

Theorem 3 (Entanglement in eigenbasis)

For every orthonormal basis $\{|i\rangle\}$ for S and every initial product state *with $\psi_0 = |j\rangle\langle j| \otimes \phi_0^B$, the* effective entanglement in the eigenbasis *(for non-degenerate $\mathscr{H}$) is on average upper bounded by*

$$\mathbb{E}_{\phi_0^B} R(|j\rangle\langle j| \otimes \phi_0^B) \leq 2\,\delta\, d_S,$$

where

$$\delta = \max_k \min_i \mathcal{D}(\mathrm{Tr}_B\, |E_k\rangle\langle E_k|, |i\rangle\langle i|)$$

is the geometric measure of entanglement *of the eigenstate $|E_k\rangle$ with respect to the basis $\{|i\rangle\}$.*

all

$^{(2)})$

[2] C. Gogolin, M. P. Mueller, and J. Eisert, PRL 106 (2011) 040401

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$$\mathcal{D}(\omega^{S(1)}, \omega^{S(2)}) \geq \mathcal{D}(\psi_0^{S(1)}, \psi_0^{S(2)}) - R(\psi_0^{S(1)}) - R(\psi_0^{S(2)})$$

$\Longrightarrow$ Refutes wide spread believe that "non-integrable models thermalize."

[2] C. Gogolin, M. P. Mueller, and J. Eisert, PRL 106 (2011) 040401

Realistic weak coupling

- Naive perturbation theory fails.
- Realistic weak coupling: $\mathrm{gaps}(\mathscr{H}_0) \ll \| \mathscr{H}_{SB} \|_\infty \ll \Delta$

[3] A. Riera, C. Gogolin, and J. Eisert, 1102.2389

Realistic weak coupling

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Theorem 4 (Corollary of a theorem from [3])

If $\| \mathscr{H}_{SB} \|_\infty \ll \Delta$ the dephased states $\omega_\sqcap^{S(0)}$ and $\omega_\sqcap^{S}$ are close to each other in the sense that

$$\mathcal{D}(\omega_\sqcap^{S}, \omega_\sqcap^{S(0)}) \lessapprox 3\sqrt{\frac{\| \mathscr{H}_{SB} \|_\infty}{2\Delta}}.$$

[3] A. Riera, C. Gogolin, and J. Eisert, 1102.2389

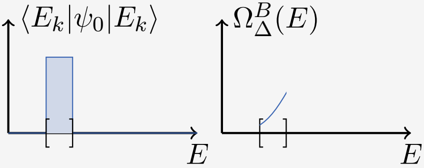
Putting everything together

Consequences

[3] A. Riera, C. Gogolin, and J. Eisert, 1102.2389

Consequences

$$\| \mathscr{H}_{SB} \|_\infty \ll \text{gaps}(\mathscr{H}_0)$$



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Consequences

$$\| \mathscr{H}_{SB} \|_\infty \gg \text{gaps}(\mathscr{H}_0)$$
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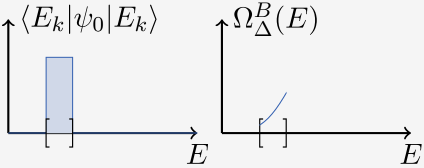

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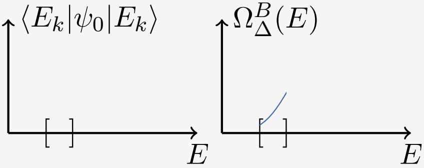

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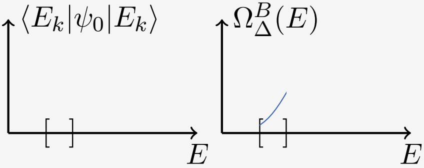

$\Longrightarrow$ "Theorem" 5 (Theorem 2 in [3])

(Kinematic) Almost all pure states from a microcanonical subspace $[E, E + \Delta]$ are locally close to a Gibbs state.

[3] A. Riera, C. Gogolin, and J. Eisert, 1102.2389

Consequences

$\| \mathscr{H}_{SB} \|_\infty \gg \mathrm{gaps}(\mathscr{H}_0)$
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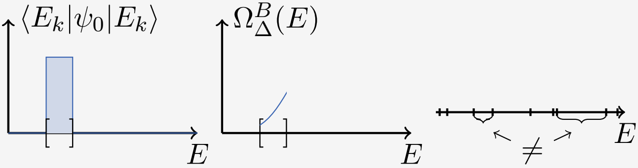

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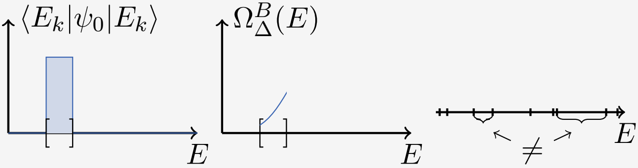

$\Longrightarrow$ "Theorem" 5 (Theorem 2 in [3])

(Kinematic) Almost all pure states from a microcanonical subspace $[E, E+\Delta]$ are locally close to a Gibbs state.

(Dynamic) All initial states $\psi_{\sqcap,0}$ locally equilibrate towards a Gibbs state, even if they are initially far from equilibrium.

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Consequences

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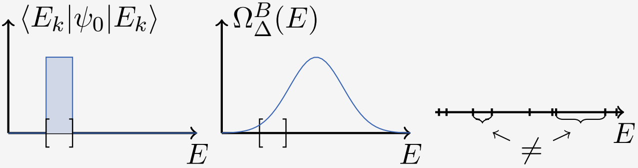

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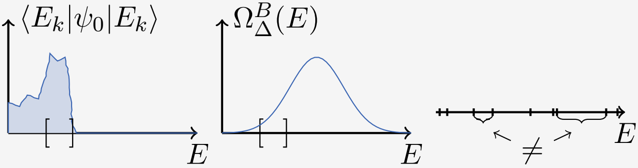

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A quantum algorithm for Gibbs state preparation

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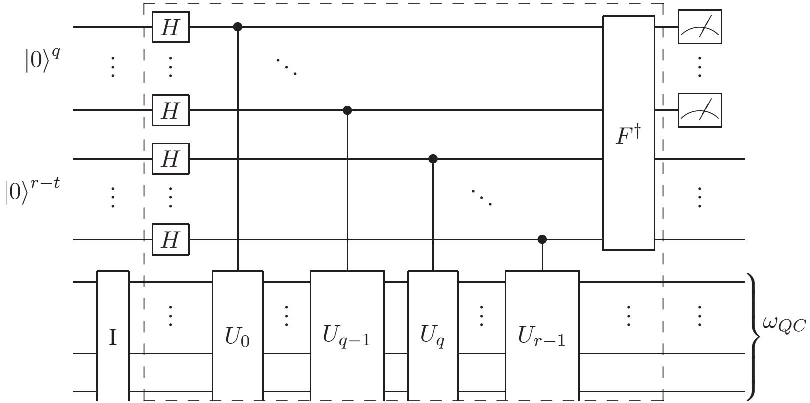
A quantum algorithm for Gibbs state preparation

Quantum circuit



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A quantum algorithm for Gibbs state preparation

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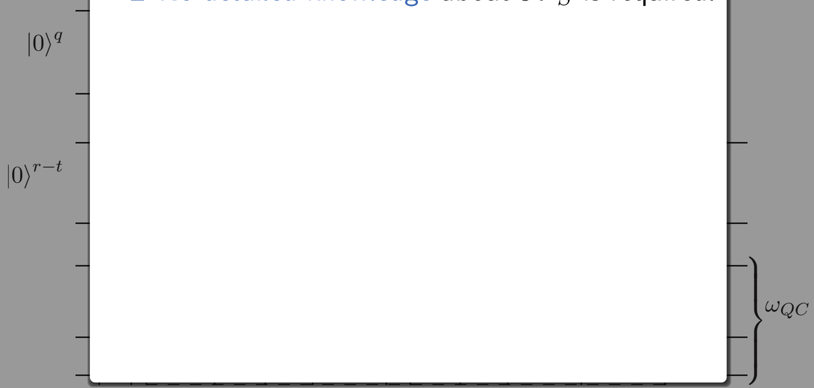

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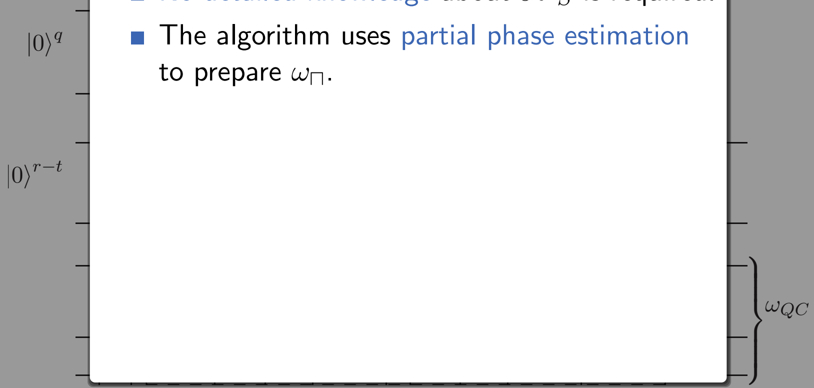
Quantum circuit



- No detailed knowledge about $\mathscr{H}_S$ is required.
- The algorithm uses partial phase estimation to prepare $\omega_{\sqcap}$.

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A quantum algorithm for Gibbs state preparation

Quantum circuit

- No detailed knowledge about $\mathscr{H}_S$ is required.
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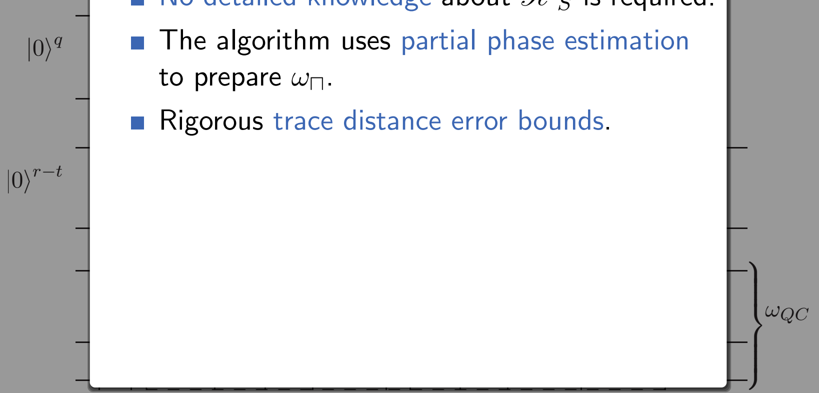
- Rigorous trace distance error bounds.



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A quantum algorithm for Gibbs state preparation

Quantum circuit

$|0\rangle^q$

$|0\rangle^{r-t}$

ω_{QC}

- No detailed knowledge about $\mathscr{H}_S$ is required.
- The algorithm uses partial phase estimation to prepare $\omega_{\sqcap}$.
- Rigorous trace distance error bounds.
- Explicit runtime (complementing quantum Metropolis).

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A quantum algorithm for Gibbs state preparation

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ω_{QC}

- No detailed knowledge about $\mathscr{H}_S$ is required.
- The algorithm uses partial phase estimation to prepare $\omega_{\sqcap}$.
- Rigorous trace distance error bounds.
- Explicit runtime (complementing quantum Metropolis).
- Complexity for fixed trace distance error:
  - polynomially many ancilla qubits
  - exponential runtime ($\Omega(\exp(\mathrm{gap}(\mathscr{H}_S)\beta))$ is necessary)

[3] A. Riera, C. Gogolin, and J. Eisert, 1102.2389

Outlook

And there is more...

What I didn't talk about:

- Thermalization in exactly solvable models [6, 7]
- A strong connection to decoherence [4]
- Measure concentration [8, 1, 9, 10]

The major open question:

- Time scales. How long does it take to equilibrate/thermalize/decohere?

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[10] C. Gogolin, Master's thesis, 2010, 1003.5058

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Andreas Winter

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Thank you for your attention!

$\longrightarrow$ slides: www.cgogolin.de

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