Quantum Large Deviations

joint work with Wojciech De Roeck and Karel Netočný

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Quantum Mathematics 10
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Two very related problems

how to count in quantum...

- 1. Establishing a microcanonical ensemble with different *noncommuting* constraints — what is a macro-state and how to study (joint) macroscopic fluctuations:
  CONFIGURATIONAL ENTROPY ?
  - equivalence with canonical framework...
  - H-theorem...

- 2. LARGE DEVIATIONS and fluctuation theory
  - equilibrium set-up...
  - nonequilibrium fluctuations...

Two very related problems

WHY DO YOU ASK?

- 1. Elements of statistical mechanics:
  - relation between fluctuation functionals and thermodynamic potentials
  - counting interpretation of entropy appears relevant for quantum information theory and for microscopic understanding of the second law.
- 2. Fluctuations in small systems:
  - quantum transport and counting statistics
  - effects of nonlocality/entanglement

Quantum macrostates

Commutative case

On a sequence of finite-dimensional Hilbert spaces $(\mathcal{H}^N)_{N\uparrow+\infty}$ consider a uniformly bounded family of observables

$$X^N = (X_1^N, \dots, X_K^N)\,, \qquad N \uparrow +\infty$$

(think of a collection of different empirical averages)

To each X_k^N assign its projection-valued measure $\mathcal{Q}_k^N$

If they mutually commute then each collection $x = (x_1, \dots, x_K)$ is associated with the projection

$$\mathcal{Q}^{N,\delta}(x) = \prod_{k=1}^{K} \mathcal{Q}_k^{N,\delta}(x) = \prod_{k=1}^{K} \int_{x_k-\delta}^{x_k+\delta} \mathcal{Q}_k^N(\mathrm{d}z_k)$$

$\longrightarrow$ quantum microcanonical ensemble

(Boltzmann-von Neumann; microcanonical) entropy function:

$$S^{N,\delta}(x) = \log \mathrm{Tr}(\mathcal{Q}^{N,\delta}(x))$$

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Von Neumann '55:
"It is a fundamental fact with macroscopic measurements that everything which is measurable at all, is also simultaneously measurable, i.e. that all questions which can be answered separately can also be answered simultaneously."

YET, while indeed averages $A = (a_1 + \ldots + a_N)/N, B = (b_1 + \ldots + b_N)/N$, for which all commutators $[a_i, b_j] = 0$ for $i \neq j$, have their commutator $[A, B] = O(1/N)$ going to zero (in the appropriate norm, corresponding to $[a_i, b_i] = O(1)$) as $N \uparrow +\infty$, it is not true in general that

$$\lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}[e^{NA}\, e^{NB}] \stackrel{?}{=} \lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}[e^{NA+NB}]$$

These generating functions are obviously important in quantum fluctuation theory...

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General case

Idea: Find a largest projection that "well approximates" each projection $\mathcal{Q}_k^{N,\delta}$, $k = 1, \ldots, K$

Def. 1. A sequence of projections $(\mathcal{P}^N)_{N\uparrow+\infty}$ is concentrating at x whenever for all $k = 1, \ldots, K$ and $\delta > 0$,

$$\lim_{N\uparrow+\infty} \frac{\mathrm{Tr}(\mathcal{P}^N \mathcal{Q}_k^{N,\delta}(x))}{\mathrm{Tr}(\mathcal{P}^N)} = 1$$

Then write $\mathcal{P}^N \to x$.

Def. 2. To any macrostate x assign the entropy function

$$s(x) = \limsup_{\mathcal{P}^N \to x} \frac{1}{N} \log \mathrm{Tr}(\mathcal{P}^N)$$

Def. 3. A sequence $\mathcal{P}^N \to x$ is called typical sequence concentrating at x iff

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General case

$\mathrm{Tr}(\mathcal{P}^N)$ along a maximal concentrating sequence $\mathcal{P}^N$ plays the role of "probability",
the entropy $s(x)$ is its well-defined rate function.

Three immediate QUESTIONS:
1. Is there an IDENTITY WITH THE CANONICAL von Neumann ENTROPY, defined for any state $\omega_N(\,\cdot\,) = \mathrm{Tr}(\sigma_N\,\cdot\,)$ as

$$H(\omega_N) = -\mathrm{Tr}(\sigma_N \log \sigma_N)$$

2. Is there an H-THEOREM? Is it a Lyapounov function?
3. Are there nontrivial EXAMPLES?

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Quantum macrostates

Generating functions and canonical ensemble

Consider the following generating functions:

$$p(\lambda) = \lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}(\exp N \sum_k \lambda_k X_k^N)$$

$$q_k(\kappa) = \lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}(\exp N \sum_k \lambda_k X_k^N \; \exp \kappa N X_k^N)\,, \qquad k = 1, \ldots, K$$

Remarks:

- $p(\lambda)$ is the "canonical pressure"

$$\omega_\lambda^N(\,\cdot\,) = \mathrm{Tr}(\sigma_\lambda^N \cdot\,) = \frac{1}{\mathcal{Z}_\lambda^N} \mathrm{Tr}(\exp N \sum_k \lambda_k X_k^N \cdot\,)$$

  parameterized by $\lambda = (\lambda_1, \ldots, \lambda_K)$
- $q_k(\kappa)$ is the large deviation generating function for the single observable X_k^N
- In general:

$$q_k(\kappa) \geq p(\lambda + (0, \ldots, (\kappa)_k, \ldots))$$

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Quantum macrostates

General case

Theorem (De Roeck, Maes, Netočný, '06). Assume that

1. $p(\lambda)$ exists and has the derivative

$$\frac{\mathrm{d}p(\kappa\lambda)}{\mathrm{d}\kappa}\Big|_{\kappa=1} = \sum_{k=1}^{K} \lambda_k x_k$$

2. $q_k(\kappa)$ exists and has the derivative

$$\frac{\mathrm{d}q_k(\kappa)}{\mathrm{d}\kappa}\Big|_{\kappa=0} = x_k$$

   for all $k = 1, \ldots, K$

Then,

$$s(x) = p(\lambda) - \sum_{k=1}^{K} \lambda_k x_k$$

Quantum macrostates

Conclusions

There are various ways how to read the above result:

(1) Note that

$$p(\lambda) - \sum_{k=1}^{K} \lambda_k x_k = \lim_{N\uparrow+\infty} \frac{H(\omega_\lambda^N)}{N}$$

is the von Neumann entropy of the (sequence of) canonical states ω_λ^N

$\longrightarrow$ the theorem is an equivalence of ensembles result

$\longrightarrow$ the von Neumann entropy gets a "counting" interpretation

Quantum macrostates

Conclusions

There are various ways how to read the above result:

(2) Under slightly stronger conditions, also

$$s(x) = \inf_{\lambda}\{p(\lambda) - \sum_k \lambda_k x_k\}$$

and the result is a noncommutative version of the Gärtner-Ellis theorem (but only under the trace state.)

LARGE DEVIATIONS

Product states

Take a matrix algebra M and consider

- the algebra of N copies: $\mathcal{U}_N = \otimes_{i=1}^N M_i$
- the product state $\omega_N = \otimes_{i=1}^N \omega_i$ where ω_i are copies of a faithful state on M

Take a self-adjoint matrix $X = X^* \in M$ and its empirical averages

$$\bar{X}_N = \frac{1}{N} \sum_{i=1}^{N} X_i$$

Question:

What is the *law* of large fluctuations of $\bar{X}_N$ over the states ω_N for large N?

Various answers, depending on the precise formulation!

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Large Deviations for Product states

Answer 1:
Spectral theorem: there is a probability measure μ_N on $\mathrm{sp}(\bar{X}_N) \subset [-\|X\|, \|X\|]$ such that

$$\omega_N(F(\bar{X}_N)) = \int \mu_N(\mathrm{d}\bar{x})\, F(\bar{x})\,, \qquad F \in C([-\|X\|, \|X\|])$$

- μ_N is physically the distribution of outcomes when measuring $\bar{X}_N$ (von Neumann measurement)
- Explicitly: for any $D \subset \mathbb{R}$ a Borel set

$$\mu_N(D) = \omega_N(\bar{\mathcal{Q}}_N(D))$$

$$= \sum_{x_1,\dots,x_N \in \mathrm{sp}(X)} \omega(\mathcal{Q}(x_1)) \dots \omega(\mathcal{Q}(x_N))\, \chi\Big(\frac{1}{N}\sum_{i=1}^{N} x_i \in D\Big)$$

where $\mathcal{Q}$ is the projection-valued measure for X and $\bar{\mathcal{Q}}_N$ the projection-valued measure for $\bar{X}_N$

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Large Deviations for Product states

Since μ_N satisfy large deviations, we have that

$$\limsup_{N\uparrow+\infty} \frac{1}{N} \log \omega_N(\bar{\mathcal{Q}}_N(D)) \le -\inf_{\bar{x}\in D} I(\bar{x}) \quad \text{for } D \text{ closed}$$

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or, equivalently, for any $-\|X\| < \bar{x} < \|X\|$,

$$\lim_{\delta\downarrow 0} \lim_{N\uparrow+\infty} \frac{1}{N} \log \omega_N(\bar{\mathcal{Q}}_N(\bar{x}-\delta, \bar{x}+\delta)) = -I(\bar{x})$$

with the rate function

$$I(\bar{x}) = \sup_t \{t\bar{x} - q(t)\}$$

$$q(t) = \lim_{N\uparrow+\infty} \frac{1}{N} \log \mu_N(e^{tN\bar{x}}) = \log \omega(e^{tX})$$

Large Deviations for Product states

Remarks:

- Note that the spectral theorem was essential here
- A *naive* attempt to repeat Cramer's lifting on the level of quantum states ω_N fails:

One might be tempted to look for a modification of the state $\omega(\,\cdot\,) = \mathrm{Tr}(e^A \,\cdot\,)$ to

$$\omega^t(\,\cdot\,) = \frac{\mathrm{Tr}(e^{A+tX}\,\cdot\,)}{\mathrm{Tr}(e^{A+tX})}$$

which makes a fixed $\bar{x}$ "typical", i.e., $\omega^t(X) = \bar{x}$
However, the heuristics

$$\omega_N(\bar{\mathcal{Q}}(\bar{x}-\delta, \bar{x}+\delta)) \simeq \left(\mathrm{Tr}(e^{A+tX})\right)^N e^{-t\bar{x}N} \underbrace{\omega_N^t(\bar{\mathcal{Q}}(\bar{x}-\delta, \bar{x}+\delta))}_{\simeq 1}$$

only works when A and X commute!

Large Deviations for Product states

Hence, the *candidate* generating function

$$\hat{q}(t) = \log \mathrm{Tr}(e^{A+tX})$$

does generally not determine the statistics of large fluctuations!
By the Golden-Thompson inequality, $\hat{q}(t) \leq q(t)$.

Large deviations for Product states

Answer 2:
Study the asymptotics of Laplace-Varadhan type:

$$\lim_{N\uparrow+\infty}\frac{1}{N}\log\operatorname{Tr}\Big(\exp\frac{1}{K}\sum_{i=1}^{N}A_i\;\exp\frac{N}{K}G(\bar{X}_N)\Big)^K$$

for various $K>0$ and $G\in C(\mathbb{R})$

- $K=1$ corresponds to the Varadhan formula over the measures μ_N:

$$\begin{aligned}\lim_{N\uparrow+\infty}\frac{1}{N}\log\omega_N\big(e^{N\,G(\bar{X}_N)}\big)\\ &=\lim_{N\uparrow+\infty}\frac{1}{N}\log\int\mu_N(\mathrm{d}\bar{x})\,e^{N\,G(\bar{x})}\\ &=\sup_{\bar{x}}\{G(\bar{x})-I(\bar{x})\}\end{aligned}$$

Large Deviations for Product states

- $K = +\infty$ corresponds to the problem

$$\lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}\Big(\exp \sum_{i=1}^{N} A_i + N\, G(\bar{X}_N)\Big)$$

(by Trotter product formula)

Theorem (Petz, Raggio, Verbeure '89).

$$\lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}\Big(\exp \sum_{i=1}^{N} A_i + N\, G(\bar{X}_N)\Big) = \sup_{\bar{x}}\{G(\bar{x}) - \hat{I}(\bar{x})\}$$

where

$$\hat{I}(\bar{x}) = \sup_{\bar{t}}\{t\bar{x} - \hat{q}(t)\}$$

The case $K = +\infty$ is very different from $K = 1$ since the former cannot be rephrased as a classical Varadhan formula upon a classical probability model!

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OUR NEW RESULTS

generalizations beyond product states

Large deviation and central limit results can be generalized in the following ways:

- Instead of product states one can consider KMS (= equilibrium) states of quantum spin lattice systems in the regimes of
  - high temperature
  - low temperature with a unique ground state and “unbiased” observables
- The method uses that the projected state on the observable’s subspace is a classical GIBBS measure. That is related to finite entanglement length.

Classical lattice spin models

Set up

- Space. $\mathbb{Z}^d$ a regular lattice, $d = 1, 2, \ldots$
- Configurations. $\Omega = \times_{i \in \mathcal{L}} \Omega_i$ where Ω_i is a finite set of "spins" at site i
- Potential. $\Phi = (\Phi(A))_{A \subset\subset \mathbb{Z}^d}$ where $\Phi(A, \cdot) : \Omega_A \mapsto \mathbb{R}$ are interactions
  - Summability condition:
  $$\sup_i \sum_{A \ni i} \|\Phi(A)\| < +\infty$$
  - Local Hamiltonians
  $$H_\Lambda(\eta) = \sum_{A \subset \Lambda} \Phi(A, \eta_A)$$
  - Local Gibbs states
  $$\mu_\Lambda^\beta(\eta) = \frac{1}{\mathcal{Z}_\Lambda^\beta} e^{-\beta H_\Lambda(\eta)} \qquad \mathcal{Z}_\Lambda^\beta = \sum_{\eta \in \Omega_\Lambda} e^{-\beta H_\Lambda(\eta)}$$

Classical lattice spin models

DLR theory

- Thermodynamic limit. Define μ^β as the weak limit (provided it exists) $\mu^\beta = \lim_\Lambda \mu^\beta_\Lambda$
  - often sufficient but not always!
- general definition of Gibbs states:
  - Relative Hamiltonians:

$$H_\Lambda(x_\Lambda \,|\, x_{\Lambda^c}) = \sum_{A \cap \Lambda \neq 0} \Phi(A, x_A)$$

  - DLR equations: for all finite Λ and μ^β−almost surely

$$\mu^\beta(x_\Lambda \,|\, x_{\Lambda^c}) = \frac{1}{\mathcal{Z}^\beta_\Lambda(x_{\Lambda^c})} e^{-\beta H_\Lambda(x_\Lambda \,|\, x_{\Lambda^c})}$$

$$\mathcal{Z}^\beta_\Lambda(x_{\Lambda^c}) = \sum_{x_\Lambda \in \Omega_\Lambda} e^{-\beta H_\Lambda(x_\Lambda \,|\, x_{\Lambda^c})}$$

- turn the logic around: a measure μ on $\Omega_{\mathbb{Z}^d}$ is Gibbs whenever it satisfies the DLR equations with some summable potential Φ

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Gibbs $\Longrightarrow$ LD $\Longrightarrow$ CLT

Theorem (Lanford, Olla,... ; simplified to level−1). If μ is a translation-invariant Gibbs measure and $F : \Omega_A \mapsto \mathbb{R}$, $A \subset\subset \mathbb{Z}^d$ a local observable, then the empirical average

$$F_\Lambda(\,\cdot\,) = \frac{1}{|\Lambda|} \sum_{i:\, i+A \subset \Lambda} F(\tau_i \,\cdot\,)$$

satisfies the large deviation principle with rate function

$$I^F(\bar{x}) = \sup_t \{t\bar{x} - q^F(t)\}$$

$$q^F(t) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \int \mathrm{d}\mu(x_\Lambda)\, e^{t|\Lambda| F_\Lambda(x_\Lambda)}$$

Note 1:
This goes beyond the Gärtner-Ellis theorem because q^F does not have to be differentiable (in phase transitions)!

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Note 2:
The generating function is (set $\beta = 1$)

$$q^F(t) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \frac{1}{\mathcal{Z}_\Lambda} \sum_{x_\Lambda \in \Omega_\Lambda} \exp -H_\Lambda(x_\Lambda) + t \sum_{i:\, i+A \subset \Lambda} F(x_\Lambda)$$
$$= P^\Phi(t) - P^\Phi$$

$P^\Phi(t)$ is the "pressure" of a modified potential!
$\Longrightarrow$ the link between LD and thermodynamic potentials

Gibbs $\Longrightarrow$ LD $\Longrightarrow$ CLT

Theorem (Bryc, '93). If the generating function $q^F(t)$ is analytic on a neighborhood of $t = 0$ then

$$W_\Lambda(x_\Lambda) = \frac{1}{\sqrt{|\Lambda|}} \sum_{i:\, i+A\subset\Lambda} \left[F(\tau_i x_\Lambda) - \int \mathrm{d}\mu(x_\Lambda)\, F(x_\Lambda)\right]$$

has the limit

$$\lim_{\Lambda\uparrow\mathbb{Z}^d} \int \mathrm{d}\mu(x_\Lambda)\, e^{itW_\Lambda(x_\Lambda)} = e^{-\frac{t^2\sigma^2}{2}}, \qquad \sigma^2 \geq 0$$

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Quantum lattice spin models

- Observables. M a finite-dimensional matrix algebra $\longrightarrow$ local algebras $\mathcal{U}_\Lambda = \otimes_{i\in\Lambda} M_i$, $\Lambda \subset\subset \mathbb{Z}^d$
- Potential. $\Phi = (\Phi_A)_{A\subset\subset\mathbb{Z}^d}$ a family of self-adjoint elements $\Phi(A) = \Phi(A)^* \in \mathcal{U}_A$
  - Local Hamiltonians

$$H_\Lambda = \sum_{A\subset\Lambda} \Phi(A)$$

  Local Gibbs states

$$\omega_\Lambda^\beta(\,\cdot\,) = \frac{1}{\mathcal{Z}_\Lambda^\beta} \mathrm{Tr}_\Lambda(e^{-\beta H_\Lambda}\,\cdot\,)\,, \qquad \mathcal{Z}_\Lambda^\beta = \mathrm{Tr}_\Lambda(e^{-\beta H_\Lambda})$$

- Thermodynamic limit. The weak limit $\omega^\beta = \lim_\Lambda \omega_\Lambda^\beta$ ($\longrightarrow$ general formalism of quantum Gibbs and KMS states)

Quantum high temperature $\Longrightarrow$ classical Gibbs

Given $X = X^* \in M$ with $\mathcal{Q}$ its projection-valued measure

- the family $(X_i)_{i\in\mathbb{Z}^d}$ of copies over $\mathbb{Z}^d$ has the common projection-valued measure

$$\mathcal{Q}_\Lambda(x_\Lambda) = \otimes_{i\in\mathbb{Z}^d}\mathcal{Q}_i(x_i)\,, \qquad x_\Lambda \in \Omega_\Lambda \equiv (\mathrm{sp}(X))^\Lambda$$

- there is the probability measure $\mu^{\beta,X}$ given on cylindric sets by

$$\mu^{\beta,X}(x_\Lambda) = \omega^\beta(\mathcal{Q}_\Lambda(x_\Lambda))$$

Theorem (De Roeck, Maes, Netočný). Let for some $\epsilon > 0$

$$\|\Phi\|_\epsilon \equiv \sup_i \sum_{A\ni i} e^{\epsilon|A|}\,\|\Phi(A)\| < +\infty$$

There there exists $\beta_0 > 0$ such that for all $|\beta| \leq \beta_0$ and for all $X = X^* \in M$, the measure $\mu^{\beta,X}$ is Gibbs.

Moreover, there is an effective potential $\Psi^{\beta,X}$ for $\mu^{\beta,X}$ such that any $\Psi^{\beta,X}(A,\cdot\,)$ is analytic in $|\beta| < \beta_0$.

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Quantum high temperature $\Longrightarrow$ classical Gibbs

In particular, one obtains the large deviation property for the empirical average

$$\bar{X}_\Lambda = \frac{1}{|\Lambda|} \sum_{i \in \Lambda} X_i$$

with the real analytic generating function

$$q(t) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \omega^\beta \left(\exp t \sum_{i \in \Lambda} X_i\right)$$

Remember:

- That $q(t)$ is not a pressure of a modified quantum systems $\longrightarrow$ it is generally difficult to prove both its existence and its smoothness!
- It is however a pressure of the modified effective classical system with the Hamiltonian

$$H_\Lambda^{\beta,X,t}(x_\Lambda) = \sum_{A \subset \Lambda} \Psi^{\beta,X}(A, x_A) + t \sum_{i \in \Lambda} x_i$$

Some related results

- *Goderis, Verbeure, Vets ‘89:* Fluctuation algebra (= CLT formalism for several observables)
- *Lebowitz, Lenci, Spohn ‘99:* LD for particle density in noninteracting quantum gases
- *Gallavotti, Lebowitz, Mastropietro ‘02:* extension for weakly interacting quantum gases
- *Netočný, Redig ‘04:* existence and real analyticity of $q(t)$ at high temperatures
- *Lenci, Rey Bellet ‘04:* existence of $q(t)$ at high temperatures
- *Abou Salem ‘07:* extension to nonequilibrium steady states
- *Hiai, Mosonyi, Ohno, Petz ’07:* free energy density for mean field perturbations of one-dimensional spin chains
- *I. Bjelakovic, J.-D. Deuschel, T. Krueger, R. Seiler, Ra. Siegmund-Schultze, A. Szkola ’07:* Sanov large deviations

Some related results

Moreover:
For general empirical averages with some $F \in \mathcal{U}_A$, $A \subset\subset \mathbb{Z}^d$,

$$F_\Lambda = \frac{1}{|\Lambda|} \sum_{i:\, i+A \subset \Lambda} \tau_i(F)$$

no associate (classical) Gibbs measure exists unless $[\tau_i(F), \tau_j(F)] = 0$, yet

- one can prove $q^F(t)$ to exist and to be analytic in a neighborhood of $t = 0$
  (NR‘04, A-S‘07 – analyticity, LR‘04 – existence)
- but no proof of existence of $q^F(t)$ for all $t \in \mathbb{R}$ is known!

Quantum Laplace-Varadhan formula

Theorem (De Roeck, Maes, Netočný). Let for some $\epsilon > 0$

$$\|\Phi\|_\epsilon \equiv \sup_i \sum_{A \ni i} e^{\epsilon |A|} \, \|\Phi(A)\| < +\infty$$

There there exists $\beta_0 > 0$ such that for all $|\beta| \leq \beta_0$, for all $X = X^* \in M$, and for all $G \in C([-\|X\|, \|X\|])$ concave,

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \frac{1}{\mathcal{Z}^\beta} \operatorname{Tr}\left(e^{-\beta H_\Lambda + |\Lambda| G(\bar{X}_\Lambda)}\right) = \sup_{-\|X\| < u < \|X\|} \{G(u) - \hat{I}(u)\}$$

where

$$\hat{I}(u) = \sup_t \{tu - \hat{q}(t)\}$$

$$\hat{q}(t) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \frac{1}{\mathcal{Z}^\beta} \operatorname{Tr}\left(\exp -\beta H_\Lambda + t \sum_{i \in \Lambda} X_i\right)$$

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Strategy of the equivalence-proof and related results

The proof consists of the next two steps:

Step 1.

$p(\kappa\lambda)$ differentiable at $\kappa = 1$

$\Longrightarrow$ the projection-valued measure $\bar{\mathcal{Q}}^N$ for $\sum_k \lambda_k X_k^N$ satisfies

$$\int_{\lambda^k x_k - \delta}^{\lambda^k x_k + \delta} \omega_\lambda^N(\bar{\mathcal{Q}}^N(\mathrm{d}z)) \geq 1 - e^{-\bar{C}(\delta)N}\,, \quad \bar{C}(\delta) > 0$$

$\Longrightarrow$ there is sequence $\delta_N \downarrow 0$ such that

$$\mathcal{P}^N := \int_{\lambda^k x_k - \delta_N}^{\lambda^k x_k + \delta_N} \bar{\mathcal{Q}}^N(\mathrm{d}z)$$

satisfies

- $\lim_{N\uparrow+\infty} \omega_\lambda^N(\mathcal{P}^N) = 1$
- $\lim_{N\uparrow+\infty} \frac{1}{N} \log \mathrm{Tr}_N(\mathcal{P}^N) = \lim_{N\uparrow+\infty} \frac{1}{N} H(\omega_\lambda^N)$

Strategy of the proof and related results

This is a special case of quantum Shannon-McMillan theorem

For a more general result of this type, see:

- *Bjelaković, Krüger, Siegmund-Schultze, Szkoła '04*

See also

- *Bjelaković, Deuschel, Krüger, Seiler, Siegmund-Schultze, Szkoła '05:* quantum Sanov theorem

Strategy of the proof and related results

The proof consists of the next two steps:

Step 2.
$q_k(\kappa)$ differentiable at $\kappa = 0$
$\Longrightarrow$ the projection-valued measure $\mathcal{Q}_k^N$ for X_k^N satisfies

$$\omega_\lambda^N(\mathcal{Q}_k^{N,\delta}(x_k)) \geq 1 - e^{-C_k(\delta)N}, \quad C_k(\delta) > 0$$

$\Longrightarrow$

$$\frac{\mathrm{Tr}_N(\mathcal{P}^N \mathcal{Q}_k^{N,\delta}(x_k))}{\mathrm{Tr}_N(\mathcal{P}^N)} \geq 1 - e^{-C_k'(\delta)N}, \quad C_k(\delta) > C_k'(\delta) > 0$$

$\Longrightarrow$ $\mathcal{P}^N$ is exponentially concentrating at x

What is a current fluctuation?

Imagine reservoirs in thermal equilibrium at inverse temperatures β_k with composite system described by

$$H_\lambda = H + \sum_{k\in K} H_k + \lambda \sum_{k\in K} \mathrm{H}_{Sk},$$

Initial state represented by density matrix ρ_0 of the form

$$\rho_0 = \rho \otimes \left[\bigotimes_{k\in K} \rho_{k,\beta_k} \right]$$

where the states ρ_{k,β_k} are equilibrium states at β_k on the k'th reservoir, and ρ is an arbitrary density matrix on the system.
QUESTION:
how much energy has flown out of/into the different reservoirs after some time t.

What is a current fluctuation?

Answer 1 Introduce "current operator"

$$I_k(t) := -\imath U^\lambda_{-t}[H_\lambda, H_k]U^\lambda_t$$

where $U^\lambda_t := \exp -\imath t H_\lambda$ generated by the total Hamiltonian H_λ and H_k is the free Hamiltonian of the k'th reservoir only.
Obviously,

$$U^\lambda_{-t} H_k U^\lambda_t - H_k = \int_0^t ds\, I_k(s)$$

Therefore heat fluctuations

$$\rho_0 \left[\exp -\imath \sum_k \kappa_k \left(U^\lambda_{-t} H_k U^\lambda_t - H_k \right) \right]$$

but not at all clear whether the operator associated to the "change of energy in the $k-$th reservoir" should really be given by that: $U^\lambda_{-t} H_k U^\lambda_t$ does not in general commute with H_k, hence their difference does not have a clear physical meaning.

What is a current fluctuation?

Answer 2 Assume for simplicity that $(H_k)_{k\in K}$ have discrete spectrum, indicating that we have not taken the thermodynamic limit and let $x \in X$ label a complete set of eigenvectors $|x\rangle$ of $(H_k)_{k\in K}$ with nondegenerate eigenvalues $(H_k)_{k\in K}(x)$. The corresponding spectral projections are denoted $P_x := |x\rangle\langle x|$.

$$\chi(\kappa, t, \lambda, \rho_0) := \sum_{x,y\in X} \mathrm{Tr}\left[P_y U_t^\lambda P_x \rho_0 P_x U_{-t}^\lambda P_y\right] \exp -\imath \sum_{k\in\mathcal{K}} \kappa_k \left(H_k(y) - H_k(x)\right)$$

Measure (thereby projecting the reservoirs on the eigenstates x), then switch on the time evolution U_t^λ, finally measure again (projecting on the eigenstates y).
Use that the initial state ρ_0 is diagonal in the basis $|x\rangle$ to rewrite

$$\chi(\kappa, t, \lambda, \rho_0) = \rho_0 \left[\exp -\imath \sum_{k\in\mathcal{K}} \kappa_k H_k U_t^\lambda \left(\exp \imath \sum_{k\in\mathcal{K}} \kappa_k H_k\right) U_{-t}^\lambda\right].$$

What is a current fluctuation?

References:
J. Derezinski, C. Maes and W. De Roeck: Fluctuations of Quantum Currents and Unravelings of Master Equations. arXiv:cond-mat/0703594.
W. De Roeck: Large deviations for currents in the spin-boson model. arXiv:0704.3400.
J. Derezinski, W. De Roeck: Reduced and Extended Weak Coupling Limit, arXiv:0704.066.
J. Derezinski, W. De Roeck: Extended Weak Coupling Limit for Pauli-Fierz Operators, arXiv:math-ph/0610054, to appear in Comm. Math. Phys.
W. De Roeck and C. Maes: Steady state fluctuations of the dissipated heat for a quantum stochastic model, Reviews in Mathematical Physics **18**, 619–653 (2006).
W. De Roeck and C. Maes: A quantum version of free energy - irreversible work relations, Phys. Rev. E **69**, 26115 (2004).

Conclusions

- For a high-temperature quantum lattice system we have constructed an effective Gibbs measure for a classical subsystem, which yields large deviations and CLT for a single observable
- As an alternative approach to quantum large deviations, we have extended the quantum Laplace-Varadhan formula of Petz, Raggio, and Verbeure to the same high-temperature regime
- Similar results can be obtained for other perturbative regimes, e.g., at low temperatures with a unique ground state
- We have discussed one approach to the problem of joint large deviations for noncommuting observables based on the construction of a generalized microcanonical ensemble; an extension from trace state to a general state remains to be understood