Typicality paradigm in Quantum Statistical Thermodynamics

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Outline

1) The framework: microcanonical statistics
   versus the dynamics of an isolated quantum system
2) Equilibrium properties and fluctuations
3) What populations? Statistical Ensemble
4) Typicality
5) Thermodynamics
6) Conclusions: an open issue and further developments

1) The framework

Dynamics of a quantum pure state for an isolated system (no interactions and entanglement with the surrounding, otherwise the system's wavefunction does not exist)

$\mathcal{H}$: Hilbert space

$\hat{\mathrm{H}}$: Hamiltonian operator for the energy

Hamiltonian (energy) eigenvalues E_k and eigenstates $|E_k\rangle$

$$\hat{H}|E_k\rangle = E_k|E_k\rangle \quad \text{for} \quad k = 1,2,\cdots$$

Schroedinger equation for the evolution of the wavefunction $|\Psi(t)\rangle$

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle \quad \text{with} \quad \langle\Psi(t)\,|\,\Psi(t)\rangle = 1$$

Density matrix operator: $\hat{\rho}(t) := |\Psi(t)\rangle\langle\Psi(t)|$

Quantum observable $a(t)$: expectation value of operator $\hat{A}$

$$a(t) := \langle\Psi(t)|\hat{A}|\Psi(t)\rangle = \mathrm{Tr}\left\{\hat{A}\hat{\rho}(t)\right\}$$

Partition of the overall system as subsystem+envinronment: reduced density matrix $\hat{\mu}(t)$ of subsystem

$$\hat{\mu}(t) := \mathrm{Tr}_{\text{envir.}}\{\hat{\rho}(t)\}$$

1) The framework

Microcanonical density matrix operator $\hat{\rho}^{\mu C}$:

$$\langle E_k | \hat{\rho}^{\mu C} | E_{k'} \rangle = \delta_{k,k'} \rho^{\mu C}_{k,k}$$

$$\rho^{\mu C}_{k,k} \begin{cases} = 1/N^{\mu C} & \text{for } E_{\min} < E_k \le E_{\max} \\ = 0 & \text{otherwise} \end{cases}$$

where $\Delta E := E_{\max} - E_{\min}$ is small enough but not too much

($E_{\max} \Rightarrow$ internal energy U of Thermodynamics)

Conventional interpretation of $\hat{\rho}^{\mu C}$: <u>average</u> of $\rho(t)$ amongst a <u>collection of system's copies</u>

1) The framework

In recent years:

1) quantum computer theory
2) decoherence program (Zurek)

Statistical Thermodynamics of a <u>single</u> <u>system</u> evolving according to the Schroedinger equation

2) Equilibrium properties and fluctuations

Quantum dynamics in a finite dimensional Hilbert space $\mathcal{H}_N$ defined by an upper energy cut-off $E_{\max}$

$$\mathcal{H}_N := \mathrm{span}\left\{ \left| E_k \right\rangle \mid E_k \le E_{\max} \right\}$$

Wavefunction expansion on the energy eigenstates

$$\left| \Psi(t) \right\rangle = \sum_{k=1}^{N} c_k(t) \left| E_k \right\rangle \qquad c_k(t) = \left\langle E_k \mid \Psi(t) \right\rangle = \mathrm{e}^{-iE_k t/\hbar} c_k(0)$$

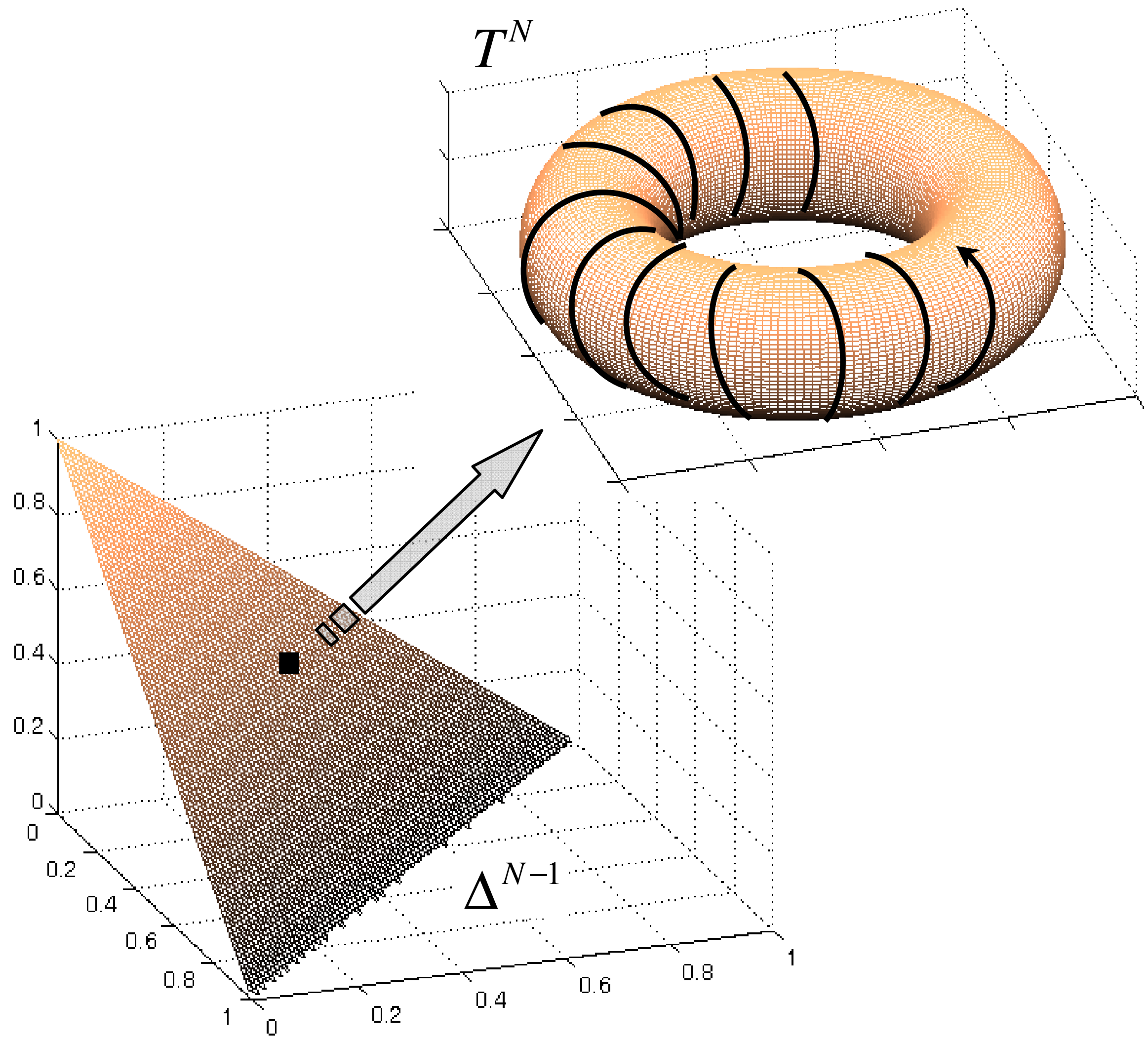
Polar representation of the coefficients: $c_k(t) = \sqrt{P_k}\, \mathrm{e}^{-i\alpha_k(t)}$

Populations: $P_k = \left| c_k(t) \right|^2 = \left| c_k(0) \right|^2$ (constants of motion!)

Phases: $\alpha_k(t) = \alpha_k(0) + E_k t / \hbar$

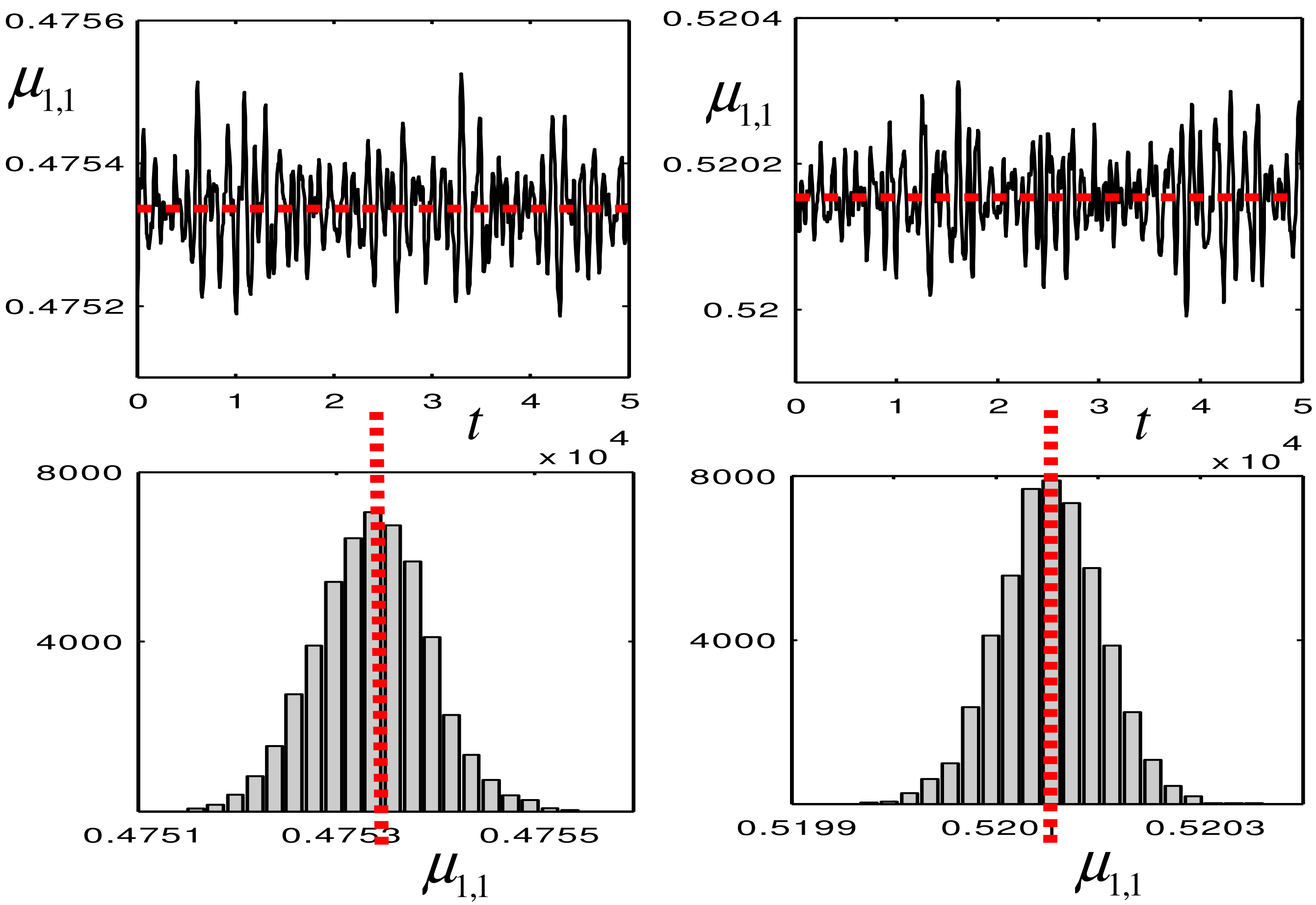
Pure State Distribution (PSD): homogeneous distribution of the phases for a given set of populations.

2) Equilibrium properties and fluctuations



2) Equilibrium properties and fluctuations

Randomly perturbed harmonic oscillators: results for the ground state element of the reduced density matrix



Two different (random) choices of the populations (or of $|\Psi(0)\rangle$)

2) Equilibrium properties and fluctuations

Equilibrium properties from the asymptotic time average

$$\overline{a} := \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^{\tau} a(t)dt = \mathrm{Tr}\left\{\hat{A}\overline{\hat{\rho}}\right\} = \overline{a}(P)$$

$$\overline{\hat{\rho}} = \sum_{k=1}^{N} P_k \left|E_k\right\rangle\left\langle E_k\right|$$

Equilibrium properties depend on the choice of the populations!

Note: PSD allows the calculations of fluctuations about
the equilibrium value

Population dependence also for the (Shannon) entropy

$$S := k_B \sum_{k=1}^{N} P_k \ln(1/P_k)$$

and the (internal) energy

$$U := \left\langle \Psi(t)\right|\hat{H}\left|\Psi(t)\right\rangle = \sum_{k=1}^{N} P_k E_k$$

3) What populations?

No way of imposing populations to a macroscopic system!

How to get predictions about a system if the populations are unknown?

The populations can be characterized only at the statistical level!

Statistical Ensemble for the populations

that is

Sample Space D + probability density $p(P)$ for the populations $P=(P_1,P_2,\cdots,P_N)$

Sample space: simplex in N dimensions $\left(\sum_{k=1}^{N} P_k = 1\right)$

Average of $f(P)$ on the Ensemble:

$$\langle f \rangle = \int_0^1 dP_1 \int_0^{1-P_1} dP_2 \cdots \int_0^{1-P_1\cdots-P_{N-2}} dP_{N-1} \left[f(P)\,p(P) \right]_{P_N=1-P_1\cdots-P_{N-1}}$$

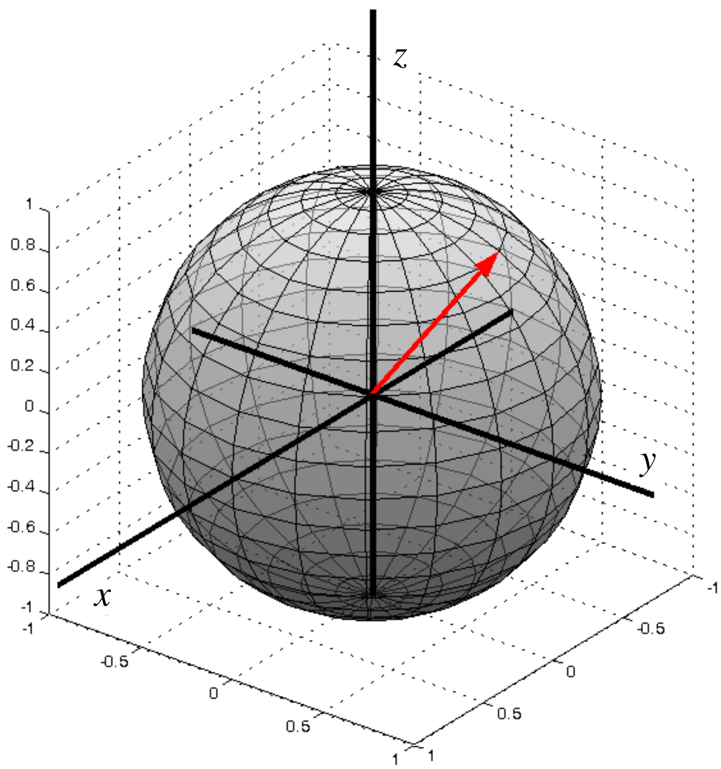
No a priori information on $p(P)$!

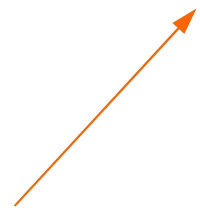
3) What populations?

From the lack of knowledge

$\Downarrow$

Random Pure State Ensemble (RPSE): homogeneous distribution of $|\Psi(0)\rangle$ on the unit sphere in $\mathcal{H}_N$





$= \quad |\Psi(0)\rangle$

$x, y, z \quad = \quad$ real or imaginary parts of $c_k(0)$

3) What populations?

From the (Euclidean) measure in $\mathcal{H}_N$: $p(P) = (N-1)!\,\delta\left(1 - \sum_{k=1}^{N} P_k\right)$

Note: RPSE is defined only in a finite dimensional Hilbert space

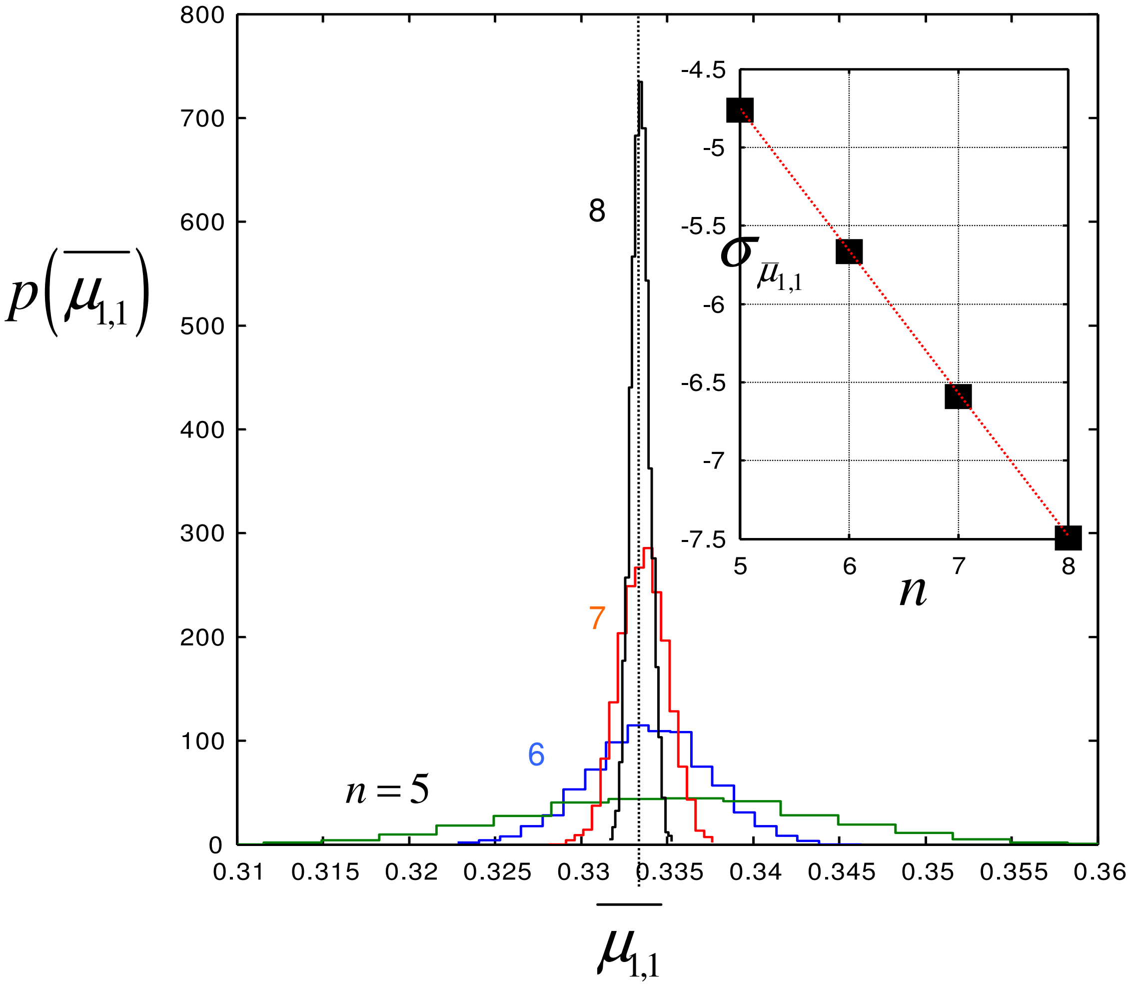
$$\Downarrow$$

necessity of the high energy cut-off $E_{\max}$

From $p(P)$: statistical sampling of the populations and of the system's (equilibrium) properties

3) What populations?

Example for randomly perturbed harmonic oscillators



$n =$ number of oscillators

$$\sigma_f = \sqrt{\left\langle \left(f - \langle f \rangle \right)^2 \right\rangle}$$

$= \text{variance of } f(P)$

3) What populations?

Different realizations of the system lead to different values of the equilibrium properties, in particular of the Entropy and of the Internal Energy

What a relation with Thermodynamical properties?

Note: standard microcanonical analysis corresponds to a specific choice of the populations

$$P_k^{\mu C} \begin{cases} = 1/N^{\mu C} & \text{for } E_{\min} < E_k \leq E_{\max} \\ = 0 & \text{otherwise} \end{cases}$$

4) Typicality

Concept of typicality from Information Theory.

$\mathcal{A}$ is a typical event in a broad meaning if

i) $\mathrm{Prob}\{\mathcal{A}\} = 1-\varepsilon$ with $\varepsilon << 1$, that is $\mathrm{Prob}\{\bar{\mathcal{A}}\} = \varepsilon$

Strong form of typicality if

ii) $\mathrm{Prob}\{\mathcal{A}\} = 1$

like the measure/probability of irrational numbers in the interval $[0,1]$

In our case:

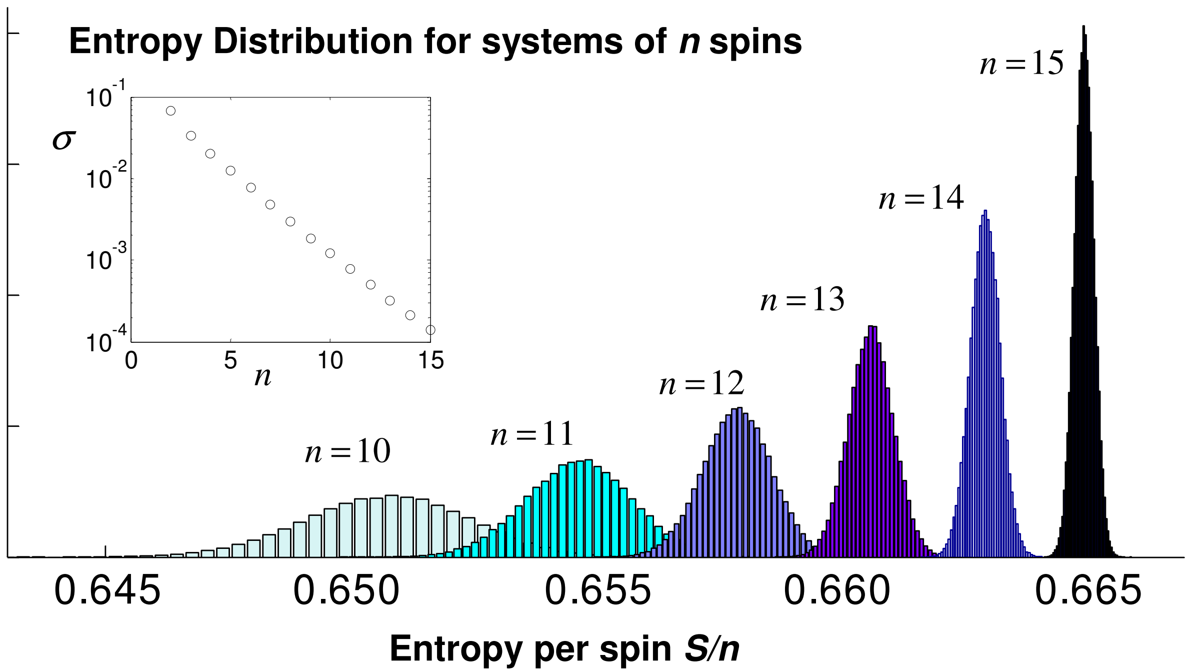
i) $\mathrm{Prob}\left\{\left|\bar{\mu}_{11} - \langle \bar{\mu}_{11} \rangle\right| \leq 2\sigma_{\bar{\mu}_{11}}\right\} \simeq 0.99$

ii) $\mathrm{Lim}_{n\to\infty} \mathrm{Prob}\left\{\left|\bar{\mu}_{11} - \langle \bar{\mu}_{11} \rangle\right| \leq K\right\} = 1 \;\; \forall\, K > 0$

Qualitatively speaking, the overwhelming majority of systems has a typical value of the property.

4) Typicality

The same behavior is found for the internal energy and the entropy



For large enough systems, the variability of populations does not influence substantially the observables which, then, can be identified with their Ensemble averages

$$\langle S \rangle \qquad \langle U \rangle \qquad \langle \bar{\mu} \rangle$$

5) Thermodynamics

Is the RPSE description consistent with the equilibrium thermodynamics of macroscopic system?

The answer is positive since, for a generic system characterized through its density of states $g(E)=\sum_k \delta(E-E_k)$

the following items are derived

a) Typicality in the thermodynamic limit (number of components $n \to \infty$) which allows the identification of the entropy ($\langle S \rangle$), of the internal energy ($\langle U \rangle$) and of the properties of a component trough $\langle \bar{\hat{\mu}} \rangle$

b) Entropy equation of state $\langle S \rangle = S(\langle U \rangle)$, by eliminating the dependence on the energy cut-off $E_{\max}$

$$\langle S \rangle = f(E_{\max}) \qquad \langle U \rangle = g(E_{\max}) \qquad \langle S \rangle = f(g^{-1}(\langle U \rangle))$$

5) Thermodynamics

c) Both $\langle S \rangle$ and $\langle U \rangle$ are extensive properties therefore the Temperature

$$\frac{1}{T} := \frac{d\langle S \rangle}{d\langle U \rangle}$$

is an intensive parameter

d) $\langle S \rangle = S(\langle U \rangle)$ is a convex increasing function of $\langle U \rangle$, therefore both $\langle S \rangle$ and $\langle U \rangle$ are increasing functions of the Temperature

e) The canonical form for the reduced density matrix of subsystem

$$\langle \bar{\mu} \rangle \propto \exp\left\{ -\hat{H}_{ss} / k_B T \right\} \qquad \hat{H}_{ss} : \text{Hamiltonian of the subsystem}$$

6) Conclusions

An open issue

1) There are other possible Statistical Ensembles for the populations.

In the past the Fixed Expectation Energy Ensemble (FEEE) having the constraint $<\Psi|\hat{H}|\Psi>=E=$constant, has been proposed as the quantum counterpart of the classical microcanonical statistical mechanics.

2) Consistency with Thermodinamics, points a) to e), as the main criterion of choice between Ensembles.

As a matter of fact, FEEE does not satisfy conditions d) and e)!

3) Further conditions to be satisfied?

1 spin + 9 spins

Switch on the interaction Hamiltonian

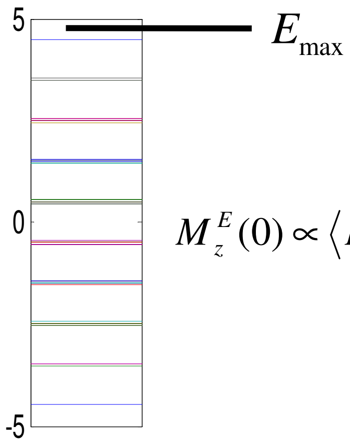
$$H = H_1 + H_E + \lambda H_{SE}$$

Solve the Schrödinger equation

$$\psi_S(0) = |\beta\rangle \qquad \psi_E(0) = \sum_{k=1}^{k_{\max}} \sqrt{P_k} e^{i\alpha_k} |M\rangle$$

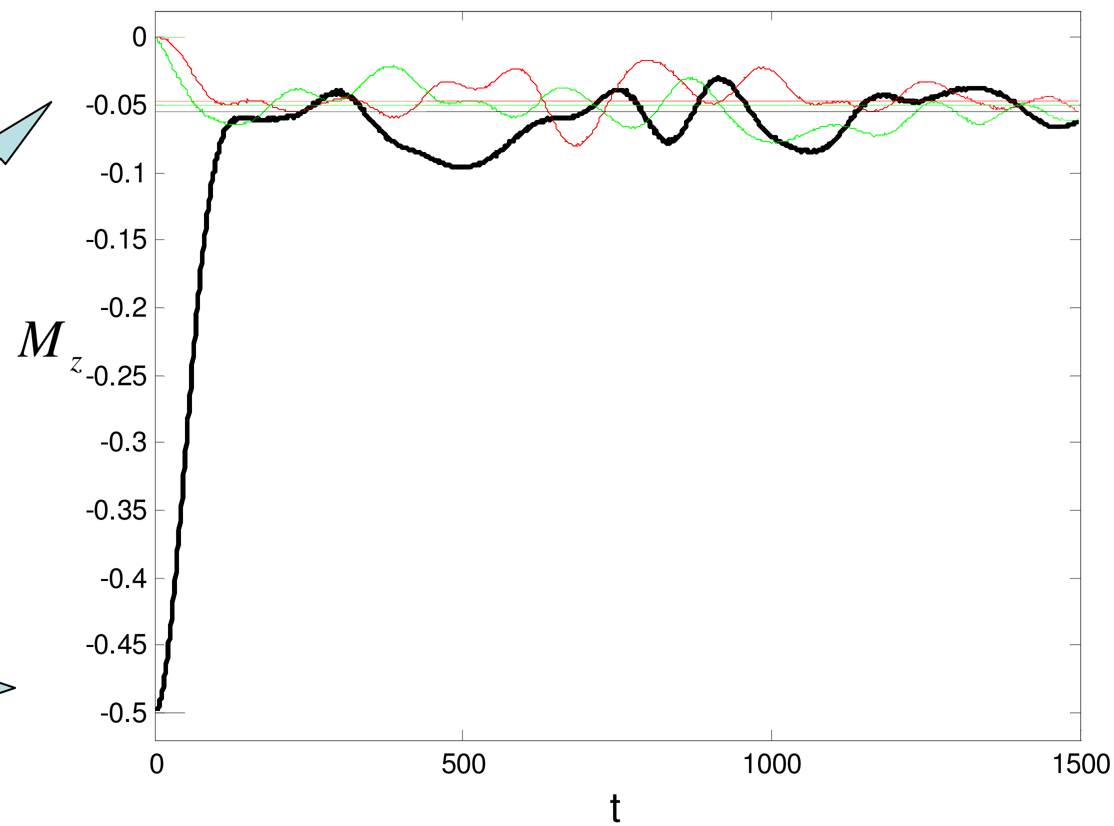
$$\psi(0) = \psi_S(0) \otimes \psi_E(0)$$

$\psi_E(0)$ from RPSE



$$M_z^E(0) \propto \langle H_E \rangle = 0$$

$$M_z(0) \propto \langle H_S \rangle =$$
$$= Tr\left(S_Z \mu(0)\right) = -0.5$$

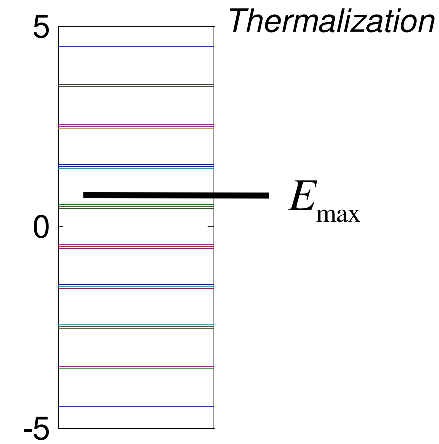


$$\psi_S(0) = \sqrt{0.34}e^{i\alpha_1}\left|\beta\right\rangle + \sqrt{0.66}e^{i\alpha_2}\left|\alpha\right\rangle$$

$$M_z^S(0) \propto \left\langle H_S \right\rangle = 0.16$$

$\psi_E(0)$ from RPSE

$$M_z^E(0) \propto \left\langle H_E \right\rangle = -0.66$$



✓ One observes relaxation toward
a well defined equilibrium state
(i.e. within the statistical uncertainty due to the finiteness of the system)

✓ The equilibrium state depends
only on the total energy of the system,
not on the initial state and equipartition of the energy is observed