Concentration of measure for thermal distributions of quantum states

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Based on joint work with Stefan Teufel and Roderich Tumulka
arXiv:2307.15624

Itinerant Quantum Math Meetings
Università degli studi di Milano, Milan
May 7, 2024

Canonical Typicality

Let $\mathcal{H}_R$ be a high-dimensional subspace of the Hilbert space $\mathcal{H}_S = \mathcal{H}_a \otimes \mathcal{H}_b$, where a is a small system with environment b in $S = a \cup b$. For $\psi \in \mathbb{S}(\mathcal{H}_R)$ let

$$\rho_a^\psi := \operatorname{tr}_b |\psi\rangle\langle\psi|$$

be the reduced density matrix and let $\rho_R = P_R/d_R$ (the normalized projection to $\mathcal{H}_R$) with $d_R := \dim \mathcal{H}_R$. Then, for most $\psi \in \mathbb{S}(\mathcal{H}_R)$,

$$\rho_a^\psi \approx \operatorname{tr}_b \rho_R,$$

where "most ψ" refers to the uniform distribution u_R over $\mathbb{S}(\mathcal{H}_R)$.

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If $\rho_R = \rho_{\mathrm{mc}}$ (micro-canonical density matrix), b is large and a and b are weakly interacting, $\mathrm{tr}_b \, \rho_{\mathrm{mc}}$ is close to a canonical density matrix $\rho_{a,\mathrm{can}} = \frac{1}{Z_a} e^{-\beta H_a}$.

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This phenomenon was discovered by several groups independently (Gemmer, Mahler (2003); Goldstein, Lebowitz, Tumulka, Zanghì (2006); Popescu, Short, Winter (2006)).

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Theorem 1 (Popescu, Short, Winter 2006)

Let $\mathcal{H}_a$ and $\mathcal{H}_b$ be Hilbert spaces of dimension $d_a, d_b \in \mathbb{N}$ respectively, $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b$, $\mathcal{H}_R$ be any subspace of $\mathcal{H}$ of dimension d_R, ρ_R be $1/d_R$ times the projection to $\mathcal{H}_R$ and u_R the uniform distribution over $\mathbb{S}(\mathcal{H}_R)$. Then for every $\varepsilon > 0$,

$$u_R\Big\{\psi \in \mathbb{S}(\mathcal{H}_R) : \big\|\rho_a^\psi - \mathrm{tr}_b\,\rho_R\big\|_{\mathrm{tr}} > \varepsilon\Big\} \leq 4d_a^2 \exp\left(-\frac{d_R \varepsilon^2}{18\pi^3 d_a^2}\right).$$

Lévy's Lemma

Theorem 2 (Lévy's Lemma)

Let $\mathcal{H}$ be a Hilbert space of finite dimension D, let $f : \mathbb{S}(\mathcal{H}) \to \mathbb{R}$ be a function with Lipschitz constant η, let u be the uniform distribution over $\mathbb{S}(\mathcal{H})$, and let $\varepsilon > 0$. Then,

$$u\{\psi \in \mathbb{S}(\mathcal{H}) : \left|f(\psi) - u(f)\right| > \varepsilon\} \leq 4 \exp\left(-\frac{\tilde{C} D \varepsilon^2}{\eta^2}\right),$$

where $\tilde{C} = \frac{2}{9\pi^3}$ and $u(f) := \int_{\mathbb{S}(\mathcal{H})} f(\psi)\, u(d\psi)$.

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$\Rightarrow$ Lipschitz functions on spheres in high-dimensional Hilbert spaces are approximately constant!

Ideas of Proof (Lévy's Lemma)

- First show an analogous fact about Gaussian distributions:

Lemma 3 (Lévy's Lemma for Gaussian random variables)

Let $X = (X_1, \ldots, X_D)$ be a vector of independent (real) standard Gaussian random variables. Let $F : \mathbb{R}^D \to \mathbb{R}$ be a Lipschitz function with constant η and let $\varepsilon > 0$. Then,

$$\mathbb{P}\left\{|F(X) - \mathbb{E}F(X)| > \varepsilon\right\} \leq 2\exp\left(-\frac{2\varepsilon^2}{\pi^2\eta^2}\right).$$

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- The proof makes heavy use of characteristics of Gaussian random variables, e.g. the invariance of X under orthogonal transformations and the form of the moment generating function of the X_i
- The link between X and the uniform distribution on $\mathbb{S}(\mathbb{R}^D)$ is given by the fact that $\frac{X}{\|X\|}$ is uniformly distributed on $\mathbb{S}(\mathbb{R}^D)$

GAP Measures

- To any probability measure μ on $\mathbb{S}(\mathcal{H})$ we can associate a density matrix ρ_μ by

$$\rho_\mu = \int_{\mathbb{S}(\mathcal{H})} \mu(d\psi) \, |\psi\rangle\langle\psi|$$

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- For any density matrix ρ on $\mathcal{H}$, the most spread-out distribution over $\mathbb{S}(\mathcal{H})$ with density matrix ρ, is known as GAP(ρ) for *Gaussian Adjusted Projected* measure; it was first introduced by Jozsa, Robb and Wootters (1994) who showed that GAP(ρ) minimizes the "accessible information" of an ensemble of wave functions under the constraint that its density matrix is ρ; therefore they called it *Scrooge measure*.

GAP Measures

- If $D = \dim \mathcal{H} < \infty$ and all eigenvalues of ρ are positive, then

$$\frac{d\mathrm{GAP}(\rho)}{du}(\psi) = \frac{D}{\det \rho} \langle \psi | \rho^{-1} | \psi \rangle^{-D-1}$$

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- GAP measures describe the thermal equilibrium distribution of the wave function of the system a if ρ is a canonical density matrix (Goldstein, Lebowitz, Mastrodonato, Tumulka, Zanghì, 2016)
- GAP measures can also be defined on separable Hilbert spaces (Tumulka, 2020)

GAP Measures – Construction

- Let ρ be a density matrix on $\mathcal{H}$ with eigenvalues p_n and let $\{|n\rangle\}$ be an ONB of eigenvectors of ρ, i.e.

$$\rho = \sum_n p_n |n\rangle\langle n|$$

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- Let Z_n be a sequence of independent $\mathbb{C}$-valued Gaussian random variables with mean 0 and variances

$$\mathbb{E}|Z_n|^2 = p_n;$$

we define $G(\rho)$ to be the distribution of the random vector

$$\Psi^G := \sum_n Z_n |n\rangle$$

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- We define the adjusted Gaussian measure $\mathrm{GA}(\rho)$ on $\mathcal{H}$ by

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- Let Ψ^{GA} be a $\mathrm{GA}(\rho)$-distributed random vector. We define $\mathrm{GAP}(\rho)$ to be the distribution of

$$\Psi^{GAP} := \frac{\Psi^{GA}}{\|\Psi^{GA}\|}$$

Generalized Canonical Typicality

Theorem 4 (Teufel, Tumulka, V. 2023)

Let $\mathcal{H}_a$ and $\mathcal{H}_b$ be Hilbert spaces with $d_a = \dim \mathcal{H}_a < \infty$ and $\mathcal{H}_b$ separable. Let ρ be a density matrix on $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b$. Then for every $\varepsilon > 0$,

$$\mathrm{GAP}(\rho)\Big\{\psi \in \mathbb{S}(\mathcal{H}) : \big\|\rho_a^{\psi} - \mathrm{tr}_b\, \rho\big\|_{\mathrm{tr}} > \varepsilon\Big\} \leq 6 d_a^2 \exp\left(-\frac{\tilde{C}\varepsilon^2}{d_a^2 \|\rho\|}\right)$$

for some universal constant $\tilde{C} > 0$.

Lévy's Lemma for GAP measures

Theorem 5 (Teufel, Tumulka, V. 2023)

Let $\mathcal{H}$ be a separable Hilbert space, let $f : \mathbb{S}(\mathcal{H}) \to \mathbb{R}$ be a function with Lipschitz constant η, let ρ be a density matrix on $\mathcal{H}$, and let $\varepsilon > 0$. Then,

$$\mathrm{GAP}(\rho)\Big\{\psi \in \mathbb{S}(\mathcal{H}) : |f(\psi) - \mathrm{GAP}(\rho)(f)| > \varepsilon\Big\} \leq 6\exp\left(-\frac{C\varepsilon^2}{\eta^2\|\rho\|}\right),$$

where $C > 0$ and $\mathrm{GAP}(\rho)(f) = \int_{\mathbb{S}(\mathcal{H})} f(\psi)\,\mathrm{GAP}(\rho)(d\psi)$.

Remarks

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- One can show that for GAP(ρ)-most $\psi \in \mathbb{S}(\mathcal{H})$ and most $t \in [0, T]$, $\rho_a^{\psi_t} \approx \text{tr}_b\, \rho_t$ ("dynamical typicality") [A statement $s(t)$ holds for most $t \in [0, T]$ if $\frac{1}{T}\lambda\{t \in [0, T] : s(t)\,\text{does not hold}\}$ is small]

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- Lévy's lemma does *not* hold for all rather-spread-out distributions on $\mathbb{S}(\mathcal{H})$ (e.g. the von-Mises-Fisher distribution); it is a non-trivial property of the family of GAP measures

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- Generalized canonical typicality is not true in general if GAP(ρ) is replaced by a different measure with density matrix ρ (e.g., the measure concentrated on the eigenvectors of ρ)
- Generalized canonical typicality is also not true in general if $\|\rho\|$ is not small, e.g. if one eigenvalue is large (and all the others small)
- Our result expresses a kind of equivalence of ensembles: If a and b interact weakly, then both ρ_{mc} and ρ_{can} in $\mathcal{H}_S = \mathcal{H}_a \otimes \mathcal{H}_b$ lead to reduced density matrices close to a canonical density matrix for a, $\mathrm{tr}_b\, \rho_{\mathrm{mc}} \approx \rho_{a,\mathrm{can}} \approx \mathrm{tr}_b\, \rho_{\mathrm{can}}$; we can start from either u_{mc} or GAP(ρ_{can}) and obtain for both ensembles of ψ that ρ_a^{ψ} is nearly constant and nearly canonical

Normal Typicality - Setting

Following von Neumann (1929) we decompose the system's (finite-dimensional) Hilbert space $\mathcal{H}$ into an orthogonal sum of subspaces ("macro spaces") $\mathcal{H}_\nu$ representing different "macro states" ν,

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Definition 6

Let $\delta > 0$. We say that a statement $s(t)$ holds for $(1-\delta)$-most $t \in [0, \infty)$, if

$$\liminf_{T\to\infty} \frac{1}{T} \lambda\{t \in [0, T] : s(t) \text{ holds}\} \geq 1 - \delta.$$

Normal Typicality

Theorem 7 (Von Neumann 1929; Goldstein, Lebowitz, Mastrodonato, Tumulka, Zanghì 2010)

Let $\varepsilon, \delta, \delta' > 0$. For $(1-\delta')$-most Hamiltonians H (where the eigenbasis of H is chosen purely randomly among all orthonormal bases) with non-degenerate eigenvalues and eigenvalue gaps, every $\psi_0 \in \mathbb{S}(\mathcal{H})$ evolves so that for $(1-\delta)$-most $t \in [0,\infty)$,

$$\left| \|P_\nu \psi_t\|^2 - \frac{d_\nu}{D} \right| < \varepsilon \frac{d_\nu}{D} \quad \text{for all } \nu,$$

if $d_\nu = \dim \mathcal{H}_\nu$ and $D := \dim \mathcal{H}$ are sufficiently large (the precise conditions involve $\varepsilon, \delta, \delta'$). Here P_ν denotes the projection onto $\mathcal{H}_\nu$. This behavior is called **normal typicality**.

Normal Typicality

Problem: Von Neumann's assumptions on H are not very realistic since for such H the decomposition of $\mathcal{H}$ and the energy eigenbasis are unrelated, which e.g. implies that one would go from any macro state immediately to the thermal equilibrium macro space (Goldstein, Hara, Tasaki 2013).

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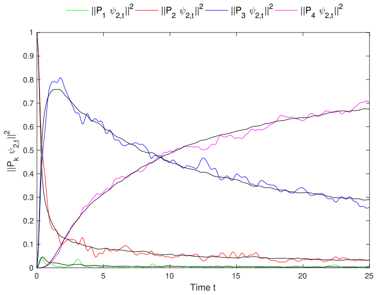
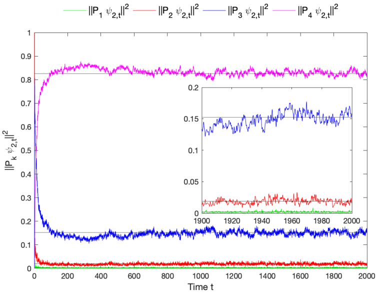
Therefore we are interested in a generalization of Normal Typicality to Hamiltonians whose energy eigenbasis is not unrelated to the decomposition of $\mathcal{H}$, e.g. where H has some kind of band structure in a basis diagonalizing the P_ν's.

Generalized Normal Typicality and Deterministic Evolution





Here the Hilbert space $\mathcal{H}$ is partitioned into four macro spaces $\mathcal{H}_\nu$ such that $d_1 \ll d_2 \ll d_3 \ll d_4$ and $\psi_0 \in \mathbb{S}(\mathcal{H}_2)$. The Hamiltonian is modelled by a random matrix with a band structure in a basis that diagonalizes the P_ν's.

Rigorous Results – Generalized Normal Typicality

For two macro states μ and ν we define

$$M_{\mu\nu} := \frac{1}{d_\mu} \sum_{e \in \mathcal{E}} \mathrm{tr}(P_\mu \Pi_e P_\nu \Pi_e)$$

where $\mathcal{E}$ is the set of the distinct eigenvalues of H. Note that $M_{\mu\nu} = \mathbb{E}_\mu \left(\overline{\|P_\nu \psi_t\|^2} \right)$, where $\overline{\|P_\nu \psi_t\|^2} = \lim_{T\to\infty} \frac{1}{T} \int_0^T \|P_\nu \psi_t\|^2 \, dt$.

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Theorem 8 (Generalized Normal Typicality; Teufel, Tumulka, V. 2022)

Let H be a Hermitian $D \times D$ matrix and let $\varepsilon, \delta \in (0,1)$. Then, $(1-\varepsilon)$-most $\psi_0 \in \mathbb{S}(\mathcal{H}_\mu)$ are such that for $(1-\delta)$-most $t \in [0,\infty)$

$$\left| \|P_\nu \psi_t\|^2 - M_{\mu\nu} \right| \leq 4 \sqrt{\frac{D_E D_G}{\delta \varepsilon d_\mu} \min\left\{1, \frac{d_\nu}{d_\mu}\right\}},$$

where D_E and D_G denote the maximum degeneracy of an eigenvalue and eigenvalue gap.

Deterministic Curves

Theorem 9 (Deterministic Curves; Teufel, Tumulka, V. 2022)

Let H be a Hermitian $D \times D$ matrix, let $\varepsilon > 0$ and $t \in [0, \infty)$. Then, $(1-\varepsilon)$-most $\psi_0 \in \mathbb{S}(\mathcal{H}_\mu)$ are such that

$$\Big| \|P_\nu \psi_t\|^2 - \mathbb{E}_\mu \|P_\nu \psi_t\|^2 \Big| \leq \frac{1}{\sqrt{\varepsilon d_\mu}}\,.$$

Moreover, for every $T > 0$, $(1-\varepsilon)$-most $\psi_0 \in \mathbb{S}(\mathcal{H}_\mu)$ are such that

$$\frac{1}{T} \int_0^T \Big| \|P_\nu \psi_t\|^2 - \mathbb{E}_\mu \|P_\nu \psi_t\|^2 \Big|^2 dt \leq \frac{1}{\varepsilon d_\mu}.$$

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The quantity $\mathbb{E}_\mu \|P_\nu \psi_t\|^2$ may be computed as

$$\mathbb{E}_\mu \|P_\nu \psi_t\|^2 = \frac{1}{d_\mu} \operatorname{tr}\left[P_\mu \exp(iHT) P_\nu \exp(-iHT)\right].$$

Generalized Normal Typicality – Relative Errors?

- Generalized Normal Typicality and the result about deterministic curves can be generalized to arbitrary linear operators instead of P_ν and Generalized Normal Typicality also to finite times (however, the equilibration times are extremely large, e.g. for a system of N particles one would need that $T \gg \exp(N)$)

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- For small d_ν, the $M_{\mu\nu}$ might become very small and then a small absolute error might not be very meaningful; therefore we are interested in relative errors for which we need lower bounds on $M_{\mu\nu}$
- If H is a random matrix with continuously distributed entries, the eigenvalues of H are, with probability 1, non-degenerate and we get

$$M_{\mu\nu} = \frac{1}{d_\mu} \sum_n \langle n|P_\mu|n\rangle \langle n|P_\nu|n\rangle,$$

where $\{|n\rangle\}$ is an ONB of eigenvectors of H

Generalized Normal Typicality - Relative Errors?

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- For $H = H_0 + V$, where H_0 is a (deterministic) Hermitian $D \times D$ matrix and V is a Hermitian Gaussian random matrix, we obtain $M_{\mu\nu} \gtrsim \left(\frac{d_\nu}{D}\right)^{16}$ (however, we expect that $M_{\mu\nu} \sim d_\nu/D$)

Remarks and Open Questions

- Can one find a (random matrix) model in which one can prove that $M_{\mu\nu} \sim d_\nu / D$, one sees the transistions through the macro spaces as in the simulations and one has "realistic thermalization times"?

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- Shiraishi and Tasaki (2024) recently proved thermalization of a free fermion chain with Hamiltonian

$$H = \sum_{x=1}^{L} e^{i\theta} c_x^\dagger c_{x+1} + e^{-i\theta} c_{x+1}^\dagger c_x \,,$$

where $\theta > 0$ is a small artificial phase to avoid eigenvalue degeneracy; more precisely they showed that if the initial state is such that all particles are in the left half of the chain, after a sufficiently large typical time, the particle number in any region of the chain is close to its equilibrium value ("$\langle \psi_t | P_{\text{neq}} | \psi_t \rangle$ is small")

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- Is it sufficient that there is an eigenbasis of H_0 that fulfills the ETH to show thermalization at least for typical (non-equilibrium) initial wave functions and typical perturbations?

Thank you for your attention!

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- WLOG $u(f) = 0$ and let $\tilde{f}(x) = ||x|| f(x/||x||)$. For any $\delta > 0$,

$$\begin{aligned} u\{|f(\psi)| > \varepsilon\} &= \mathbb{P}\left\{|\tilde{f}(x)| > \varepsilon ||x||\right\} \\ &\leq \mathbb{P}\left\{|\tilde{f}(x)| > \delta\varepsilon\sqrt{D}\right\} + \mathbb{P}\left\{||x|| < \delta\sqrt{D}\right\} \\ &\leq \mathbb{P}\left\{|\tilde{f}(x)| > \delta\varepsilon\sqrt{D}\right\} + \mathbb{P}\left\{\Big|||x|| - \mathbb{E}||x||\Big| > \mathbb{E}||x|| - \delta\sqrt{D}\right\}. \end{aligned}$$

Now apply Lévy's Lemma for Gaussian random variables to the Lipschitz functions $\tilde{f}(x)$ and $g(x) = ||x||$.

Ideas of Proof (Canonical Typicality)

- Let $(U_a^j)_{j=0}^{d_a^2-1}$ be an orthogonal operator basis for $\mathcal{L}(\mathcal{H}_a)$ such that $\mathrm{tr}_a(U_a^{j*}U_a^k) = d_a\delta_{jk}$ and write

$$\rho_a^\psi = \frac{1}{d_a}\sum_j C_j(\rho_a^\psi)U_a^j$$

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- This implies

$$\begin{aligned} u_R & \left\{\psi \in \mathbb{S}(\mathcal{H}_R) : \|\rho_a^\psi - \mathrm{tr}_b\, \rho_R\|_{\mathrm{tr}} > \varepsilon d_a\right\} \\ & \leq u_R \left\{\psi \in \mathbb{S}(\mathcal{H}_R) : \exists j : \left|C_j(\rho_a^\psi) - C_j(\mathrm{tr}_b\, \rho_R)\right| > \varepsilon\right\} \\ & = u_R \left\{\psi \in \mathbb{S}(\mathcal{H}_R) : \exists j : \left|\mathrm{tr}_a(U_a^j \rho_a^\psi) - \mathrm{tr}_a(U_a^j\, \mathrm{tr}_b\, \rho_R)\right| > \varepsilon\right\} \end{aligned}$$

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- Finally apply Lévy's Lemma to $f : \mathbb{S}(\mathcal{H}_R) \to \mathbb{R}$, $f(\psi) = \mathrm{tr}_a(U_a^j \rho_a^\psi)$

Ideas of Proof (Lévy's Lemma for GAP measures)

- An application of Lévy's Lemma for Gaussian random variables to $F \circ \sqrt{\rho/2} : \mathbb{C}^D \to \mathbb{R}$ shows that for every $\varepsilon > 0$,

$$\mathbb{P}\left\{|F(Z) - \mathbb{E}F(Z)| > \varepsilon\right\} \leq 2\exp\left(-\frac{4\varepsilon^2}{\pi^2\eta^2\|\rho\|}\right).$$

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- First assume that $D < \infty$. Wlog $\mathrm{GAP}(\rho)(f) = 0$ and for $0 < r < 1$ define $\tilde{f} : \mathcal{H} \to \mathbb{R}$ by

$$\tilde{f}(\psi) = \begin{cases} f\left(\frac{\psi}{\|\psi\|}\right) & \text{if } \|\psi\| \geq r, \\ r^{-1}\|\psi\| f\left(\frac{\psi}{\|\psi\|}\right) & \text{if } \|\psi\| \leq r. \end{cases}$$

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- We find

$$\mathrm{GAP}(\rho)\left\{|f(\psi)| > \varepsilon\right\} \leq \mathrm{GA}(\rho)\left\{\left|\tilde{f}(\psi) - \mathrm{GA}(\rho)(\tilde{f})\right| > \varepsilon - |\mathrm{GA}(\rho)(\tilde{f})|\right\}$$
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- In the infinite-dimensional case consider

$$\rho_n := \sum_{m=1}^{n-1} p_m |m\rangle\langle m| + \left(\sum_{m=n}^{\infty} p_m\right) |n\rangle\langle n|\,,$$

note that $\|\rho_n - \rho\|_{\mathrm{tr}} \to 0$ and therefore $\mathrm{GAP}(\rho_n) \Rightarrow \mathrm{GAP}(\rho)$

Ideas of Proof (Lévy's Lemma for GAP measures)

- Portmanteaus's Theorem states that a sequence (μ_n) of probability measures on a measurable space $(E, \mathcal{B})$ converges weakly to a probability measure μ on $(E, \mathcal{B})$ if and only if $\liminf_{n\to\infty} \mu_n(O) \geq \mu(O)$ for all open sets $O \in \mathcal{B}$

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- Let $\varepsilon' > 0$. With $A_\varepsilon := \{\psi \in \mathbb{S}(\mathcal{H}) : |f(\psi)| > \varepsilon\}$ it follows from Portmanteau's Theorem that

$$\mathrm{GAP}(\rho)(A_\varepsilon) \leq \liminf_{n\to\infty} \mathrm{GAP}(\rho_n)(A_\varepsilon) \leq \mathrm{GAP}(\rho_N)(A_\varepsilon) + \varepsilon'$$

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- Generalized Canonical Typicality follows from Lévy's Lemma for GAP measures similarly as in the case of Canonical Typcality (with some extra steps needed for covering infinite dimensions)