The BMV Conjecture:

an adventure in mathematical physics

Une aventure en Physique Mathématique
La Conjecture BMV

- 1975 Berni Rousset Villani
  - Review Rousset 2000

- 2003 Lieb Seiringer
Monotonic converging variational approximations to the functional integrals in quantum statistical mechanics

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We show, by making use of the functional integral technique, that, for a large class of useful quantum statistical systems, the partition function is, with respect to the coupling constant, the Laplace transform of a positive measure. As a consequence, we derive an infinite set of monotonically converging upper and lower bounds to it. In particular, the lowest approximation appears to be identical to the Gibbs–Bogolioubov variational bound, while the next approximations, for which we give explicit formulas for the first few ones, lead to improve the previous bound. The monotonic character of the variational successive approximations allows a new approach towards the thermodynamical limit.


Equivalent Forms of the Bessis–Moussa–Villani Conjecture

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The BMV conjecture for traces, which states that $\text{Tr} \exp(A - \lambda B)$ is the Laplace transform of a positive measure, is shown to be equivalent to two other statements: (i) The polynomial $\lambda \mapsto \text{Tr}(A + \lambda B)^p$ has only non-negative coefficients for all $A, B \geq 0, p \in \mathbb{N}$ and (ii) $\lambda \mapsto \text{Tr}(A + \lambda B)^{-p}$ is the Laplace transform of a positive measure for $A, B \geq 0, p > 0$.

KEY WORDS: BMV conjecture; Laplace transform; Padé approximants.

Dedicated with best wishes to Giovanni Jona-Lasinio on his 70th birthday
Original 1975 evaluation: Quantum Statistical Mechanics

\[ Z_\beta (A) = \text{Tr} (e^{-\beta H}) = \text{Tr} \exp (A - \beta B) \]
with \( A = -\beta H_0 \) \( B = -\beta H_1 \)
\( H = H_0 - \lambda H_1 \)

(Example in \( L^2(\mathbb{R}^n) \))
\( H_0 = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i,j=1}^{N} V(r_{ij}) \)
with \( \vec{p_i} = \frac{1}{2} \frac{\partial}{\partial \vec{r_i}} \) \( H_1 = V(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \)
(Schrödinger N-body equation)

Observation: if we have
\[ Z_\beta (A) = \int_0^\infty e^{-\beta \lambda} d\mu_\beta (\lambda) \]
we can obtain upper and lower bounds for \( Z_\beta (A) \) using a finite number of terms in the perturbation expansion (a perturbation parameter) if we have such a property (kernel of the laplacian \( e^{-\Delta} \) is positive), but positivity disappears with arbitrary multiplicity (Pauli)
* additional problem with \( N \rightarrow \infty \) limit
Lieb & Seiringer Theorem:

Let $A, B$ be Hermitian matrices $n \times n$, then the following statements are equivalent:

1. Suppose $A, B > 0$ and $p$ arbitrary integer. Then $Tr ((A+B)^p) = \sum_{k=0}^{p} \binom{p}{k} S_{kp}(A,B)$ and $S_{kp} > 0$ for all $0 \leq k \leq p$ with $A$ and $B$.

2. The function $\mathcal{Z}(\lambda) = Tr (\exp(A-\lambda B))$ is the Laplace transform $\mathcal{Z}(\lambda) = \int_0^\infty e^{-\lambda x} \, dp(x)$ where $p$ is a positive measure for any $A, B$ with $B > 0$.

3. For $A$ positive and $B$ positive definite and all $p > 0$ then the function $Tr ((A+B)^p)$ is the Laplace transform of a positive measure for any such $A$ and $B$.

* In fact, one needs

1. $B$ fixed
2. Any $A$ of the form $A+x B + c I$

provided that $c$ large enough to get $A+x B + c I > 0$.
Proof

1 \to 2 : \quad \text{Tr} \exp (A - \lambda B) = \sum_{k=0}^{\infty} \frac{1}{k!} \text{Tr}(A - \lambda B)^k

is a serie in \(-\lambda\) with only positive coefficients.

Therefore \((-1)^n \frac{d^n}{d\lambda^n} \text{Tr} \exp (A - \lambda B)\) is positive

for any \(\lambda > 0\)

Bernstein's Theorem implies that it is a

Laplace Transform of a positive measure.

2 \to 3 \quad \text{Use:}

\[
\frac{1}{(A + \lambda B)^p} = \frac{1}{\Gamma(p)} \int_0^\infty \exp(-t(A + \lambda B)) t^{-p} \, dt
\]

and take the trace (needs a without the condition \(A > 0\)).

3 \to 1 \quad \text{let } p \text{ integer, set } A = a^{-1}, B = a^{-1/2} ba^{-1/2}

an algebraic lemma shows that:

\[
\left. \frac{d^n}{d\lambda^n} \frac{1}{(A + \lambda B)^p} \right|_{\lambda = 0} = \frac{p}{p+n} \left. \text{Tr}(A + \lambda B)^{p+n} \right|_{\lambda = 0}
\]

\(\uparrow\)

Use 3

(Note 3 for \(p\) integer \(\to 1 \to 2 \to 3\) for any \(p\))

in the last proof the case \(A\) non invertible is

obtained by continuity.
Conjecture (BMV)

The propositions 1, 2, 3 hold for any $A, B > 0$ hermitian
any dimension

- Proposition 1 extend to any $A$ hermitian operator
  (bounded from below)
- True for $n=2$
- Non-explicit for $n=3 < \forall$ any counter example!
- It is sufficient to prove the case $A, B$ real symmetric
- True under the following positivity hypothesis:

In a basis where $B$ is diagonal,
the off diagonal elements $A_{ij}$ are real
and positive

$\Rightarrow$ Schoenberg case

- Partial results $n=3$. Parametrize $A, B$ as

$$B = \begin{pmatrix} b_1 & 0 & 0 \\ 0 & b_2 & 0 \\ 0 & 0 & b_3 \end{pmatrix}$$

$$A = \begin{pmatrix} a_1 & z & ye^{i\varphi} \\ z & a_2 & x \\ ye^{i\varphi} & x & a_3 \end{pmatrix}$$

$A_{ij}$ are real

$\Delta = \begin{pmatrix} 1 & 1 & 1 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{pmatrix}$

$b_1 < b_2 < b_3$

Conjecture holds if one (at least) of the two numbers

$$\begin{align*}
2XYZ \cos \varphi + \Delta \frac{y^2}{b_3-b_1} \\
2XYZ \cos \varphi - \Delta \inf \left\{ \frac{z^2}{b_2-b_1}, \frac{x^2}{b_3-b_2} \right\}
\end{align*}$$

- In particular Conjecture holds if $\cos \varphi > 0$

- Additional result by Drineas et al. (in one case
  with $a_1=a_2=a_3=0$ and $e^{i\varphi}=-1$)
- The Conjecture holds for some set of random matrices (Fannes-Petz) (2001)

- The Conjecture holds for some infinite dimensional $C^*$ Algebra (Bożejko) 2008 amounts to the case when $A$ and $B$ are in a 3-442 Fock space.

  - Remark: this is for infinite dimensional case when only case 2-3 hold in Lieb's proof

- What is the density in the Laplace transform?

  $n=2$: Bessel Function

  $n=3$: Very complicated expression in terms of hypergeometric functions

  (Drmota, Schachermayer, Teichmann) (2005)

  Using these conjectures: important numerical investigation by Grafendorfer (2009)

  No counterexample found.
Some unsuccessful attempts for the exponential form

- No generalization possible to more than one variable \( \text{Tr} \exp(A-xB_1-x_2B_2) \) \( (Gaudin) 1978 \)

- An inequality quoted by Lieb, Dyson, Simon \( (1978) \) in an attempt to prove existence of phase transition for Heisenberg (quantum) model appeared to be wrong. BMV would have been a corollary

- Conjecture wrong if we replace \( \text{Tr} \) by \( \text{Tr} P \) where \( P \) is a projector on one eigenvalue of \( B \). Counterexample by Froissart \( \approx 1976 \)

- Variational approach

\[
\Omega_n(A|B) = (-1)^n \frac{d^n}{dx^n} \left|_{x=0} \text{Tr} \left( \exp(A-xB) \right) \right|
\]

has only minima (no max, no saddle points) under variation of \( B \) at fixed \( A \).
However domain unbounded \( (Lecoultre 1978) \)
Polynomial Version

Since 2004 many workers of different hand tried to approach the Conjecture

\[ S_{kn}(A;B) \geq 0 \quad \text{Tr} (A + xB)^{2} = \sum_{k=0}^{n} x^{k} S_{kn}(A;B) \]

\[ A, B > 0 \]

* Hillar and his workers, Hagele

Look at algebraic equation between words with two letters:

\[ S_{kn}(A;B) = \sum \text{words with} \ \{ \text{letters starting} \ \& \ \text{in-lating} \ A \} \]

Try to express such a word as a sum of "squared" words + commutation

In such a case potentially obtained (Hagele for S_{kn} for n \leq 7 angle)

- If some S_{kn} < 0, then for any S_{kn'} with n' > n there exist A;B such that S_{kn'} < 0
Asymptotic results
(Fleischhack and Friedrich 2009)

There exists $N(A, B, k)$ such that
$S_{km} \geq 0$ if $Tr(AB) > 0$ and $m > N(A, B, k)$

more precisely $AB=0 \implies [A,B]=0$

* Burgdorf (2009)
$S_{m4} \geq 0$

* Kopp Schweighöfer
$S_{mk} \geq 0$ for $m \leq 13$

* Connection with C* Algebra problem

Gauss embedding theorem
Conclusion

Still improved since 35 years for the exponential version, 5 years for the algebraic one.

- Difficult because if counterexamples exist they can involve $m$ large coefficients even may be too large for easy computation.

- Reason to believe in the validity
  - Tractable numerics in dimension 3 and unexpected pattern in the set of already proven for
  - Random matrices
  - Looking carefully at Le Cointeau's

- Variational approach leads to a mystery: why doesn't it work?

See you again within 35 years!