What Really Lies Behind the Grand-Canonical Ensemble in Quantum Mechanics

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The Gibbs ensembles in quantum mechanics

Density matrices:

$$\begin{aligned} \text{micro-canonical} \quad & \hat{\rho}_{\mathrm{mc}} = Z_{\mathrm{mc}}^{-1}\, 1_{[E-\Delta E, E]}(\hat{H}) \\ \text{canonical} \quad & \hat{\rho}_{\mathrm{can}} = Z_{\mathrm{can}}^{-1} \exp(-\beta \hat{H}) \\ \text{grand-canonical} \quad & \hat{\rho}_{\mathrm{gc}} = Z_{\mathrm{gc}}^{-1} \exp\big(-\beta(\hat{H} - \mu_1 \hat{N}_1 - \ldots - \mu_r \hat{N}_r)\big) \end{aligned}$$

But also probability distributions . . .

[Bloch 1950s, Goldstein et al. 2006]

. . . of the wave function in the unit sphere $\mathbb{S}(\mathscr{H}) = \{\psi \in \mathscr{H} : \|\psi\| = 1\}$,

$$\mathbb{P}_{\mathrm{mc}}(d\psi) = u_{\mathbb{S}(\mathscr{H}_{[E-\Delta E,E]})}(d\psi) \quad \text{uniform}$$

$$\mathbb{P}_{\mathrm{can}}(d\psi) = \mathrm{GAP}_{\hat{\rho}_{\mathrm{can}}}(d\psi)$$

$$\mathbb{P}_{\mathrm{gc}}(d\psi) = \ldots \quad \text{later}$$

$\mathrm{GAP}_{\hat{\rho}}$ (Gaussian adjusted projected measure) = "Scrooge measure" [Jozsa et al. 1994, Goldstein et al. 2006] is the most spread-out measure on $\mathbb{S}(\mathscr{H})$ with density matrix given by $\hat{\rho}$.

Density matrix of a measure μ on $\mathbb{S}(\mathscr{H})$: $\hat{\rho}_\mu = \int_{\mathbb{S}(\mathscr{H})} \mu(d\psi)\, |\psi\rangle\langle\psi|$

The justification of $\hat\rho_{\mathrm{can}}, \hat\rho_{\mathrm{gc}}, \mathbb{P}_{\mathrm{can}}, \mathbb{P}_{\mathrm{gc}}$ has to do with...

...weakly coupling the quantum system S to another quantum system B ("bath") much bigger than S but finite.

Precise sense in which a distribution μ on $\mathbb{S}(\mathscr{H})$ is "correct":

μ agrees with the distribution of the conditional wave function ψ^S [Dürr et al. 1992]: Given $\Psi \in \mathscr{H} = \mathscr{H}^S \otimes \mathscr{H}^B$ and ONB $b = \{|b_1\rangle, |b_2\rangle, \ldots\}$ of $\mathscr{H}^B$, ψ^S is the random wave function one would obtain for S if one carried out a quantum measurement of b,

$$\psi^S = \frac{\langle b_J|\Psi\rangle_B}{\|\langle b_J|\Psi\rangle_B\|} \text{ with } \mathbb{P}(J=j) = \|\langle b_j|\Psi\rangle_B\|^2 .$$

Sense in which $\hat\rho_{\mathrm{can}}$ is "correct": reduced density matrix (partial trace)

1. $\hat\rho^S_{\mathrm{can}} \approx \mathrm{tr}^B\, \hat\rho^{S\cup B}_{\mathrm{mc}}$
2. $\hat\rho^S_{\mathrm{can}} \approx \mathrm{tr}^B\, |\Psi\rangle\langle\Psi|$ for most $\Psi \in \mathbb{S}(\mathscr{H}^{S\cup B}_{[E-\Delta E, E]})$ ("canonical typicality") [Gemmer et al. 2004, Popescu et al. 2005, Goldstein et al. 2005].

The first statement is the average of the second.

Contrasting with a standard way of justifying $\hat{\rho}_{\mathrm{can}}$:

$\hat{\rho}_{\mathrm{can}}$ maximizes the von Neumann entropy

$$S_{\mathrm{vN}} = -k_{\mathrm{B}}\, \mathrm{tr}(\hat{\rho} \log \hat{\rho})$$

under the constraint that the expected energy is fixed, $\mathrm{tr}(\hat{\rho}\hat{H}) = E$ (and $\hat{\rho}_{\mathrm{gc}}$ if in addition the particle numbers $\mathrm{tr}(\hat{\rho}\hat{N}_i) = n_i$ are fixed).

Disadvantages of a derivation of $\hat{\rho}_{\mathrm{can}}$ based on this fact:

- The maximizer represents an observer's knowledge (subjective probability). If statistical mechanics were limited to subjective probability, then it would not be justified in most applications (e.g., the formation of stars before humans existed). In contrast, canonical typicality shows how $\hat{\rho}_{\mathrm{can}}$ occurs in nature.
- Unclear why one should constrain the expectation value. If the observer had knowledge that the energy lies in $[E - \Delta E, E]$, then one should constrain on this subspace, not the expectation.

Side remark

Aren't also $\hat{\rho}_{\mathrm{mc}}, \mathbb{P}_{\mathrm{mc}}$ expressions of subjective probability?

No, they are expressions of thermal equilibrium: it is the nature of thermal equilibrium that micro states in thermal equilibrium behave like *most* micro states with approximately given E (etc.).

Two situations in which the grand-canonical ens. arises

(classically or quantum-mechanically)

1. spatial equilibrium: S is a spatial region that molecules can enter or leave, so their number n^S can change.
2. chemical equilibrium: a chemical reaction such as

$$A + B \leftrightharpoons C + \delta E$$

can change the numbers n_A, n_B, n_C of molecules;
δE = energy released (or, if negative, consumed).

Many textbooks focus on 1. I will talk a lot about 2.

Questions:

- What are the numbers $n_{\mathrm{eq},i}$ of $i \in \{A, B, C\}$ in chemical equilibrium?
- How can grand-canonical density matrices be used for calculating them?

But isn't it obvious?

Everyone would guess $n_{\mathrm{eq},i} = \mathrm{tr}(\hat{\rho}_{\mathrm{gc}}\, \hat{N}_i)$.

Questions remain:

- Why is this correct? Justification from quantum mechanics?
- How do we know which values of μ_i to use? We know E and δE.

Chemical equilibrium (1)

Key consideration:

- conserved observables (such as $\hat{Q}_1 := \hat{N}_A - \hat{N}_B$ and $\hat{Q}_2 := \hat{N}_C + \hat{N}_A$ for $A + B \leftrightharpoons C + \delta E$)
- more abstract perspective of "generalized Gibbs ensemble" [Balian 1982, Rigol et al. 2007, precursor Landau-Lifshitz 1939]

$$\hat{\rho}_{\mathrm{gG}} = Z_{\mathrm{gG}}^{-1} \,\exp\Bigl(\sum_{k=1}^{K} \lambda_k \hat{Q}_k\Bigr)\,,$$

  where $\hat{Q}_1, \ldots, \hat{Q}_K$ are the macroscopic conserved observables, commute with each other (one of them is $\hat{H}$).
- $\Rightarrow$ K-parameter family of thermal equilibrium states

Chemical equilibrium (2)

- Define generalized micro-canonical subspace

$$\mathscr{H}_{\mathrm{gmc}} := \mathrm{span}\Big\{\phi \in \mathscr{H} \ : \ \forall k : \hat{Q}_k \phi = q_k \phi, \ q_k \in [Q_k - \Delta Q_k, Q_k]\Big\}$$

with intervals that are short on the macroscopic scale but allow $\dim \mathscr{H}_{\mathrm{gmc}} \gg 1$. Set $\hat{\rho}_{\mathrm{gmc}} = (\dim \mathscr{H}_{\mathrm{gmc}})^{-1} \hat{P}_{\mathrm{gmc}}$.

General Gibbs Principle

Suppose the self-adjoint operators $\hat{Q}_1, \ldots, \hat{Q}_K$ commute with each other. Then, in relevant senses of equivalence of ensembles, $\hat{\rho}_{\mathrm{gmc}}$ is equivalent to $\hat{\rho}_{\mathrm{gG}}$ with λ_k chosen so that

$$\mathrm{tr}(\hat{\rho}_{\mathrm{gG}} \, \hat{Q}_k) = Q_k \, .$$

Specific sense: Def $\hat{\rho}_1$ is *locally equivalent* to $\hat{\rho}_2$ $:\Leftrightarrow$ for every small spatial region S (with complement $S^c = \Lambda \setminus S$), $\mathrm{tr}^{S^c} \hat{\rho}_1 \approx \mathrm{tr}^{S^c} \hat{\rho}_2$.

Use of $\hat\rho_{\mathrm{gc}}$ for chemical reactions (1)

- Possible chemical reactions

$$\nu_{\ell 1} A_1 + \ldots + \nu_{\ell r} A_r \leftrightharpoons \tilde\nu_{\ell 1} A_1 + \ldots + \tilde\nu_{\ell r} A_r + \delta E_\ell$$

  with $\ell = 1, \ldots, L$ and $\nu_{\ell i}, \tilde\nu_{\ell i} \in \{0, 1, 2, \ldots\}$ the number of molecules A_i.
- $\mathscr{H} = \mathscr{F}_1 \otimes \cdots \otimes \mathscr{F}_r$ with Fock space $\mathscr{F}_i = \bigoplus_{n_i=0}^{\infty} \mathscr{F}_i^{(n_i)}$
- Of $\hat H$, we assume that molecules, when separated by a sufficient microscopic distance, hardly interact.
- Let $\hat H_{1i}$ be the 1-molecule operator including kinetic energy of the center of mass and external fields.
- Let $\hat H_{0i}$ be the second quantization of $\hat H_{1i}$ (acting like $\hat H_{1i}$ on each particle of type i).
- Let $\hat H_0 = \sum_{i=1}^r \hat H_{0i}$ ("free Hamiltonian").
- Let E_{0i} be the *rest energy* of each i-molecule (= rest mass $\times c^2$ + ground state energy).
- Let $\hat H_* := \hat H_0 + \sum_{i=1}^r E_{0i} \hat N_i$, so

$$\hat H = \hat H_* + \hat V$$

  with $\hat V$ mostly negligibly small; $\hat V$ contains transition elements for each reaction but not otherwise.

Use of $\hat{\rho}_{\mathrm{gc}}$ for chemical reactions (2)

- Consider $\mathbb{R}^r$ with axes labeled $n_1 \ldots, n_r$.
- Let $\mathcal{L}$ be the subspace spanned by the L vectors $(\nu_{\ell 1} - \tilde{\nu}_{\ell 1}, ..., \nu_{\ell r} - \tilde{\nu}_{\ell r})$. Any change in particle numbers due to reactions lies in $\mathcal{L}$. Any conserved linear combination of $n_1 ... n_r$ is $\perp \mathcal{L}$.
- Choose a complete set $F_1, \ldots, F_{K-1}$ of conserved linear combinations (with $K := r + 1 - \dim \mathcal{L}$).
  That is, choose a linear mapping $F : \mathbb{R}^r \to \mathbb{R}^{K-1}$ with kernel $F^{-1}(0) = \mathcal{L}$. Then F has full rank $K - 1$, and each $F_k(n_1, \ldots, n_r)$ (for $k \leq K - 1$) is conserved in every reaction. Thus, the
  $$\hat{Q}_k := F_k(\hat{N}_1, \ldots, \hat{N}_r)$$
  commute with $\hat{Q}_K := \hat{H}$ and with each other.
- Now $\hat{\rho}_{\mathrm{gG}} = Z_{\mathrm{gG}}^{-1} \exp(\sum_{k=1}^{K} \lambda_k \hat{Q}_k)$ is defined. Choose λ_k so that $\mathrm{tr}(\hat{\rho}_{\mathrm{gG}} \hat{Q}_k) = Q_k$. If we had chosen F differently, $\hat{\rho}_{\mathrm{gG}}$ would have been the same.
- Choose suitably small ΔQ_k; now $\hat{\rho}_{\mathrm{gmc}}$ is defined.

Use of $\hat\rho_{\mathrm{gc}}$ for chemical reactions (3)

Now apply the general Gibbs principle:

- $\hat\rho_{\mathrm{gmc}}$ and $\hat\rho_{\mathrm{gG}}$ are equivalent ensembles.
- There is a K-parameter family of thermal equilibrium states.
- $$\hat\rho_{\mathrm{gG}} \approx \hat\rho_{\mathrm{gc}} = Z_{\mathrm{gc}}^{-1} \exp\Bigl(-\beta\bigl(\hat H_0 - \sum_{i=1}^{r} \mu_{0i} \hat N_i\bigr)\Bigr)$$

  with $r+1$ parameters
  - $\beta = -\lambda_K$ (> 0 assuming unbounded $\hat H \geq 0$)
  - $\mu_{0i} = \beta^{-1} \sum_{k=1}^{K-1} \lambda_k F_{ki} - E_{0i}$

  determined by the conditions

  $$(1) \quad \sum_{i=1}^{r} (\mu_{0i} + E_{0i})(\nu_{\ell i} - \tilde\nu_{\ell i}) = 0 \quad \bigl(\Leftarrow \; F(\mathcal{L}) = 0\bigr) \text{ for } \ell = 1, \ldots, L$$

  $$(2) \quad \mathrm{tr}(\hat\rho_{\mathrm{gG}}\, \hat Q_k) = Q_k \quad \text{for } k = 1, \ldots, K-1$$

  of which $r+1$ are independent.

In particular, $n_{\mathrm{eq},i} \approx \mathrm{tr}(\hat\rho_{\mathrm{gc}} \hat N_i)$, answering the question we asked.
Meaning of μ_{0i}: $\hat\rho_{\mathrm{gc}}$ looks as if canonical with ground state energy $-\mu_{0i}$.

Remarks

- The rest energies E_{0i} are usually not known. They don't need to be, because β and μ_{0i} can be determined by Eq.s (1) and (2). (In particular, different values $\tilde{E}_{0i}$ consistent with the δE_ℓ would lead to the same $\hat{\rho}_{\mathrm{gc}}$.)
- For spatial regions $\Lambda = \Lambda_1 \cup \Lambda_2 \subset \mathbb{R}^3$ bordering along surface Σ (most volume not close to Σ), usually $\hat{H}_0(\Lambda) \approx \hat{H}_0(\Lambda_1) \oplus \hat{H}_0(\Lambda_2)$. E.g., 1D negative discrete Laplacian in $\varepsilon\mathbb{Z}$ with $\Lambda_1 = \varepsilon\mathbb{Z} \cap [0,\infty)$, $\Lambda_2 = \varepsilon\mathbb{Z} \cap (-\infty, 0)$ has $\varepsilon^2 \hat{H}_0(\Lambda) = -\varepsilon^2 \Delta =$

$$\left[\begin{array}{ccc|ccc}
\ddots & -1 & & & & \\
-1 & 2 & -1 & & & \\
 & -1 & 2 & -1 & & \\
\hline
 & & -1 & 2 & -1 & \\
 & & & -1 & 2 & -1 \\
 & & & & -1 & \ddots
\end{array}\right] \approx \left[\begin{array}{ccc|ccc}
\ddots & -1 & & & & \\
-1 & 2 & -1 & & & \\
 & -1 & 2 & & & \\
\hline
 & & & 2 & -1 & \\
 & & & -1 & 2 & -1 \\
 & & & & -1 & \ddots
\end{array}\right]$$

Plausibility argument for the general Gibbs principle

$\hat{\rho}_{\mathrm{gmc}} \propto \hat{P}_{\mathrm{gmc}}$ is an equivalent ensemble to $\hat{\rho}_{\mathrm{gG}} \propto \exp\left(\sum_k \lambda_k \hat{Q}_k\right)$.

- Any ONB $\{\phi_j\}$ that jointly diagonalizes $\hat{Q}_1, \ldots, \hat{Q}_K$ also diagonalizes $\hat{\rho}_{\mathrm{gmc}}$ and $\hat{\rho}_{\mathrm{gG}}$.
- For $\alpha = \mathrm{gmc}$ and $\alpha = \mathrm{gG}$, consider the Born distribution in $\mathbb{R}^K$,

$$p_\alpha(q_1, \ldots, q_K) = \mathrm{tr}\Big(\hat{\rho}_\alpha\, \hat{P}\big(\hat{Q}_1 = q_1, \ldots, \hat{Q}_K = q_K\big)\Big)\,.$$

- Both are sharply peaked at $(q_1, \ldots, q_K) = (Q_1, \ldots, Q_K)$:
  - $\hat{\rho}_{\mathrm{gmc}}$ because it is concentrated in $\prod_k [Q_k - \Delta Q_k, Q_k]$
  - $\hat{\rho}_{\mathrm{gG}}$ because its expectation is $(Q_1, \ldots, Q_K)$, much larger values of q_k are suppressed by exponential dependence, much smaller values are suppressed provided the joint "density of states" increases quickly with each q_k (as for energy or particle number).
- The peaks may have different width (Q_k/N for gmc and $Q_k/\sqrt{N}$ for gG), but macro observables (or partial traces in small regions S) should not detect that.

Our main claims (1)

- Let $\Lambda \subset \mathbb{R}^3$ ("the available volume"), $S^c := \Lambda \setminus S$.
- Suppose for every region $S \subseteq \Lambda$, $\mathscr{H} = \mathscr{H}^S \otimes \mathscr{H}^{S^c}$.
- Suppose $\hat{Q}_1, \ldots, \hat{Q}_K$ commute with each other and are approximately additive (extensive), i.e., for any $S \subseteq \Lambda$,

$$\hat{Q}_k \approx \hat{Q}_k^S \otimes \hat{I}^{S^c} + \hat{I}^S \otimes \hat{Q}_k^{S^c}\,.$$

- As a consequence,

$$\hat{\rho}_{\mathrm{gG}} \approx \hat{\rho}_{\mathrm{gG}}^S \otimes \hat{\rho}_{\mathrm{gG}}^{S^c} \text{ and } \mathrm{tr}^{S^c}\,\hat{\rho}_{\mathrm{gG}} \approx \hat{\rho}_{\mathrm{gG}}^S\,.$$

Statement 1 (reduced $\hat{\rho}_{\mathrm{gmc}}$)

If $\lambda_1, \ldots, \lambda_K$ are chosen so that $\mathrm{tr}(\hat{\rho}_{\mathrm{gG}}\hat{Q}_k) = Q_k$, then for small $S \subset \Lambda$,

$$\mathrm{tr}^{S^c}\,\hat{\rho}_{\mathrm{gmc}} \approx \hat{\rho}_{\mathrm{gG}}^S\,.$$

In particular, $\hat{\rho}_{\mathrm{gmc}}$ is locally equivalent to $\hat{\rho}_{\mathrm{gG}}$.

Our main claims (2)

- Special case $\hat{N}_i$: Let $\mathscr{H} = \mathscr{F}_1 \otimes \cdots \otimes \mathscr{F}_r$ with $\mathscr{F}_i$ the (bosonic or fermionic) Fock space over the 1-particle space $\mathscr{H}_{1i}$. Suppose

$$\hat{H} \approx \hat{H}_* = \hat{H}_0 + \sum_{i=1}^{r} E_{0i} \hat{N}_i \,, \qquad \hat{H}_0 = \sum_{i=1}^{r} d\Gamma(\hat{H}_{1i}) \,,$$

$$\mathscr{H}_{1i} = \mathscr{H}_{1i}^{S} \oplus \mathscr{H}_{1i}^{S^c} \,, \qquad \hat{H}_{1i} \approx \hat{H}_{1i}^{S} \oplus \hat{H}_{1i}^{S^c} \,.$$

  Define $\hat{Q}_k := F_k(\hat{N}_1, \ldots, \hat{N}_r)$ and $\hat{Q}_K := \hat{H}$.
  For β, μ_{0i} satisfying (1) and (2), $\hat{\rho}_{\mathrm{gmc}}$ is locally equivalent to $\hat{\rho}_{\mathrm{gc}}$.

Our main claims (3)

Theorem [Popescu, Short, Winter 2005]

For any $\mathscr{H}^S, \mathscr{H}^B$ of finite dimension, any high-dimensional subspace $\mathscr{H}_R \subseteq \mathscr{H}^S \otimes \mathscr{H}^B$, and most pure states $\Psi \in \mathbb{S}(\mathscr{H}_R)$,

$$\mathrm{tr}^B \, |\Psi\rangle\langle\Psi| \approx \mathrm{tr}^B \, \hat{\rho}_R$$

with $\hat{\rho}_R = (\dim \mathscr{H}_R)^{-1} \hat{P}_R =$ normalized projection to $\mathscr{H}_R$.

As a consequence:

Statement 2 (ensemble typicality)

In the setting of Statement 1, for small $S \subset \Lambda$ and most $\Psi \in \mathbb{S}(\mathscr{H}_{\mathrm{gmc}})$,

$$\mathrm{tr}^{S^c} \, |\Psi\rangle\langle\Psi| \approx \hat{\rho}^S_{\mathrm{gG}} \, .$$

- Special case $\hat{N}_i$ (grand-canonical typicality): for small $S \subset \Lambda$ and most $\Psi \in \mathbb{S}(\mathscr{H}_{\mathrm{gmc}})$, $\mathrm{tr}^{S^c} \, |\Psi\rangle\langle\Psi| \approx \hat{\rho}^S_{\mathrm{gc}}$.
  (Note: in $\mathscr{H}_{\mathrm{gmc}}$ we constrain also $\hat{Q}_k = F_k(\hat{N}_1 \ldots \hat{N}_r)$.)

The GAP measure

Def of $\mathrm{GAP}_{\hat\rho}$ for any density matrix $\hat\rho : \mathscr{H} \to \mathscr{H}$

Let $\mathrm{G}_{\hat\rho}$ be the Gaussian measure on $\mathscr{H}$ with mean 0 and covariance $\hat\rho$.
Let $\mathrm{GA}_{\hat\rho}(d\psi) = \|\psi\|^2 \, \mathrm{G}_{\hat\rho}(d\psi)$ ("Gaussian adjusted measure").
Let Ψ^{GA} have distribution $\mathrm{GA}_{\hat\rho}$; then $\mathrm{GAP}_{\hat\rho}$ is the distribution of $\Psi^{\mathrm{GAP}} := \Psi^{\mathrm{GA}}/\|\Psi^{\mathrm{GA}}\|$ ("Gaussian adjusted projected measure").

- $\hat\rho_{\mathrm{GAP}_{\hat\rho}} = \hat\rho$
- $\mathrm{GAP}_{\hat\rho_{\mathrm{gmc}}} = u_{\mathbb{S}(\mathscr{H}_{\mathrm{gmc}})}$ uniform
- $\mathrm{GAP}_{\hat\rho}$ is the natural measure on $\mathbb{S}(\mathscr{H})$ with density matrix $\hat\rho$.
- Continuous dependence: If $\hat\rho_1 \approx \hat\rho_2$, then $\mathrm{GAP}_{\hat\rho_1} \approx \mathrm{GAP}_{\hat\rho_2}$.

Our main claims (4)

- Let $\mathscr{L}_X$ denote the distribution of the random variable X.
- Let ψ^S denote again the conditional wave function for given $\Psi \in \mathbb{S}(\mathscr{H}^S \otimes \mathscr{H}^B)$ and ONB b of $\mathscr{H}^B$: the (pure) state of S after a measurement of b on Ψ.

Theorem [Goldstein et al. 2015]

For any $\mathscr{H}^S$ of finite dimension, any $\mathscr{H}^B$ of high dimension, and most ONBs $b = \{|b_1\rangle, |b_2\rangle, \ldots\}$ of $\mathscr{H}^B$,

$$\mathscr{L}_{\psi^S} \approx \mathrm{GAP}_{\mathrm{tr}^B |\Psi\rangle\langle\Psi|} \,.$$

As a consequence,

Statement 3 ($\mathbb{P}_{\mathrm{gG}}$ for typical ONB)

In the setting of Statement 1, for any small $S \subset \Lambda$, most $\Psi \in \mathbb{S}(\mathscr{H}_{\mathrm{gmc}})$, and most ONBs b of $\mathscr{H}^{S^c}$,

$$\mathscr{L}_{\psi^S} \approx \mathrm{GAP}_{\hat\rho^S_{\mathrm{gG}}} \,.$$

- Special case $\hat N_i$ (grand-canonical): $\mathscr{L}_{\psi^S} \approx \mathrm{GAP}_{\hat\rho^S_{\mathrm{gc}}}$

We are particularly interested in the position basis

- The concept of conditional wave function originated in Bohmian mechanics [Dürr et al. 1992], where the basis b is the position (i.e., configuration) basis.
- Is the position basis a typical basis?
- A typical basis is unrelated to either $\hat{H}$ or $\hat{Q}_k$.
- However, the position basis diagonalizes all $\hat{N}_i$, and thus all $\hat{Q}_k$ $(k \leq K-1)$ in the grand-canonical case.
- That is why we are also interested in ONBs b that diagonalize the $\hat{N}_i$ (or the $\hat{Q}_k$) and are otherwise typical.

Our main claims (5)

Notation $\mu = \bigoplus_j p(j)\,\mu_j$ for the prob. distribution that is the mixture of the prob. distributions μ_j with weights $p(j) \geq 0$, $\sum_j p(j) = 1$

Statement 4 ($\mathbb{P}_{\mathrm{gc}}$ for ONB diagonalizing $\hat{N}_i^{S^c}$)

In the grand-canonical setting, suppose $\Delta Q_k = 0$ and Q_k is an eigenvalue of $\hat{Q}_k$. Then for any small $S \subset \Lambda$, most $\Psi \in \mathbb{S}(\mathscr{H}_{\mathrm{gmc}})$ and most ONBs b of $\mathscr{H}^{S^c}$ that diagonalize $\hat{N}_1^{S^c}, \ldots, \hat{N}_r^{S^c}$,

$$\mathscr{L}_{\psi^S} \approx \mathbb{P}_{\mathrm{gc}} := \bigoplus_{q_1^S,\ldots,q_{K-1}^S} p(q_1^S, \ldots, q_{K-1}^S)\,\mathrm{GAP}_{\hat{\rho}^S(q_1^S,\ldots,q_{K-1}^S)}$$

with $p(q_1^S, \ldots, q_{K-1}^S) = \mathrm{tr}(\hat{\rho}_{\mathrm{gc}}^S \hat{P})$, $\hat{P}$ the projection to the joint eigenspace of $\hat{Q}_1^S, \ldots, \hat{Q}_{K-1}^S$ with eigenvalues $q_1^S, \ldots, q_{K-1}^S$, and $\hat{\rho}^S(q_1^S, \ldots, q_{K-1}^S) = p(q_1^S, \ldots, q_{K-1}^S)^{-1}\,\hat{P}\,\hat{\rho}_{\mathrm{gc}}^S\,\hat{P}$.

Instead of a GAP measure, $\mathbb{P}_{\mathrm{gc}}$ is a *mixture* of GAP measures with weights given by the Born distribution of $\hat{Q}_k^S$.

Approach (time evolution) to thermal equilibrium

- "Approach" means that for most $t \geq 0$ in the long run, S is in thermal equilibrium [von Neumann 1929].
- Here, "thermal equilibrium" means that $\mathrm{tr}^{S^c} |\Psi_t\rangle\langle\Psi_t| \approx \hat{\rho}^S_{\mathrm{gc}}$ and $\mathscr{L}_{\psi^S(t)} \approx \mathbb{P}_{\mathrm{gc}}$ ("microscopic thermal equilibrium," MITE), as opposed to thermalization of macro observables ("macroscopic thermal equilibrium," MATE) [Goldstein et al. 2010, 2017].
- We use the eigenstate thermalization hypothesis (ETH) for MITE (in the version of [Srednicki 1996]): for eigenvectors $\phi_1, \phi_2 \in \mathbb{S}(\mathscr{H}_{\mathrm{gmc}})$ of $\hat{H}$ with different eigenvalues,

$$\mathrm{tr}^{S^c} |\phi_1\rangle\langle\phi_1| \approx \mathrm{tr}^{S^c} \hat{\rho}_{\mathrm{gmc}}\,, \qquad \mathrm{tr}^{S^c} |\phi_1\rangle\langle\phi_2| \approx 0\,. \tag{3}$$

Statement 5 (approach to thermal equilibrium)

In the grand-canonical setting, suppose $\hat{H}$ satisfies the ETH (3). Then for every $\Psi_0 \in \mathbb{S}(\mathscr{H}_{\mathrm{gmc}})$ for most $t \geq 0$,

$$\mathrm{tr}^{S^c} |\Psi_t\rangle\langle\Psi_t| \approx \hat{\rho}^S_{\mathrm{gc}}\,.$$

Furthermore, for every $\Psi_0 \in \mathbb{S}(\mathscr{H}_{\mathrm{gmc}})$ for most ONBs b diagonalizing the $\hat{N}_i^{S^c}$ for most $t \geq 0$, $\mathscr{L}_{\psi^S(t)} \approx \mathbb{P}_{\mathrm{gc}}$.

Thank you for your attention