Large Deviations in Quantum Spin Systems

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Goals:

Classically thermodynamic formalism (i.e. pressure, entropy, variational principle) is intimately linked with large deviations of macroscopic observables.

Do we have the same connection in quantum systems?

Problems:

• No quantum equivalent of empirical measures.

• Non-commutativity.

• Lack of understanding of basic properties of quantum states (Even Bulk/boundary estimates !)

• No formulation of proper quantum, non-commutative large deviations.

Today's program

1) A quantum version of Laplace-Varadhan Lemma

or more precisely

a variational principle for spin systems with short range and mean-field interactions (with De Roeck, Maes, Netockny). Published in RMP 2010

2) Large deviations in quantum spin systems via Ruelle-Lanford functions (with Ogata). Published in RMP 2011

Laplace-Varadhan

Suppose the sequence of measures μ_n satisfies a large deviation principle, on the scale v_n with rate function $I(x)$, i.e.

$$\mu_n(A) \asymp \exp\left(-v_n \inf_{x \in A} I(x)\right)$$

then the Laplace-Varadhan Lemma tells us that for G continuous and bounded

$$\lim_{n\to\infty} \frac{1}{v_n} \log \int \exp\left(v_n G(x)\right) d\mu_n(x) = \sup_x \left\{G(x) - I(x)\right\} .$$

Quantum Lattice Systems

• Lattice $\mathbf{Z}^d$, write $\Lambda \subset \mathbf{Z}^d$ for finite box (cube), and $\Lambda \nearrow \mathbf{Z}^d$ means limit taken along a increasing sequence of cubes.

• Hilbert space: At each lattice site there is a finite level quantum system (a spin) with finite dimensional Hilbert space $\mathcal{H}_x \cong \mathbf{C}^N$.

For $\Lambda \subset \mathbf{Z}^d$ the Hilbert space is $\mathcal{H}_\Lambda = \otimes_{x\in\Lambda}\mathcal{H}_x$

• Observable algebras: For a finite volume Λ

$$\mathcal{O}_\Lambda = \mathcal{B}(\mathcal{H}_\Lambda) = \{A : \mathcal{H}_\Lambda \to \mathcal{H}_\Lambda, \text{linear}\}$$

and there is a natural inclusion $\mathcal{O}_\Lambda \subset \mathcal{O}'_\Lambda$ for $\Lambda \subset \Lambda'$.

The algebra of observable for the infinite system is the C^*-algebra

$$\mathcal{O} = \overline{\cup_\Lambda \mathcal{O}_\Lambda}$$

• Interactions and Hamiltonians The interactions between the spins is specified by the collection

$$\Phi = \{\phi_X \;\; X \subset \mathbf{Z}^d \text{ finite}\}$$

where $\phi_X = \phi_X^*$ describes the multi-body interactions for spins in X and we will always assume that ϕ_X is translation invariant.

Finite-volume Hamiltonians

$$H_\Lambda = \sum_{X \subset \Lambda} \phi_X \qquad \text{free boundary conditions}$$

and one assumes, for example, that

$$\|\Phi\| = \sum_{X \in x} |X|^{-1} \|\phi_X\| < \infty$$

(i.e., the energy per site is bounded).

For example we can assume finite range interactions, $\phi_X = 0$ if diam$(X) > R$.

The variational principle

Let ω be a translation invariant state for the infinite system ($=$ positive normalized linear functional on $\mathcal{O}$) and write ω_Λ for the restriction of ω to $\mathcal{O}_\Lambda$

Facts: The following limits exist

Specific entropy $s(\omega) = \lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} S(\omega_\Lambda)$

Specific energy $e_\Phi(\omega) = \lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} \omega(H_\Lambda)$

Pressure $p(\beta\Phi) = \lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} \log Z_\Lambda = \lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} \log \mathrm{tr}(e^{-\beta H_\Lambda})$

Theorem: (Variational Principle) The functional $\omega \mapsto s(\omega) - \beta e(\omega)$ is upper-semicontinuous and

$$p(\beta\Phi) = \lim_{n\to\infty} \frac{1}{|\Lambda|} \log \mathrm{tr}\,(\exp(-\beta H_\Lambda)) = \sup_{\omega\ trans.inv.} \{s(\omega) - \beta e_\Phi(\omega)\}$$

Morever we can write

$$p(\beta\Phi) = \sup_e \{s(e) - \beta e\}$$

where $s(e)$ is the microcaconical entropy

Relation with large deviations and Laplace-Varadhan: $-s(e)$ is the microcanonical entropy, i.e. the rate function function for

$$\mu_\Lambda(A) = \mathrm{tr}\left(\mathbf{I}_A\left(\frac{H_\Lambda}{|\Lambda|}\right)\right) \asymp \exp(|\Lambda| \sup_{e\in A} s(e))$$

(Use this to prove equivalence of micro and macro ensembles!)

Short range and long range interactions

Two interactions Φ and Ψ with Hamiltonians H_Λ, K_Λ

G a continuous functions on $[-\|\Psi\|, \|\Psi\|]$

What is

$$\lim_{n\to\infty} \frac{1}{|\Lambda|} \log \mathrm{tr} \left[\exp\left(-\beta H_\Lambda + |\Lambda| G\left(\frac{K_\Lambda}{|\Lambda|} \right) \right) \right] \text{ ?}$$

Example: $K_\Lambda = \sum_{x\in\Lambda} \psi_x$ and $G(z) = z^2$ then

$$|\Lambda| G(K_\Lambda) = \frac{1}{|\Lambda|} \sum_{x,y\in\Lambda} \psi_x \psi_y \,, \text{ Mean - field interaction}$$

Pressure for systems with short range and mean field interactions.

In collaboration with De Roeck, Maes, Netockny (see also Hiai, Mosonyi, Ohno , Petz).

Let g be a continuous function and G is a quantization of g, i.e.,

- $G(X,Y) = G(X,Y)^*$ for $X = X^*, Y = Y^*$
- $G(x,y) = g(x,y)$ for $x, y \in \mathbf{R}$

Theorem For any quantization of G we have

$$\lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} \log \mathrm{tr} \left[\exp \left(-\beta H_\Lambda + |\Lambda| G \left(\frac{K_{\Lambda,1}}{|\Lambda|}, \frac{K_{\Lambda,2}}{|\Lambda|} \right) \right) \right]$$

$$= \sup_\omega \{ g\left(e_{\Psi_1}(\omega), e_{\Psi_2}(\omega)\right) + s(\omega) - \beta e_\Phi(\omega) \}$$

We also have the formula

$$\lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} \log \operatorname{tr}\left[\exp\left(-\beta H_\Lambda + |\Lambda| G\left(\frac{K_{\Lambda,1}}{|\Lambda|}, \frac{K_{\Lambda,2}}{|\Lambda|}\right)\right)\right]$$

$$= \sup_{x_1, x_2 \in \mathbf{R}^2} \{g(x_1, x_2) - I(x_1, x_2)\} \tag{1}$$

where

$$I(x,y) = \lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} \log \operatorname{tr}\left[\exp(-\beta H_\Lambda + x_1 K_{\Lambda,1} + x_2 K_{\Lambda,2})\right]$$

Here the connection with large deviations is somewhat lost.

Proof:

• The lower bound use the standard trick + approximation of any state by ergodic states

• Upper bound: Reduction to a product state on a coarse lattice + slight extension of the Petz-Raggio-Verbeure bound.

Open problem: Existence of the specific relative entropy

Variational Principle and Gibbs states

$$p(\beta\Phi) = \sup_{\omega \; trans.inv.} \{s(\omega) - \beta e_{\Phi}(\omega)\}$$

A translation invariant state $\omega^{\beta\Phi}$ is a (infinite volume) Gibbs state if

$$p(\beta\Phi) = s(\omega) - \beta e_{\Phi}(\omega)$$

and let us denote by $\Omega(\beta\Phi)$ the set of Gibbs states.

Relative entropy

For two states ω_Λ and ω'_Λ with density matrices σ_Λ and σ'_Λ the relative entropy of ω_Λ with respect to ω'_Λ

$$S(\omega_\Lambda | \omega'_\Lambda) = \mathrm{tr}\left(\sigma_\Lambda \left(\log \sigma_\Lambda - \log \sigma'_\Lambda\right)\right)$$

Let $\omega^{\beta\Phi}$ be an equilibrium state at temperature β and let $\omega_\Lambda^{\beta\Phi}$ its restriction to $\mathcal{O}_\Lambda$.

Open Problem: Prove that for any translation invariant state ω the limit

$$s(\omega \,|\, \omega^\beta) = \lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} S(\omega_\Lambda \,|\, \omega_\Lambda^{\beta\Phi})$$

exists and that

$$s(\omega \,|\, \omega^\beta) = -s(\omega) + \beta e(\omega) + p(\beta)\,.$$

Equivalent reformulation of the variational principle:

Let $\omega^{\beta\Phi}$ be a Gibbs state. Then we have

$$s(\omega\,|\omega^{\beta\Phi}) = 0 \quad \text{iff} \quad \omega \in \Omega^{\beta}$$

Not known if the the specific relative entropy $s(\omega\,|\,\omega^{\beta\Phi})$ exists for a general quantum Gibbs state $\omega^{\beta\Phi}$!

Known for

- Classical case
- Quantum case, β sufficently small (high-temperature)
- Quantum case, $d = 1$, finite range interactions.

If $\omega^{\beta\Phi}_{\Lambda,can}$ is the finite volume Gibbs state (i.e. with free boundary conditions) then the existence of the limit

$$\lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} S(\omega_\Lambda \,|\, \omega^{\beta\Phi}_{\Lambda,can})$$

is (very easy)

Control the boundary terms!

$\omega^{\beta\Phi}_{\Lambda,can}$ vs $\omega^{\beta\Phi}_{\Lambda}$

Classical : use DLR condition

Quantum : use Araki-Gibbs condition, but...

Asymptotic decoupling property

If $\omega^{\beta\Phi} \in \Omega^{\beta\Phi}$ is a Gibbs state then there exist constants $C(\Lambda)$ with

$$\lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{c(\Lambda)}{|\Lambda|} = 0$$

such that

$$e^{-c(\Lambda)} \, \sigma_\Lambda^{\beta\Phi} \leq \frac{e^{-\beta H_\Lambda}}{\mathrm{tr}(e^{-\beta H_\Lambda})} \leq e^{c(\Lambda)} \, \sigma_\Lambda^{\beta\Phi}$$

The proof in the classical case is very easy, at high temperature not too difficult, in dimension 1 quite hard (based on hard estimates by Araki on the dynamics)

This implies that for $A \in \mathcal{O}_\Lambda$, $B \in \mathcal{O}_{\Lambda^C}$ we have

$$e^{-c(\Lambda)} \omega^{\beta\Phi}(A)\omega^{\beta\Phi}(B) \leq \omega^{\beta\Phi}(AB) \leq \omega^{\beta\Phi}(A)\omega^{\beta\Phi}(B) e^{c(\Lambda)}$$

Ruelle-Lanford functions and large deviations

see Ruelle and Lanford and Lewis, Pfister & Sullivan

Consider a sequence of measures $\{\mu_n\}$ and a scal v_n. For simplicity assume $\{\mu_n\}$ supported on some compact set of $\mathbf{R}$

Define the set functions

$$\overline{m}(B) \equiv \limsup_n \frac{1}{v_n} \log \mu_n(B) \qquad \underline{m}(B) \equiv \liminf_n \frac{1}{v_n} \log \mu_n(B)$$

and the Ruelle-Lanford functions

$$\overline{s}(x) = \inf_\epsilon \overline{m}(B_\epsilon(x)) \qquad \underline{s}(x) = \inf_\epsilon \underline{m}(B_\epsilon(x))$$

Facts:

- If

$$\underline{s}(x) = \overline{s}(x) \equiv s(x)$$

then μ_n satisfy a LDP with rate function $I(x) = -s(x)$

- By Laplace-Varadhan lemma the moment generating function

$$e(\alpha) = \lim_n \frac{1}{v_n} \log \mu_n \left(\exp(v_n \alpha x)\right)$$

exists. Suppose, in addition, that $s(x)$ is concave then by convex duality

$$s(x) = \inf_\alpha \{e(\alpha) - \alpha x\}$$

Application to quantum spin systems

Consider the probability measures (with $v_n = |\Lambda|$)

$$\mu_\Lambda(A) = \omega^{(\beta\Phi)}\left(\mathbf{I}_A\left(\frac{K_\Lambda}{|\Lambda|}\right)\right)$$

with

$\mathbf{I}_A(X)$ = spectral projection onto the eigenspaces of X corresponding to eigenvalues in A.

$\omega^{\beta\Phi}$ a Gibbs measure at inverse temperature β.

Various previous results obtained by Lebowitz-Lenci-Spohn, Gallavotti-Lebowitz-Mastropietro, Netocny-Redig, Lenci-R.B., Petz-Hiai-Mosonyi, Ogata, ...

Novelty: (Joint work with Yoshiko Ogata)

• Characterization of the large deviation function in terms of classical (!) relative entropy

• Proof of large deviation theorems done in "Ruelle-Lanford's spirits", i.e. use only subadditivity arguments, so no cluster expansion, transfer operators, etc... As a result proofs are very short and fairly straightforward.

Classical Observables

Assume

• The state $\omega = \omega^{(\beta\Phi)}$ is asymptotically decoupled quantum or classical Gibbs state.

• The observable K_Λ is a classical observable e.g.

$$K_\Lambda = \sum_{x\in\Lambda} \Psi_x\,, \qquad \text{one} - \text{site observables}$$

or

$$K_\Lambda = \text{energy for a classical spin systems}$$

In both cases there exists a classical subalgebra $\mathcal{O}^{(cl)}$ such that $\psi_X \in \mathcal{O}^{(cl)}$ for all X.

Theorem: The family of measures $\mu_n(A) = \omega^{(\beta\Phi)}\left(\mathbf{I}_A\left(\frac{1}{|\Lambda(n)|}K_{\Lambda(n)}\right)\right)$ satisfies a large deviation principle with a convex rate function $-s(x)$ with

$$s(x) = \inf_\alpha \{e(\alpha) - \alpha x\}$$

where

$$e(\alpha) = \lim_{n\to\infty} \frac{1}{|\Lambda(n)|} \log \omega^{(\beta\Phi)}(\exp(\alpha K_{\Lambda(n)})) . \quad \text{(Relative pressure)}$$

This is not the translated pressure $P(\beta\Phi - \alpha\Psi)$.

Moreover we have

$$s(x) = \sup\left\{-s_{cl}(\nu|\omega|_{\mathcal{O}}^{(cl)})\,;\,\nu \text{ state on } \mathcal{O}^{(cl)}\,, \nu(A_\Psi) = x\right\}$$

This rate function is expressed using the classical relative entropy h_{cl}, in particular

$$s(x) \neq \sup\{-s\,(\nu|\omega)\,;\,\nu \text{ state on } \mathcal{O}\,, \nu(A_\Psi) = x\}$$

Dimension 1

Assume

- $\omega^{\beta\Phi}$ is a Gibbs state for a finite range interaction Φ

- The observable K_Λ is a macroscopic observable for a finite-range interaction Ψ.

Theorem:

$$\omega^{\beta\Phi}\left(\mathbf{I}_A\left(\frac{K_\Lambda}{|\Lambda|}\right)\right) \asymp e^{-|\Lambda| \inf_{x\in A} I(x)}$$

with

$$I(x) = \inf\left\{s_\Psi(\omega \,|\, \omega^{\beta\Phi})\,,\, e_\psi(\omega) = x)\,,\right\}$$

with

$$s_\Psi(\omega \,|\, \omega') = \lim_{|\Lambda|\nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} S(\omega_\Lambda|_{\mathcal{O}_{\Lambda,\Psi}} \,|\, \omega'_\Lambda|_{\mathcal{O}_{\Lambda,\Psi}})$$

and $\mathcal{O}_{\Lambda,\psi}$ is the classical subalgebra generated by K_Λ.

Basic idea to prove the existence of a concave Ruelle-Lanford function.

Pick x, x_1, x_2 such that $x = \frac{1}{2}x_1 + \frac{1}{2}x_2$ arbitrary.

Pick $\epsilon > \epsilon'$ arbitrary.

Show that

$$\underline{m}(B_\epsilon(x)) \geq \frac{1}{2}\left(\overline{m}(B_{\epsilon'}(x_1)) + \underline{m}(B_{\epsilon'}(x_2))\right)$$

Take a cube Λ of side length $n = kl$ and write

$$K_\Lambda = \sum_{j=1}^{k^d} K_{C_j} + W$$

where the C_j are disjoint cubes of sidelength l and W is the interaction energy between the C_j's.

Main problem: Control the projections the difference between the projections

$$\mathbf{I}_{B_\epsilon(x)}(K_\Lambda) \quad \text{and} \quad \mathbf{I}_{B_{\epsilon'}(x)}(\sum_j K_{C_j})$$

Proposition: Assume $d = 1$, then for any $\epsilon > \epsilon'$ and any $\alpha > 0$

$$\limsup_{\Lambda \nearrow \mathbf{Z}} \frac{1}{|\Lambda|} \log \left\| \mathbf{I}_{B_\epsilon(x)}(K_\Lambda) \mathbf{I}_{B_{\epsilon'}(x)^C}(\sum_j K_{C_j}) \right\| \leq -\alpha(\epsilon - \epsilon')$$

Related problems

(1) Show the existence of the specific relative entropy. For translation invariant ω the limit

$$s(\omega \,|\, \omega^{\beta\Phi}) = \lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} S(\omega_\Lambda \,|\, \omega_\Lambda^{\beta\Phi})$$

exist.

(2) Consider two families of Hamiltonians H_Λ and K_Λ. Prove the existence of the limit

$$\lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|} \log \mathrm{tr}\left(e^{H_\Lambda} e^{K_\Lambda}\right)$$

Also useful in quantum information theory (Hypothesis testing:Chernoff and Hoefding bounds)

(3) Obtain bounds on imaginary time-evolution

$$e^{izH_\Lambda} A e^{-izH_\Lambda}$$

uniformly in $|\Lambda|$. In 1-dimension it is an entire-analytic function (Araki) for local A and $\Lambda \nearrow \mathbf{Z}^d$.