Concentration of measure and the mean energy ensemble

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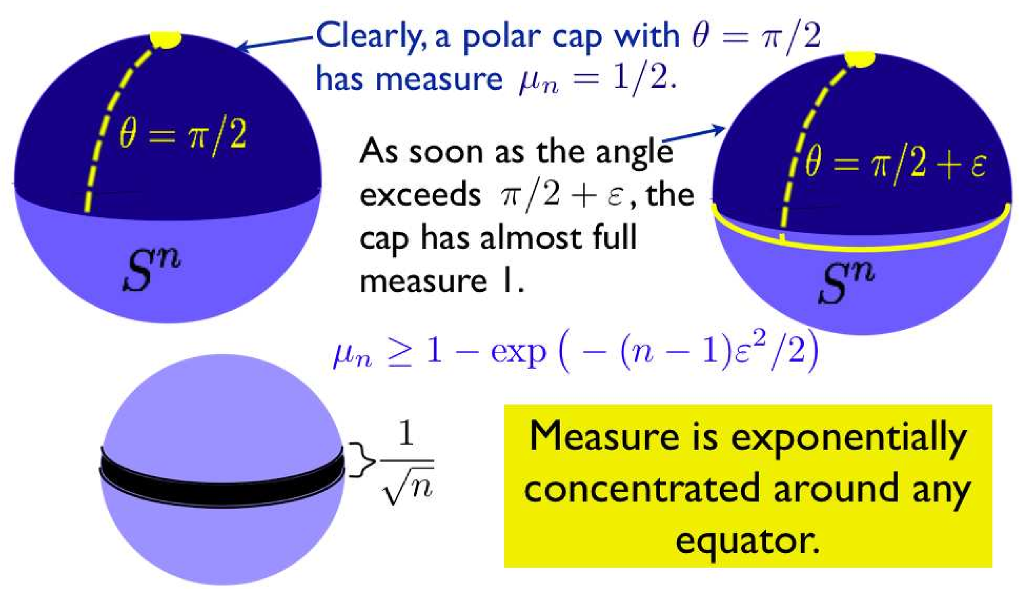
Given some Hamiltonian H on a finite-dimensional quantum system, we investigate the typical properties of pure quantum states $|\psi\rangle$ that have a fixed energy expectation value $\langle\psi|H|\psi\rangle = E$ with respect to H. Under some moderate conditions on the spectrum, we prove that this manifold of quantum states shows a concentration of measure phenomenon: values of Lipschitz-continuous functions on the states are almost everywhere close to their mean. Moreover, the resulting distribution can be efficiently sampled by drawing quantum states randomly with respect to a Boltzmann-Gaussian amplitude distribution. We use this result to give explicit formulas for the reduced density matrix of typical states in bipartite quantum systems with weak interaction, and discuss the dependence of concentration from the energy spectrum.

Concentration of measure in quantum information theory...

- What do random quantum states look like?
- Drawing a pure state in $\mathbb{C}^d$ randomly wrt. the unitarily invariant measure corresponds to picking a point on the unit sphere S^{2d-1} in $\mathbb{R}^{2d}$. In high dimensions, most of the uniform measure on the sphere is strongly concentrated around any equator.



- Consequence: Lévy's Lemma. *Let $f : S^n \to \mathbb{R}$ be a function with $\|\nabla f\| \leq \eta$ and a point $x \in S^n$ chosen uniformly at random. Then,*

$$\mathrm{Prob}\{|f(x) - \mathbb{E}f| > \varepsilon\} \leq 2\exp\left(-c(n+1)\varepsilon^2/\eta^2\right),$$

where $c := (9\pi^3 \ln 2)^{-1}$ is a constant.

- Sample application: Most bipartite quantum states are highly entangled [1]. *Let $|\psi\rangle$ be a random pure state on $A \otimes B$, with $d_B \geq d_A \geq 3$. Then*

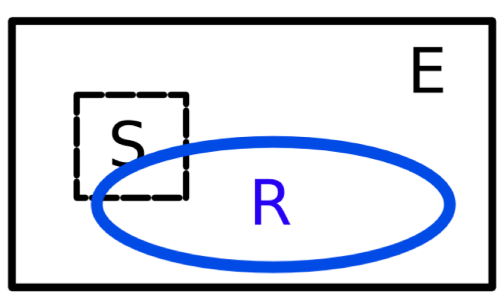
$$\mathrm{Prob}\left\{S(\psi_A) < \log d_A - \alpha - \beta\right\} \leq \exp\left(-\frac{(d_A d_B - 1)c\alpha^2}{(\log d_A)^2}\right),$$

where $\beta = \frac{d_A}{d_B \ln 2}$, and $c = (8\pi^2 \ln 2)^{-1}$.

- Most famous application: M. Hastings' counterexample to the additivity conjecture [2].

... and typicality in statistical mechanics

Consider a subspace $\mathcal{H}_R \subset \mathcal{H}_S \otimes \mathcal{H}_E$. Example: S=system, E=environment, R=subspace spanned by global energy eigenstates in $[E - \Delta E, E + \Delta E]$.



Statistical mechanics recipe: equidistribution on R gives "microcanonical ensemble" $\Omega_S := \mathrm{Tr}_E(\mathbf{1}_R/d_R)$. Popescu et al. [3] use measure concentration to prove the following:

- Given fixed $|\psi\rangle \in \mathcal{H}_R$, the reduced state is $\psi_S := \mathrm{Tr}_E|\psi\rangle\langle\psi|$.
- It turns out that for "almost all" $|\psi\rangle$, it holds $\psi_S \approx \Omega_S$. In more detail, if $|\psi\rangle$ is drawn randomly in R, then

$$\mathrm{Prob}\left\{\|\psi_S - \Omega_S\|_1 \geq \varepsilon + \frac{d_S}{\sqrt{d_R}}\right\} \leq 2\exp\left(-Cd_R\varepsilon^2\right),$$

where $C = 1/18\pi^3$, $d_R = \dim \mathcal{H}_R$, $d_S = \dim \mathcal{H}_S$.

- In this sense, most single pure quantums states locally look like the ensemble average.

Under additional assumptions on the spectrum, Goldstein et al. [4] show that Ω_S is a Gibbs state, i.e. $\Omega_S \sim e^{-\beta H}$.

However, treating all states in subspaces R in equal footing is sometimes criticized as unphysical ("nature lives in a small corner of Hilbert space"). Hence it makes sense to ask for similar results for more natural subsets of states R:

Problem: What if the restriction R is not given by a subspace, but by a *nonlinear* constraint?
As a physical example, *what if the mean energy $\langle\psi|H|\psi\rangle$ is fixed instead* – do similar results hold?

The mean energy ensemble M_E

Several authors [5, 6] have suggested to define a "quantum microcanonical ensemble" differently: instead of fixing the energy subspace, fix the energy expectation value to equal some value E:

$$M_E := \{|\psi\rangle \in \mathbb{C}^n \mid \langle\psi|H|\psi\rangle = E, \quad \|\psi\| = 1\},$$

where $H = H^\dagger$ is an arbitrary fixed Hamiltonian on $\mathbb{C}^n$.

- This is not a subspace, but a submanifold of real dimension $2n - 2$.
- As such, it carries a natural geometric volume measure inherited from the unitarily invariant measure.
- It is the simplest example of a "non–linear ensemble", natural to consider in quantum information and statistical mechanics. → prototype for more general situations

Problem: Can we prove concentration of measure (analog of Lévy's Lemma) for M_E? If so, what do reduced density matrices (and other properties) typically look like?

Main Results

If H's eigenvalues are $E_1, E_2, \ldots, E_n$, then M_E is invariant wrt. energy shifts $E'_k := E_k + s$, $E' := E + s$. While the arithmetic mean $E_A := \frac{1}{n}\sum_k E_k$ is shifted as well (i.e. $E'_A = E_A + s$), the harmonic mean $E_H := \left(\frac{1}{n}\sum_k \frac{1}{E_k}\right)^{-1}$ changes in a non–linear way. Choosing s appropriately, we can shift the energies such that $E' = E'_H$ if $E_{min} < E < E_A$.

Main Theorem 1. Suppose that $E > E_{min}$ is an arbitrary energy value such that E is not too close to the "infinite temperature" energy E_A, i.e.

$$E \leq E_A - \frac{2E_{max}}{\sqrt{2n-1}}\left(\sqrt{\log(2n-1)} + \sqrt{\frac{\pi^3}{2}}\right).$$

If $f : M_E \to \mathbb{R}$ is any function with $\|\nabla f\| \leq \lambda$ and median $\bar{f}$, then the value $f(\psi)$ evaluated on a randomly chosen state $|\psi\rangle \in M_E$ satisfies

$$\mathrm{Prob}\left\{|f(\psi) - \bar{f}| > \lambda t\right\} \leq a \cdot n^{\frac{3}{2}} \cdot e^{-cn\left(t - \frac{1}{4n}\right)^2 + \varepsilon\sqrt{n}}.$$

The constants a, c and ε depend on the spectrum. They can be determined in the following way:

- Find an energy shift (which is always possible, see above) such that $E' = \left(1 + \frac{1}{n}\right)\left(1 + \frac{\varepsilon}{\sqrt{n}}\right)E'_H$ for some $\varepsilon > 0$ which is arbitrary, but must be large enough such that the constant a (described below) is positive.
- Compute $c = \frac{3E'_{min}}{64E'}$, $E'_Q := \left(\frac{1}{n}\sum_k {E'_k}^{-2}\right)^{-\frac{1}{2}}$, and $a = 3040{E'_{max}}^2\left[E'^2\left(1 - \frac{E'^2}{\varepsilon^2 {E'_Q}^2}\right)\right]^{-1}$.

Then, how do we compute the median $\bar{f}$ on the energy manifold M_E? We can do it by integrating over an ellipsoid (in spherical coordinates):

Main Theorem 2. The median $\bar{f}$ can be estimated as follows. Let N be the full ellipsoid of vectors $z \in \mathbb{C}^n$ with $\langle z|H|z\rangle \leq E'\left(1 + \frac{1}{2n}\right)$, then

$$|\bar{f} - \mathbb{E}_N f| \leq \mathcal{O}\left(n^{-\frac{1}{4}}\right),$$

where the exact constants depend on the spectrum. Applying this to the reduced density matrix elements $\psi_A := \mathrm{Tr}_B|\psi\rangle\langle\psi|$ for random states $|\psi\rangle \in A \otimes B$ with Hamiltonian $H = H_A + H_B$ yields in particular

$$\psi_A \approx \frac{E'}{n+1}\begin{pmatrix} \sum_{i=1}^{|B|}\frac{1}{E'^A_1 + E'^B_i} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sum_{i=1}^{|B|}\frac{1}{E'^A_{|A|} + E'^B_i} \end{pmatrix}$$

with high probability, where $\{E'^A_i\}_i$ and $\{E'^B_j\}$ are the energy eigenvalues of H'_A and H'_B respectively.

Thus, the typical reduced density matrix is not of the Gibbs form in general.

A simple example

Suppose we have a bipartite Hilbert space $A \otimes B$ with $A = \mathbb{C}^3$, $\dim B = n$, and a Hamiltonian $H = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 3 \end{pmatrix} \otimes \mathbf{1}_B$.

- Choose ψ randomly under the constraint $\langle\psi|H|\psi\rangle = \frac{3}{2}$. Then, the reduced density matrix ψ^A is typically close to

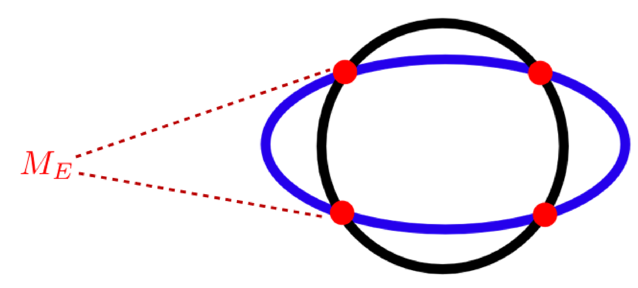
$$\rho_c := \frac{1}{12}\begin{pmatrix} 5 + \sqrt{7} & 0 & 0 \\ 0 & 2(4 - \sqrt{7}) & 0 \\ 0 & 0 & -1 + \sqrt{7} \end{pmatrix}.$$

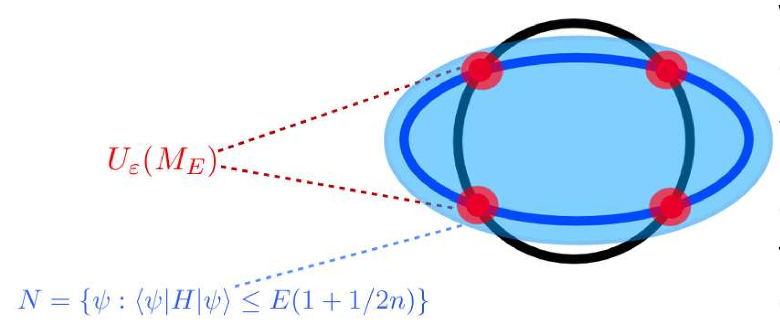
- More in detail, for all $t > 0$ and $n \geq 8193$

$$\mathrm{Prob}\left\{\left\|\psi^A - \rho_c\right\|_2 > 3\sqrt{8}\left(t + \frac{59}{\sqrt[4]{n}}\right)\right\} \leq 369960\, n^{\frac{3}{2}} \times$$
$$\times e^{-\frac{3}{64}n\left(t - \frac{1}{4n}\right)^2 + 4\sqrt{n}}.$$

Proof idea and tools: integral geometry

Geometrically, M_E is the intersection of a sphere (normalization) and an ellipsoid (energy expectation value).





We get solid objects by considering the ε-neighbourhood of M_E, and the full (enlarged) ellipsoid.

- By standard results, we have concentration of measure in the full ellipsoid N.
- If $U_\varepsilon(M_E)$ covers a lot of N, then M_E "inherits" measure concentration from the surrounding ellipsoid N.
- This is the case if $\mathbb{E}_N\|x\|^2 \approx 1$, such that "most" points in N are close to the sphere. It turns out that E must be close to the harmonic energy E_H such that this is true.

This proof strategy is inspired by M. Gromov [7] and uses techniques from geometric probability theory.

Approximate Gaussian sampling of M_E

As a by–product, we get the following method to sample points randomly from the energy manifold M_E:

Draw $|\psi\rangle = (\psi_1, \ldots, \psi_n)$ randomly by choosing real and imaginary part x_k of each $\psi_k \in \mathbb{C}$ independently according to the distribution with density proportional to

$$e^{-n\frac{E_k}{E}x_k^2/2}.$$

In the thermodynamic limit $n \to \infty$, the resulting measure gets close to the geometric volume measure on M_E (assuming concentration depending on the spectrum). The error bounds can be given explicitly.

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