Geometry, Topology, and Dynamics of Many-Body Systems: Quantum and Classical Perspectives

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PhD Defense

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2) Mixed Quantum States: Entanglement and Quantum Correlations
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Part I:

Entanglement and Quantum Correlations

1) Pure Quantum States: Entanglement and Correlation Patterns

1) Pure Quantum States: Entanglement and Correlation Patterns

Quantum entanglement, a direct consequence of the specificities of measurement processes in **Quantum Mechanics**: ***measuring a quantum object modifies its state*.**

First noticed by EPR in 1935, named by Schrödinger on the same year.

Inconsistency of **quantum theory** (hidden variables)?

Bell's inequalities: proof that entanglement cannot come from **hidden variables**.
Aspect's experiments showed violation of **Bell's inequalities**.

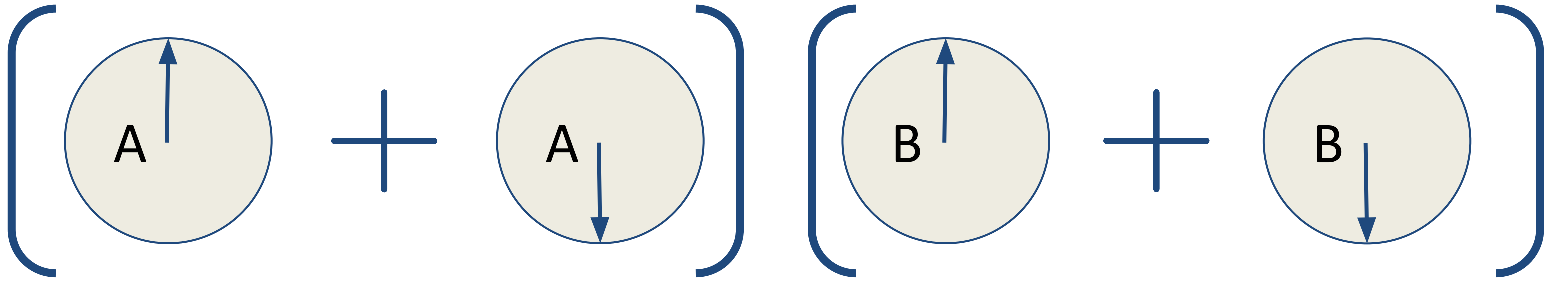
Of major importance in today's quest for achieving the **quantum computer**.

A. Einstein, B. Podolsky, and N. Rosen, "*Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?*", Phys. Rev., 1935
E. Schrödinger, "*Discussion of Probability Relations between Separated Systems*", Math. Proc. of the Cambridge Philo. Soc., 1935
J. S. Bell, "*On the Einstein Podolsky Rosen paradox*", Physics Physique Fizika,1964
A. Aspect, P. Grangier, and G. Roger, "*Experimental Tests of Realistic Local Theories via Bell's Theorem*", Physical Review Letters, 1981
R.P. Feynman, *Simulating physics with computers*. *Int J Theor Phys*, 1982

1) Pure Quantum States: Entanglement and Correlation Patterns

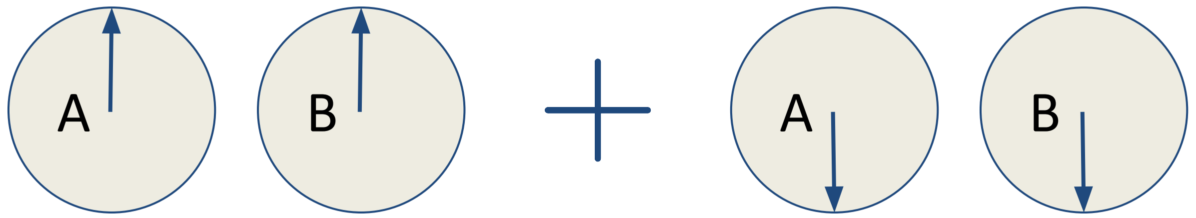
Product state:

$$|\varphi\rangle = (|\uparrow\rangle + |\downarrow\rangle) \otimes (|\uparrow\rangle + |\downarrow\rangle)/2$$



Entangled state (here, **Bell state**):

$$|\psi_+\rangle = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$$



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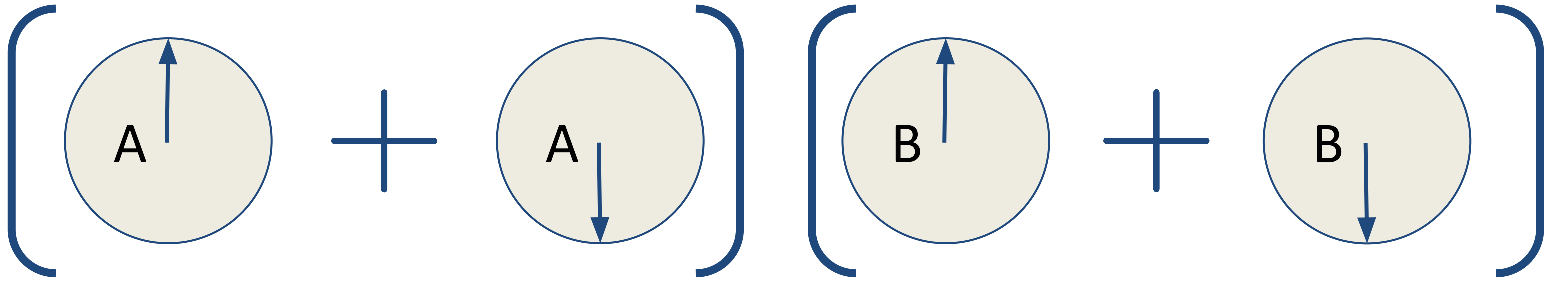
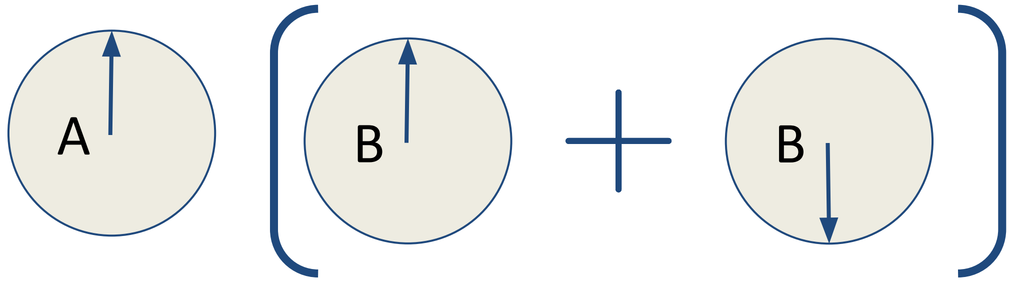


Measuring A pointing upward:



does not affect the state of B.

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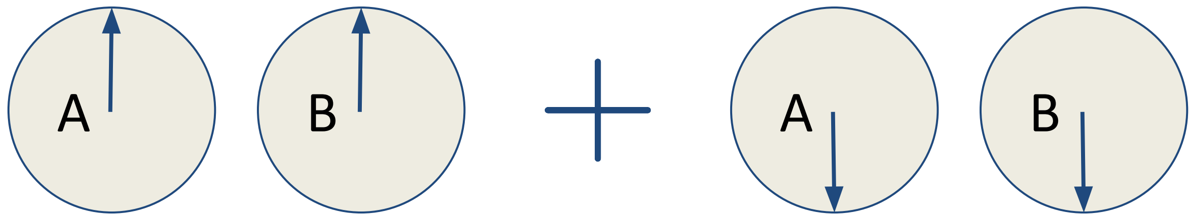

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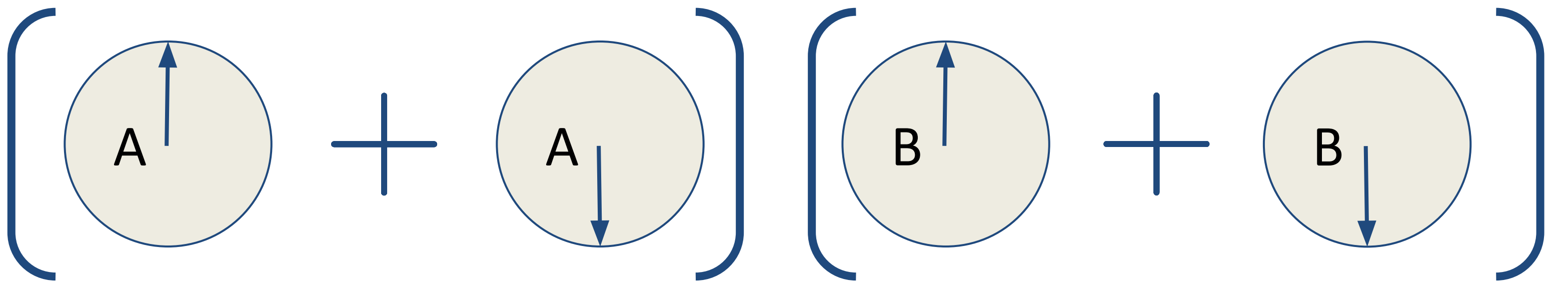

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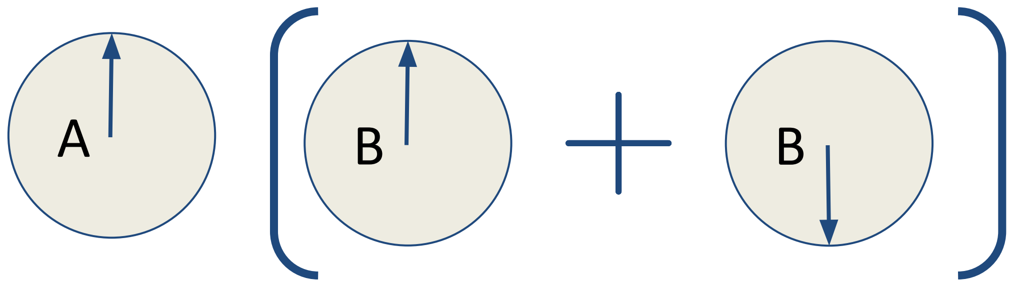

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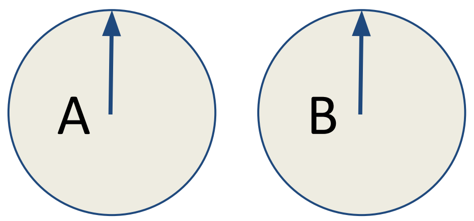

projects B onto the upward-pointing state.

I. Entanglement and Quantum Correlations

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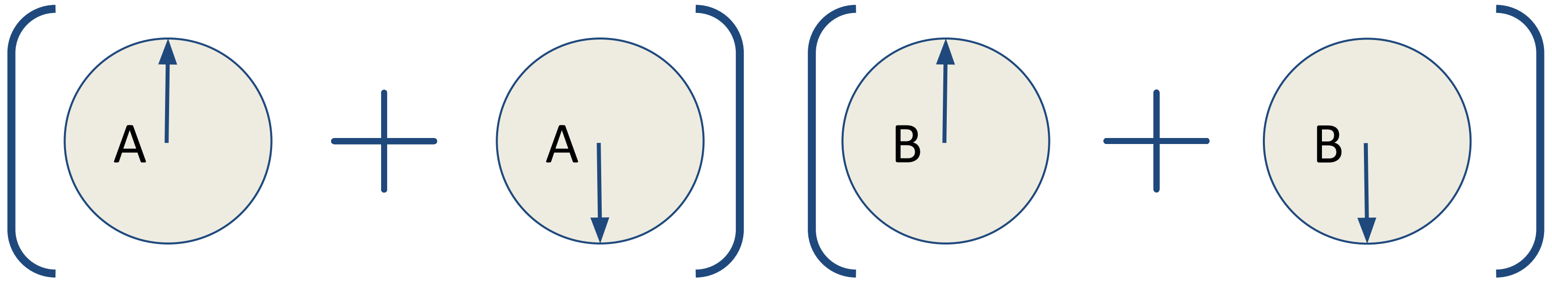

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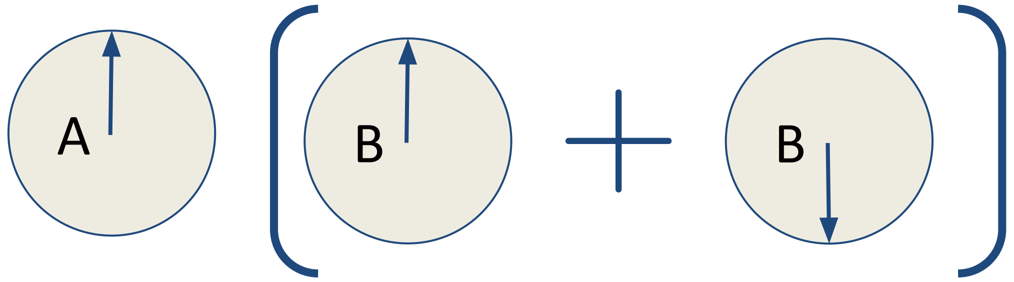

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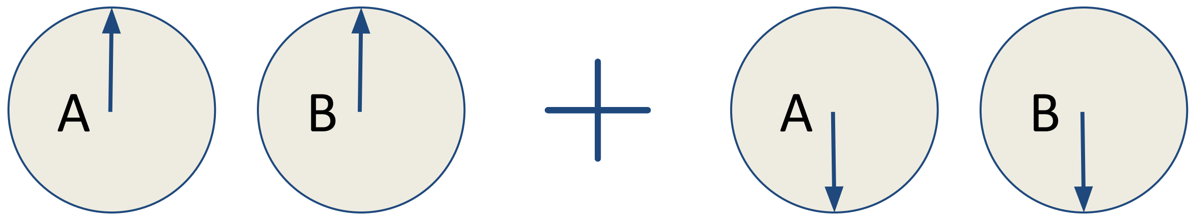

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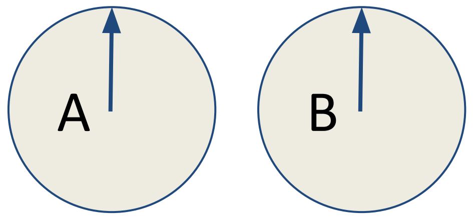


projects B onto the upward-pointing state.

Entangled pair : **measurement** on A **may** modify the state of B.

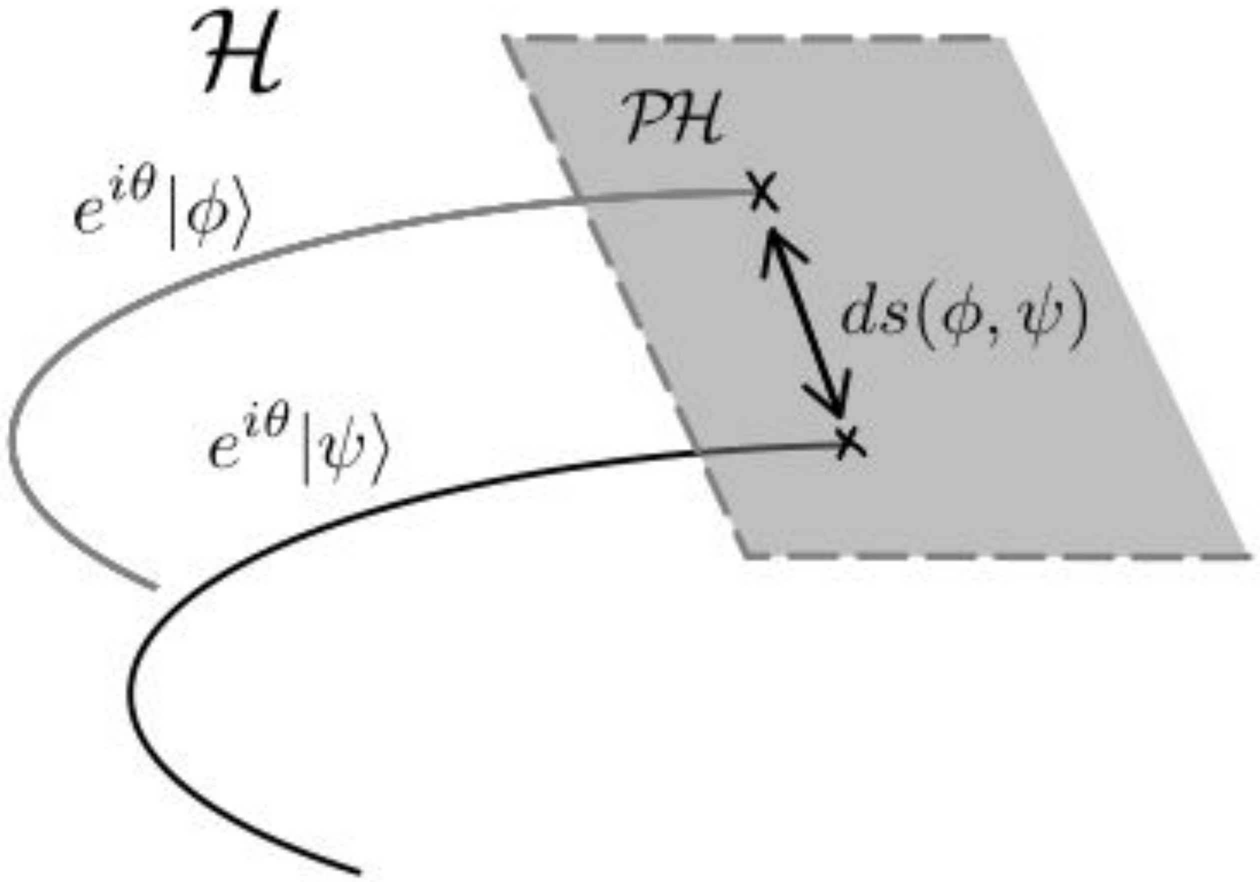
1) Pure Quantum States: Entanglement and Correlation Patterns

- State vectors: $|\psi\rangle \in \mathcal{H}$

- **Physically equivalent** if they differ by a global phase:

$$|\phi\rangle = e^{i\theta}|\psi\rangle \Leftrightarrow |\phi\rangle \sim |\psi\rangle$$

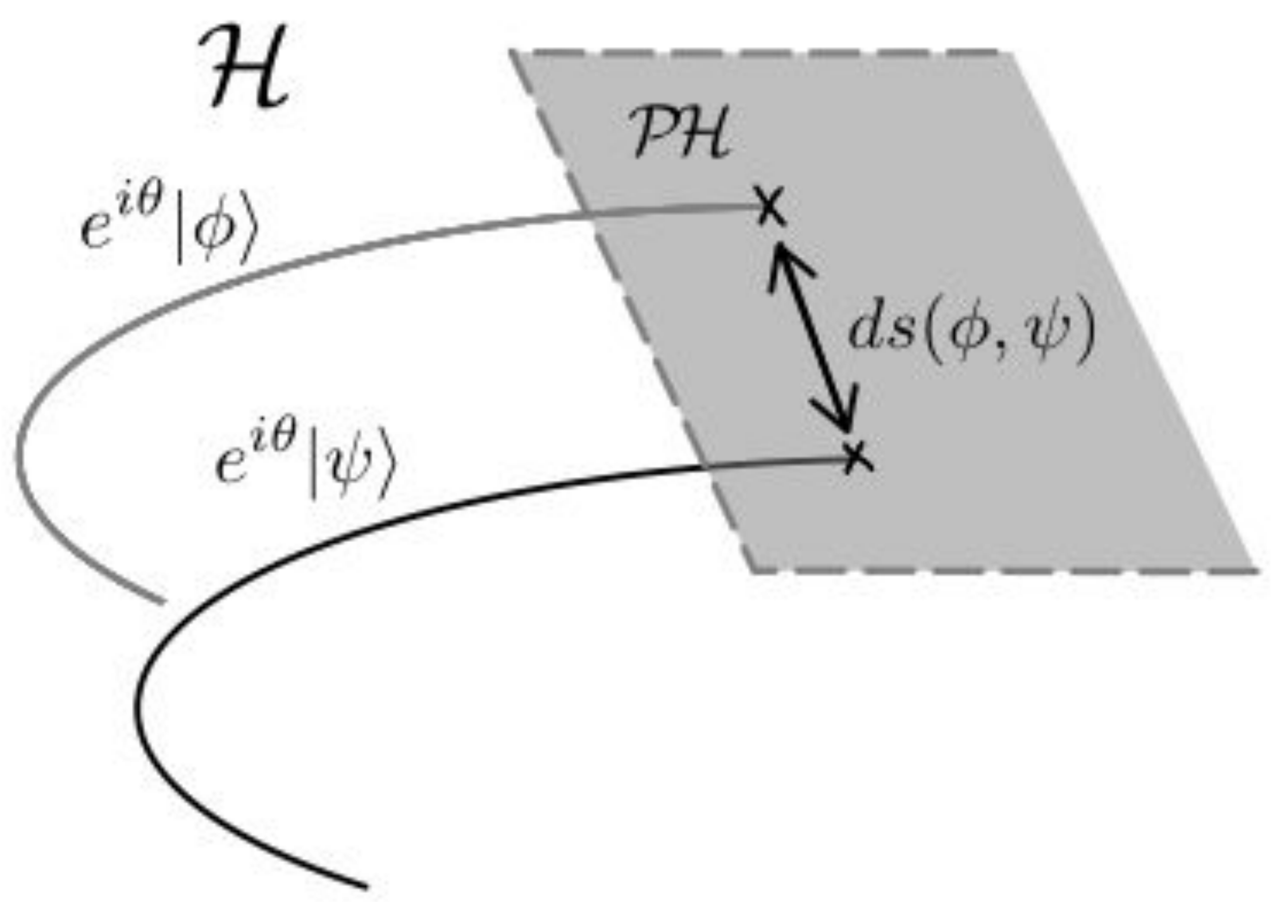
- The *physically meaningful* space of quantum states is the **projective Hilbert space** collapsing each of these **rays** into a **point**.



1) Pure Quantum States: Entanglement and Correlation Patterns

Infinitesimal squared distance in this projective space

$$ds^2 = \langle d\psi | d\psi \rangle - \langle d\psi | \psi \rangle \langle \psi | d\psi \rangle = \sum_{\mu\nu} g_{\mu\nu} d\xi^\mu d\xi^\nu$$



With the **Fubini-Study metric**

$$g_{\mu\nu} = \langle \partial_\mu \psi | \partial_\nu \psi \rangle - \langle \partial_\mu \psi | \psi \rangle \langle \psi | \partial_\nu \psi \rangle$$

by construction invariant under the **gauge transformations**

$$|\psi(\xi))\rangle \to e^{i\alpha(\xi)} |\psi(\xi))\rangle$$

We adapted it to define other projective spaces, considering an alternative **equivalence class**.

1) Pure Quantum States: Entanglement and Correlation Patterns

States with the exact same statistical properties are ***local-unitary (LU) equivalent***.

(Rotating the frame does not change the physics!)

Thus, we considered the **LU equivalence class**:

$$|\phi\rangle = e^{i\alpha}\prod_{\mu} U^{\mu}|\psi\rangle \Leftrightarrow |\phi\rangle \underset{l.u.}{\sim} |\psi\rangle$$

And we defined the ***Entanglement Metric***:

$$g_{\mu\nu}(|\psi\rangle, \{\mathbf{v}^{\mu}\}) = \langle\psi|\sigma^{\mu}_{\mathbf{v}}\sigma^{\nu}_{\mathbf{v}}|\psi\rangle - \langle\psi|\sigma^{\mu}_{\mathbf{v}}|\psi\rangle\langle\psi|\sigma^{\nu}_{\mathbf{v}}|\psi\rangle$$

with $\sigma^{\mu}_{\mathbf{v}} = \sum_{j=x,y,z} v^{\mu}_{j}\,\sigma^{\mu}_{j}$

D. Cocchiarella, S. Scali, S. Ribisi, B. Nardi, G. Bel-Hadj-Aissa, and R.Franzosi, "*Entanglement distance for arbitrary M-qudit hybrid systems*",Phys. Rev. A, 2022
A. Vesperini, G. Bel-Hadj-Aissa, L. Capra, and R. Franzosi, *"Unveiling the geometric meaning of quantum entanglement"*, arXiv:2307.16835, 2023

1) Pure Quantum States: Entanglement and Correlation Patterns

We define the **Entanglement Distance (ED)** as the minimum of its diagonal elements

$$E_\mu(|\psi\rangle) = \min_{\mathbf{v}^\mu} \; g_{\mu\mu}(|\psi\rangle, \mathbf{v}^\mu) = 1 - \sum_{j=x,y,z} |\langle\psi|\sigma_j^\mu|\psi\rangle|^2$$

Entanglement monotone: does not increase, in average, under ***Local Operations and Classical Communication*** (**LOCC**), i.e. the operations that cannot generate entanglement.

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1) Pure Quantum States: Entanglement and Correlation Patterns

Projective measurement: $|s\rangle \longrightarrow |s'\rangle = \frac{P^{\nu}_{\mathbf{m}}|s\rangle}{\sqrt{\langle s|P^{\nu}_{\mathbf{m}}|s\rangle}}$

Maximum correlation

Operators and **projective measures** are equivalent (**have the same effect on *s***):

$$\langle s|\sigma^{\mu}_{\mathbf{v}}\sigma^{\nu}_{\mathbf{u}}|s\rangle = 1$$
$$\sigma^{\nu}_{\mathbf{u}}|s\rangle = \sigma^{\mu}_{\mathbf{v}}|s\rangle$$
$$P^{\nu}_{\mathbf{u}}|s\rangle = P^{\mu}_{\mathbf{v}}|s\rangle = P^{\nu}_{\mathbf{u}}P^{\mu}_{\mathbf{v}}|s\rangle$$

Maximally entangled in μ and ν

Post-measurement expectation value equates **pre-measurement correlator**:

$$\langle s'|\sigma^{\mu}_{\mathbf{v}}|s'\rangle = \langle s|\sigma^{\mu}_{\mathbf{v}}\sigma^{\nu}_{\mathbf{m}}|s\rangle$$

Entanglement-breaking: $\exists \mathbf{v}^{\mu}$ s.t. $\langle s|\sigma^{\mu}_{\mathbf{v}}\sigma^{\nu}_{\mathbf{m}}|s\rangle = 1 \Leftrightarrow E_{\mu}(|s'\rangle) = 0$

A. Vesperini, "*Correlations and projective measurements in maximally entangled multipartite states*," Annals of Physics, 2023

1) Pure Quantum States: Entanglement and Correlation Patterns

For some states (in particular, most states useful for **quantum computation**), the **Entanglement Metric *g*** is **block-diagonal**, **filled with 0 and 1**.

The number *n* of blocks provides an **upper bound** to the ***persistency of entanglement***: $P_e \leq n$

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1) Pure Quantum States: Entanglement and Correlation Patterns

$$P_e \leq n$$

E.g. : Briegel-Raussendorf State of 5 qubits $|\phi_N\rangle = \prod_{\mu=0}^{N-2} \frac{1}{2}\left(\mathbb{I} - \sigma_z^\mu + \sigma_z^{\mu+1} + \sigma_z^\mu \sigma_z^{\mu+1}\right)|+\rangle^{\otimes N}$

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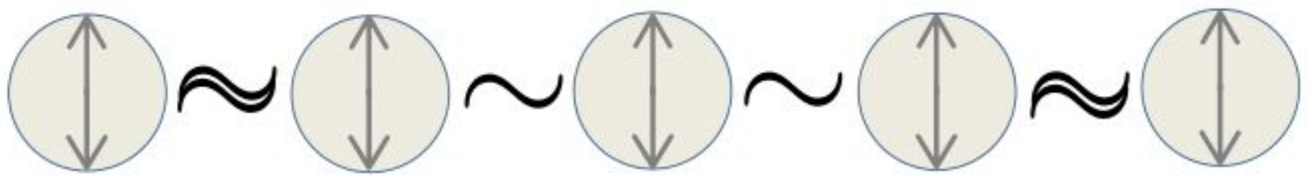

$$\tilde{g}(|\phi_5\rangle) = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$

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2) Mixed Quantum States: Entanglement and Quantum Correlations

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Density matrices can describe **statistical mixtures of quantum states**: $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$

A **density matrix** describes a **statistics**.
It contains information on the ***probability of experimental outcomes***, not on the ***underlying phenomenon***.

There exists an infinite variety of mixtures **realizing** the exact same **statistics**,
hence an infinite number of **realization / decomposition** for a given density matrix.

e.g.: $$\rho = \frac{1}{2}(|\psi_+\rangle\langle\psi_+| + |\psi_-\rangle\langle\psi_-|) = \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|)$$

A mixed state is

- ***entangled*** *<u>if and only if</u> each of its decompositions contains* ***entangled sub-states****,*
- ***separable*** *otherwise.*

2) Mixed Quantum States: Entanglement and Quantum Correlations

The most common way to adapt for **mixed states** an **entanglement monotone** defined on **pure states** is by **convex roof construction**:

$$E_\mu(\rho) := \min_{\{p_j,\psi_j\}} \sum_j p_j E_\mu(|\psi_j\rangle)$$

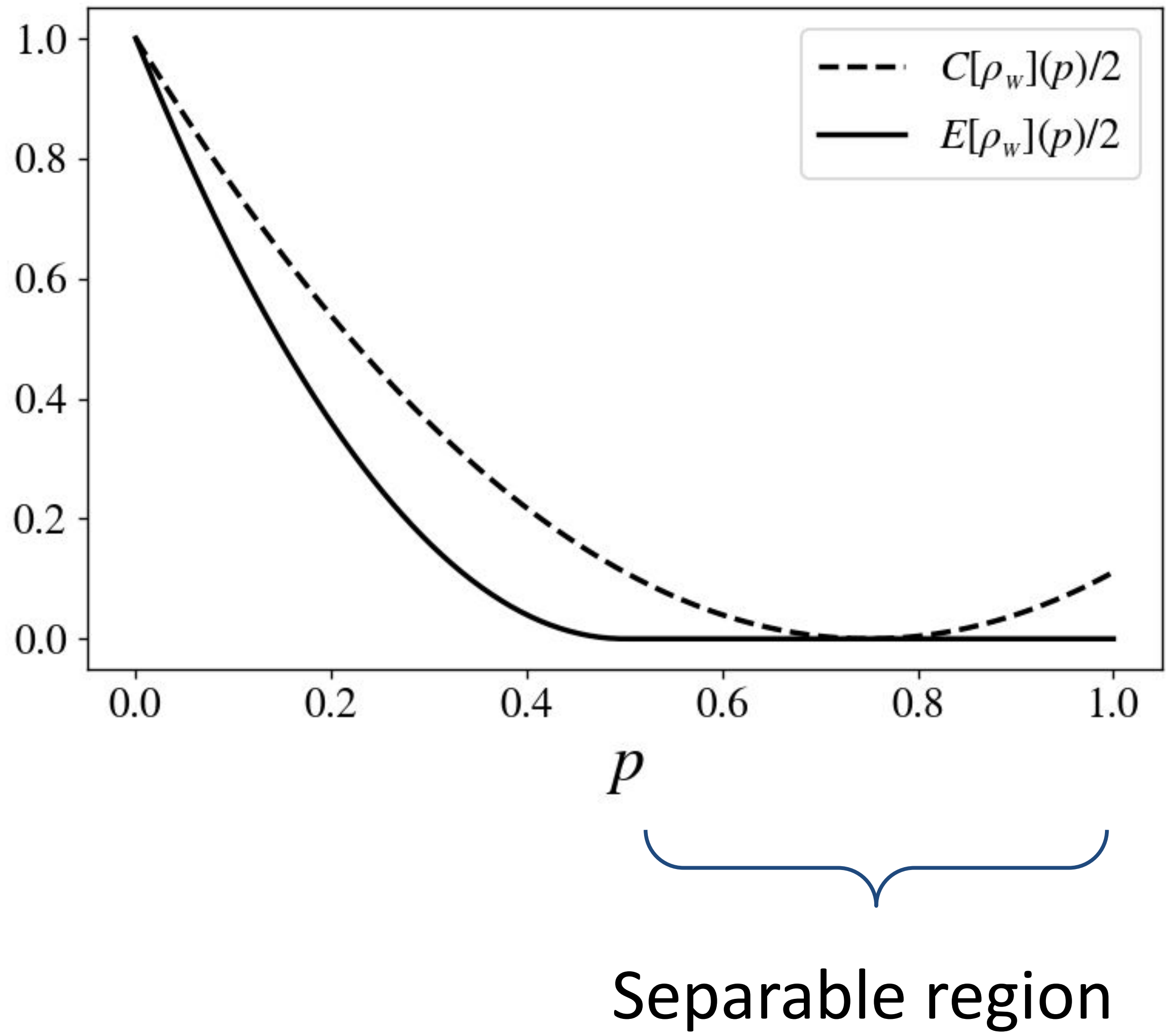
But this *optimization procedure* is **practically intractable**, as the dimensionality of the space to explore **scales exponentially** with the size of the system.

2) Mixed Quantum States: Entanglement and Quantum Correlations

Again, using the **FS-metric**, we obtained a measure of **quantum correlations** for mixed states, the **Quantum Correlation Distance (QCD)**:

$$C_\mu(\rho) = \mathrm{Tr}(\rho^2) - \lambda_{\max}\left(A^\mu(\rho)\right)$$
$$A^\mu_{ij}(\rho) = \mathrm{Tr}[\rho\sigma^\mu_i \rho\sigma^\mu_j]$$

$$\rho_W = \frac{4p}{3}\frac{\mathbb{I}_4}{4} + \left(1 - \frac{4p}{3}\right)|\phi_-\rangle\langle\phi_-|$$



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2) Mixed Quantum States: Entanglement and Quantum Correlations

For a **classical state**, there always exists a (unique) **measurement $\mathcal{M}$*** leaving the state **unchanged**:

$$\exists ! \mathcal{M}^* \,\middle|\, \mathcal{M}^*[\rho] = \rho$$

Quantum correlations: any property breaking this rule.

Pure states: **entanglement** is the only type of **quantum correlation**.

Mixed states: there exists another type of **quantum correlations**.

G. Adesso, T. R. Bromley, and M. Cianciaruso, *"Measures and applications of quantum correlations"*, Journal of Physics A: Mathematical and Theoretical, 2016

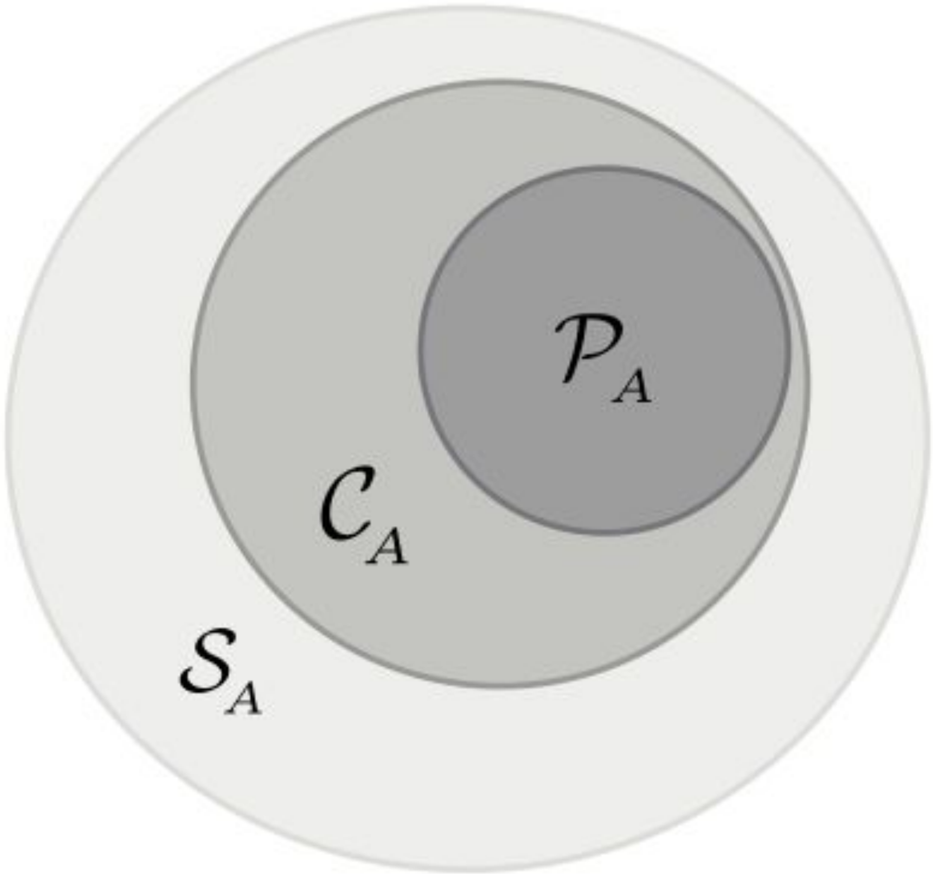
2) Mixed Quantum States: Entanglement and Quantum Correlations

Density matrices have a richer zoology of quantum correlations:

$$\mathcal{P}_A := \{\rho^{AB} |\, \rho^{AB} = \rho^A \otimes \rho^B\} = \mathcal{P}_B$$

$$\mathcal{C}_A := \left\{\rho^{AB} |\, \rho^{AB} = \sum_k p_k |k\rangle\langle k|^A \otimes \rho_k^B\right\} \neq \mathcal{C}_B$$

$$\mathcal{S}_A := \left\{\rho^{AB} |\, \rho^{AB} = \sum_k p_k \rho_k^A \otimes \rho_k^B\right\} = \mathcal{S}_B$$



Quantum dissonance:

$$\rho \in \mathcal{S}_A \setminus \mathcal{C}_A \Leftrightarrow \rho = \sum_k p_k \rho_k^A \otimes \rho_k^B,$$

$$\mathrm{Tr}[\rho_k^A \rho_l^A] \neq \delta_{kl}$$

At variance with **classical systems**, where **distinct states are always orthogonals**: "Measuring X implies non-Y ."

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2) Mixed Quantum States: Entanglement and Quantum Correlations

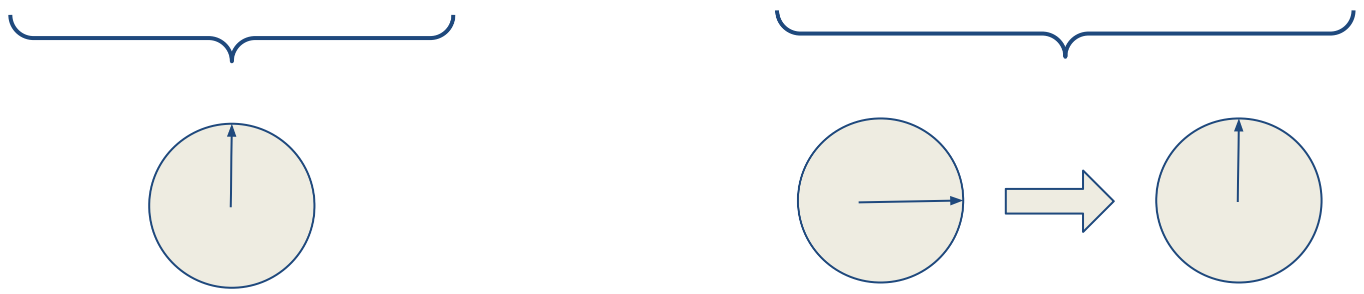
Ideally, we need a mapping $\Phi : \mathcal{S}_A \to \mathcal{C}_A$

Since **separable yet quantum correlated states** differ from **classical states** by a **local-unitary operation on the sub-states *of a given decomposition***, we devised the **regularization procedure:**

$$\rho_U\left(\{p_k, \rho_k, U_k\}\right) = \sum_k p_k U_k \rho_k U_k^\dagger$$

e.g. : $\rho = p|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + (1-p)|\rightarrow\rightarrow\rangle\langle\rightarrow\rightarrow|$

$$\rho_U = p|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + (1-p)U|\rightarrow\rightarrow\rangle\langle\rightarrow\rightarrow|U^\dagger = |\uparrow\uparrow\rangle\langle\uparrow\uparrow|$$



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$$\rho_U\left(\{p_k, \rho_k, U_k\}\right) = \sum_k p_k U_k \rho_k U_k^\dagger$$

and the induced **regularized entangled distance**:

$$E(\rho) = \min_{\{p_k,\rho_k\}} \left\{ \sum_{\mu=1}^{M-1} \min_{\{U_k\}} C_\mu\left(\rho_U\left(\{p_k, \rho_k, U_k\}\right)\right) \right\}$$

Very similar to the **convex roof construction** but, at least **for some special cases**, and choosing the appropriate **decomposition** (*not necessarily the separable one*), the optimization is much simpler.

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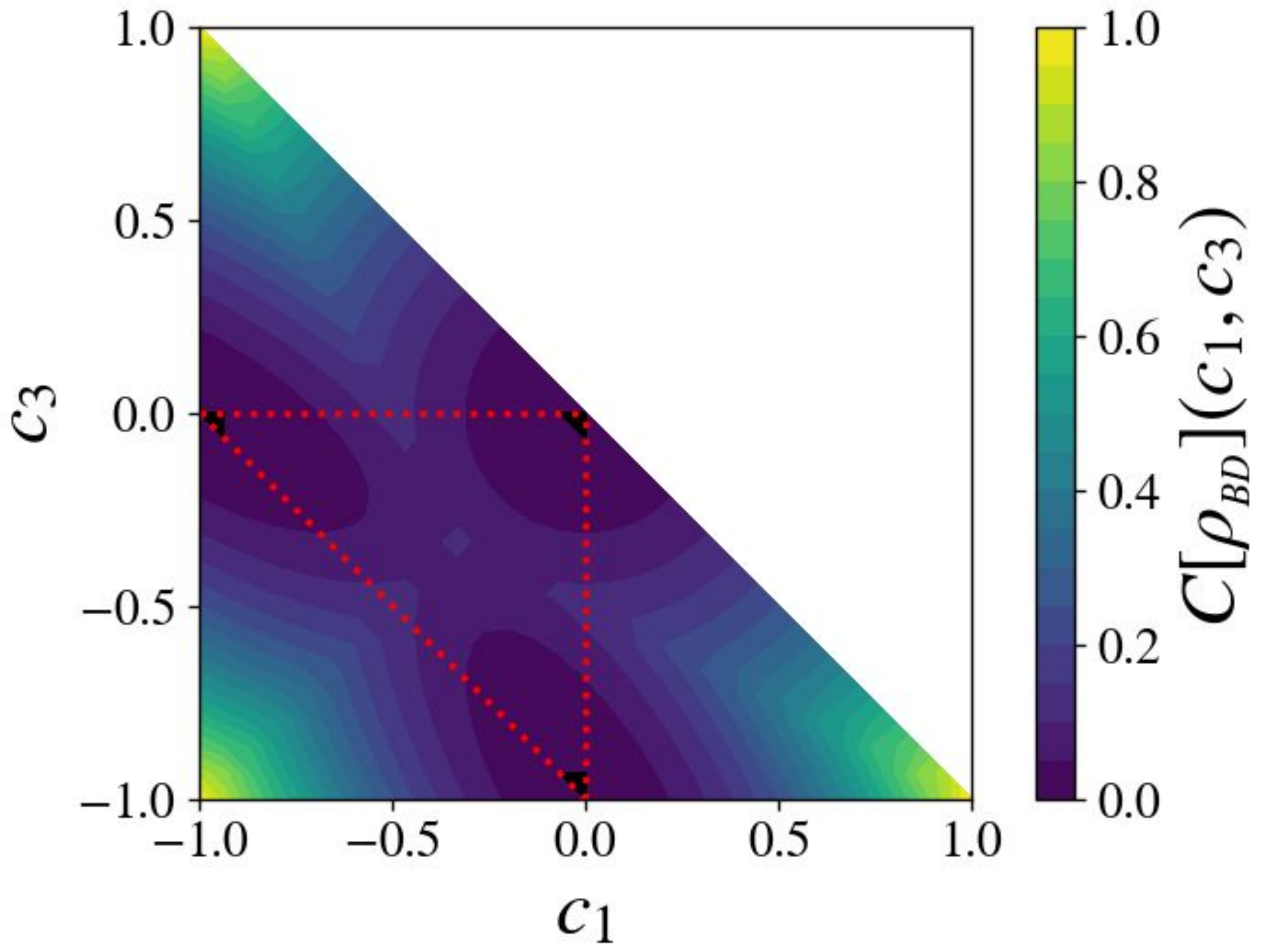
2) Mixed Quantum States: Entanglement and Quantum Correlations

Application on **Bell-diagonal states** (mixture of Bell states):

$$\rho_{BD}(\{p_\alpha\}) = \sum_{\alpha=1}^{4} p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$$



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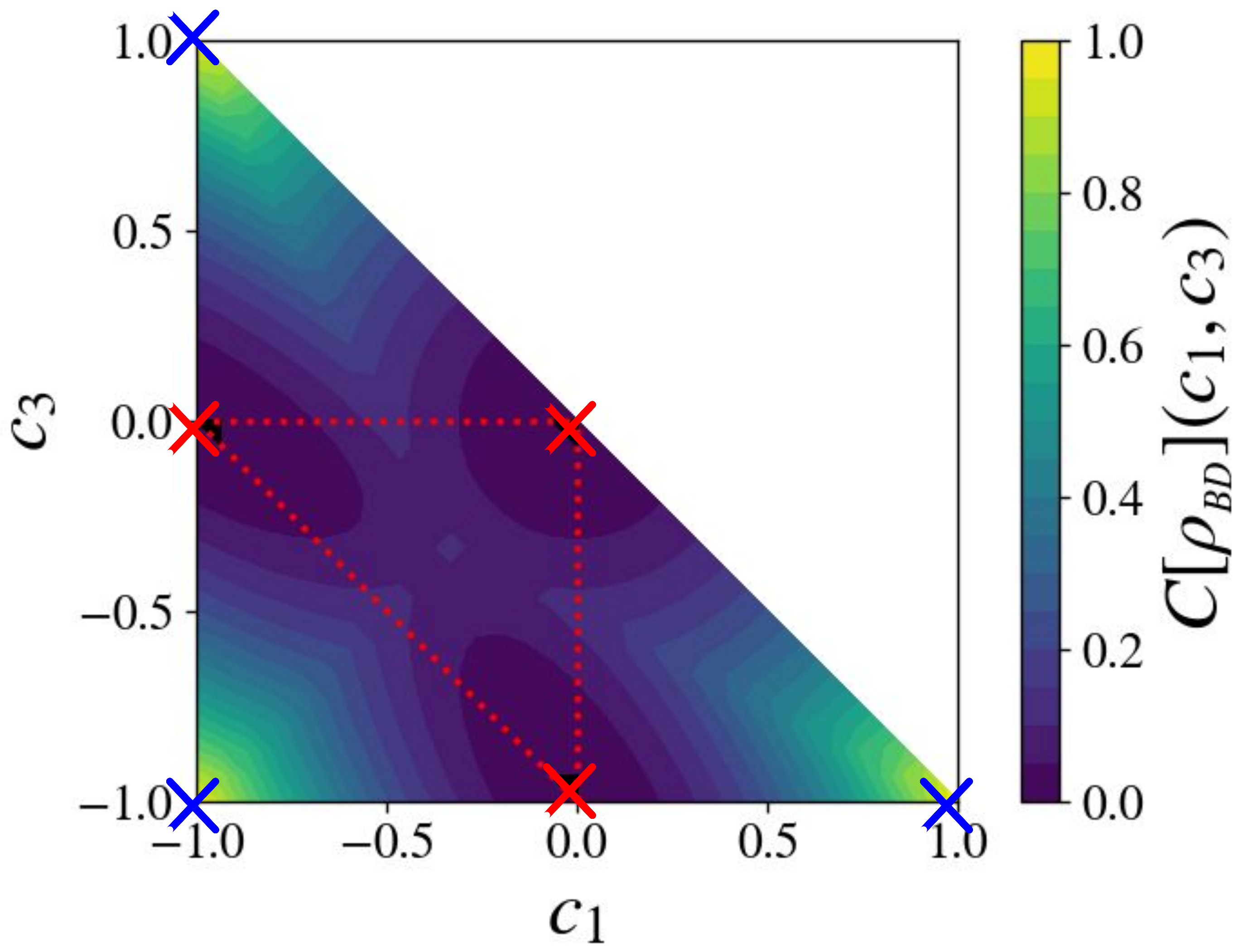

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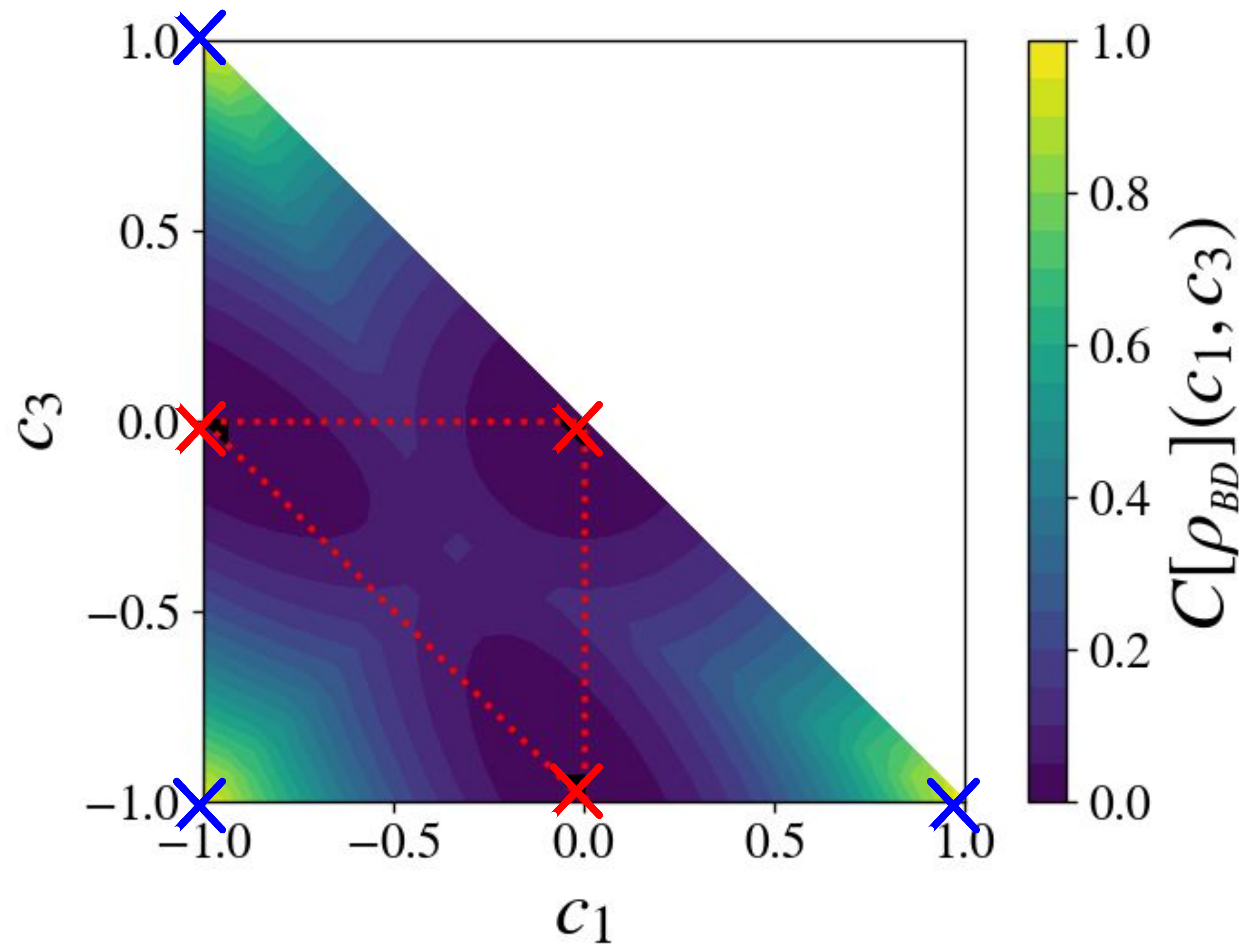
$$\rho_{BD}(\{p_\alpha\}) = \sum_{\alpha=1}^{4} p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| \longrightarrow \rho_{BD}^{U}(\{p_\alpha, U_\alpha\}) = \sum_{\alpha=1}^{4} p_\alpha U_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| U_\alpha^\dagger$$



A. Vesperini, G. Bel-Hadj-Aissa, and R. Franzosi, *"Entanglement and quantum correlation measures for quantum multipartite mixed states"*, Scientific Reports, 2023

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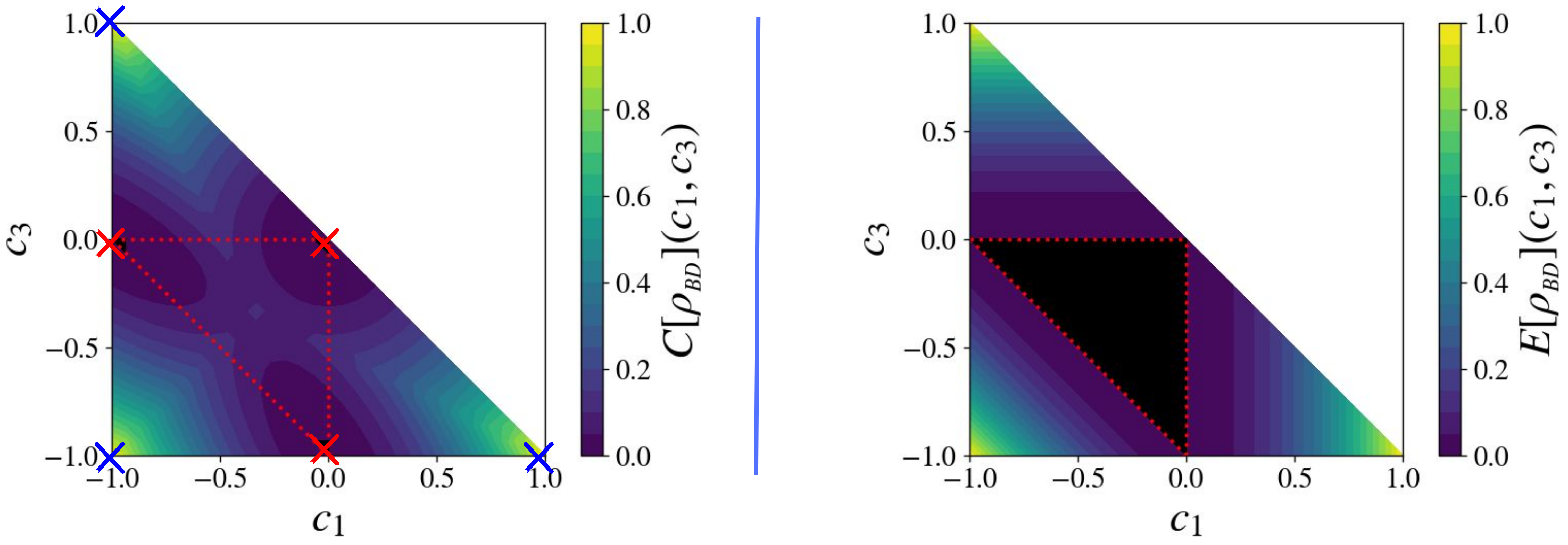

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3) Quantum Phase Transition in the Tavis-Cummings Model

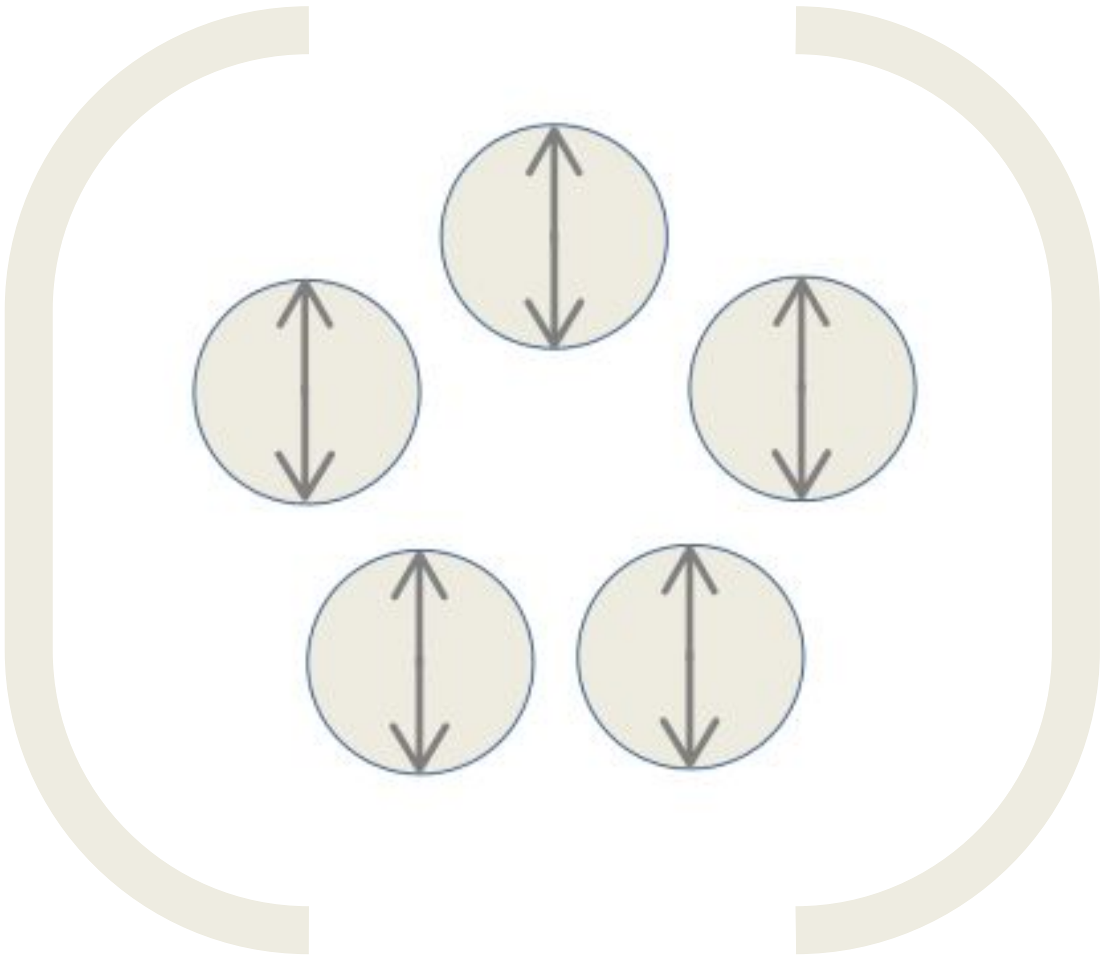
3) Quantum Phase Transition in the Tavis-Cumming Model

A model describing an assembly of **two-level atoms** in a **single-mode electromagnetic cavity**:

$$H = \underbrace{\omega_c a^\dagger a}_{\text{Field}} + \underbrace{\omega_z S_z}_{\text{Atoms}} \underbrace{- \frac{\lambda}{\sqrt{N}}(a^\dagger S_- + a S_+)}_{\text{Coupling}}$$

Quantum phase transition: structural changes of the ground state happen at **zero temperature**, brought by varying the parameter

$$g = \frac{\lambda}{\sqrt{\omega_c \omega_z}}$$



3) Quantum Phase Transition in the Tavis-Cumming Model

$$H = H_I + H_{II}$$

$$H_I = \omega_c(a^\dagger a + S_z)$$

$$[H, H_I] = 0$$

A. Vesperini, M. Cini, and R. Franzosi, *"Entanglement signature of the Superradiant Quantum Phase Transition"*, Manuscript in preparation

3) Quantum Phase Transition in the Tavis-Cumming Model

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$$[H, H_I] = 0$$

We used this **conserved quantity** to exploit the **block structure** of the **infinite-dimensional Hamiltonian** into **finite sub-eigenspace**.

$$H = \begin{pmatrix} H_0 & \cdots & \cdots & \cdots \\ \vdots & \ddots & & \\ \vdots & & H_k & \\ \vdots & & & \ddots \\ \vdots & & & \end{pmatrix}$$

A. Vesperini, M. Cini, and R. Franzosi, *"Entanglement signature of the Superradiant Quantum Phase Transition"*, Manuscript in preparation

I. Entanglement and Quantum Correlations

3) Quantum Phase Transition in the Tavis-Cumming Model

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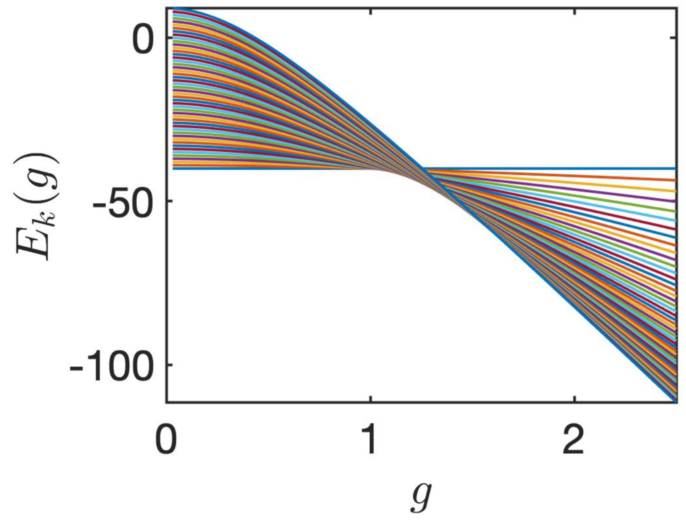
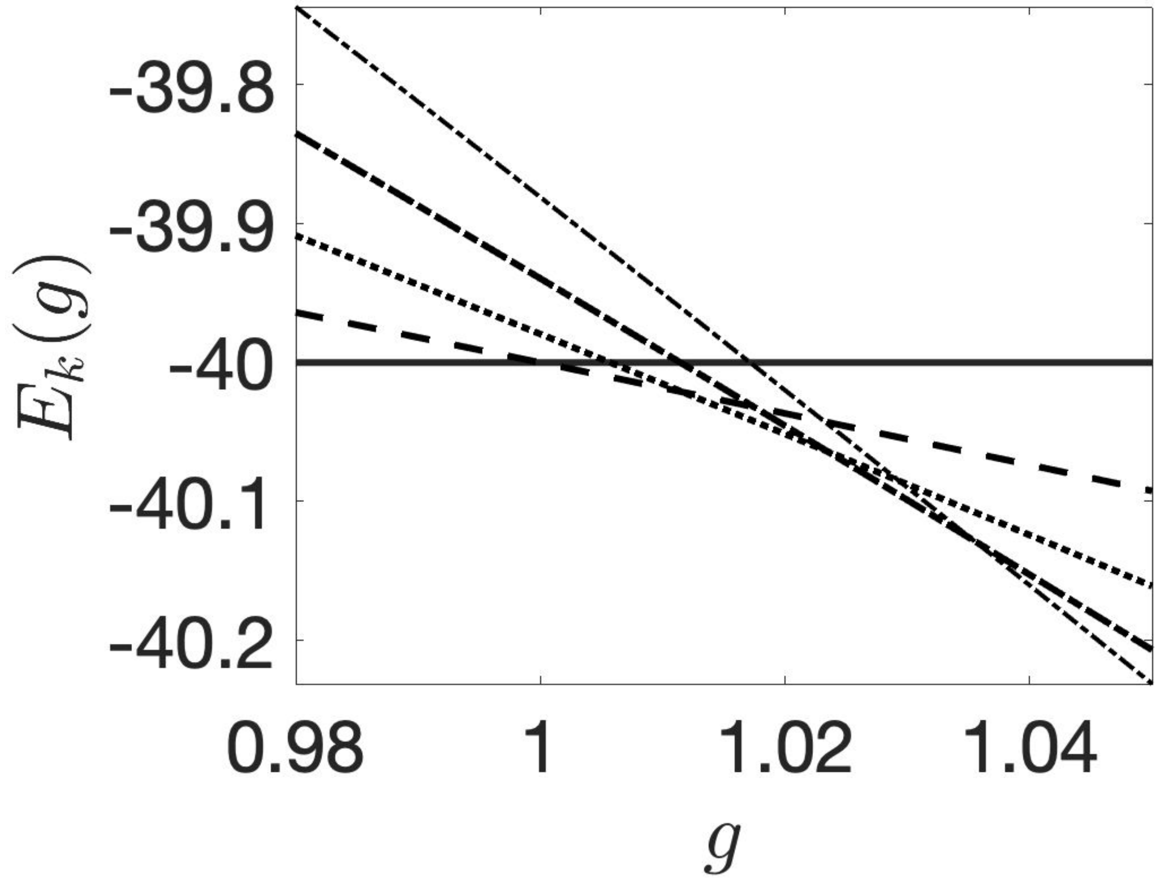
As *g* varies, the **ground state** (**GS**) changes of sub-space, with an **increase** of ***k***, thus of:

- the **number of photons**
- the **total spin**
- the **degeneracy**

Symmetry breaking at g=1 .





A. Vesperini, M. Cini, and R. Franzosi, *“Entanglement signature of the Superradiant Quantum Phase Transition”*, Manuscript in preparation

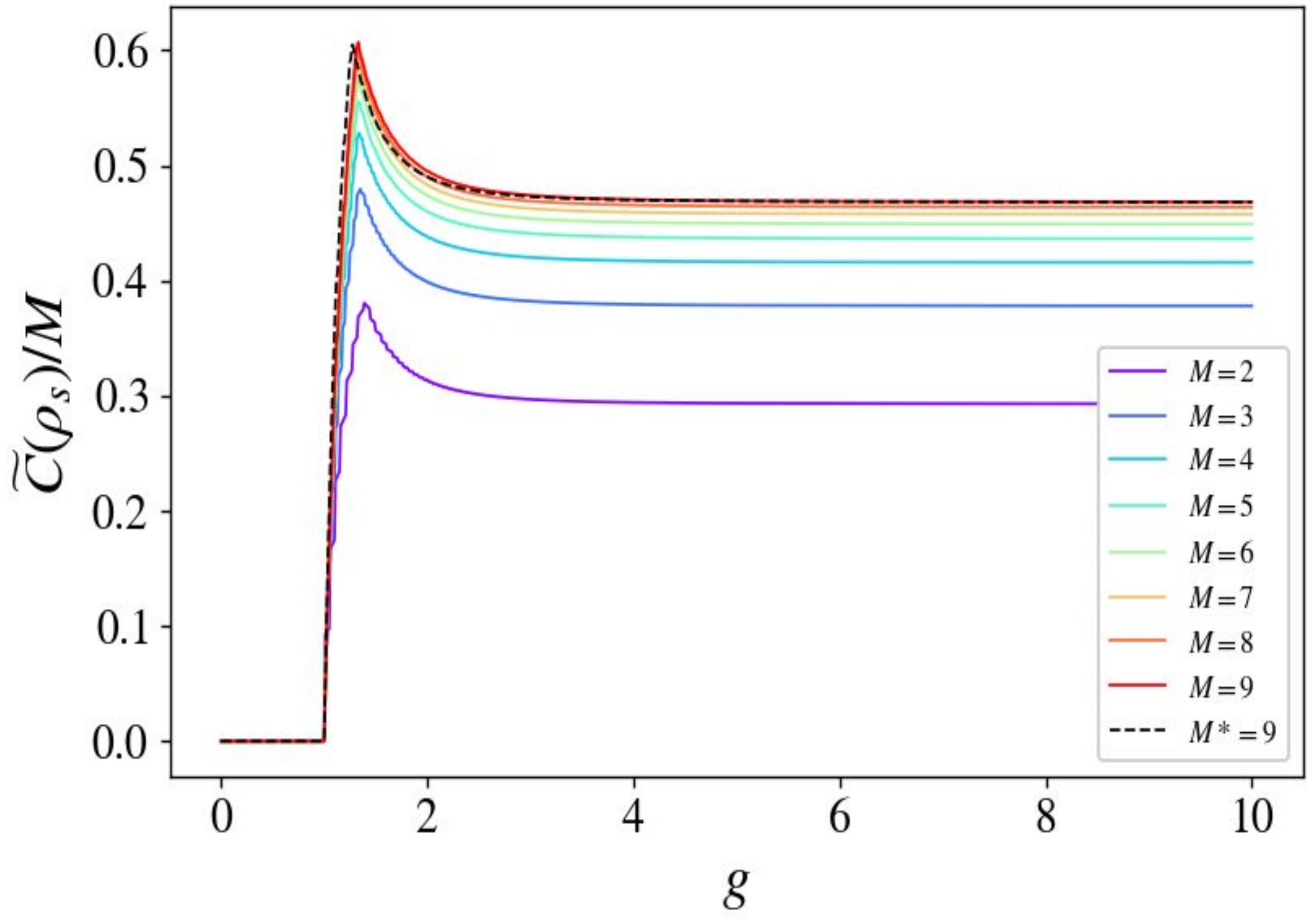
3) Quantum Phase Transition in the Tavis-Cumming Model

Discarding the **field part** of the GS, the remaining **atomic part of the GS** is a **mixture of Dicke state**

$$\rho_s = \sum_{n=0}^{M} p_n |D_{M-n}^{M}\rangle\langle D_{M-n}^{M}|$$

where *n* is the number of excitations.

We found, using the **QCD**, that ϱ_s is **quantum correlated** for ***g>1***, with a peak close to ***g=1***.
It **converges** to a **finite value** with increasing *M*.



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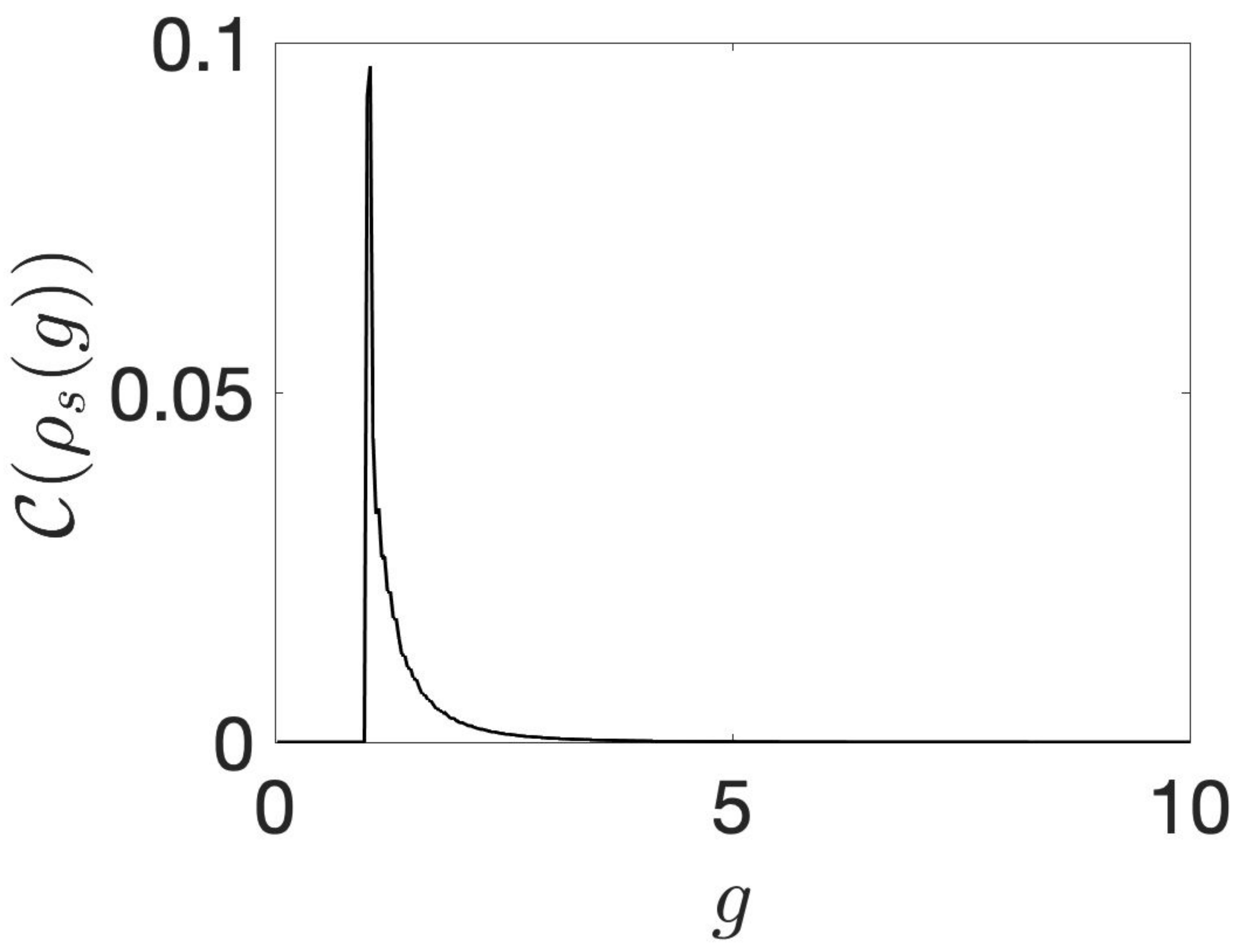
3) Quantum Phase Transition in the Tavis-Cumming Model

We confirmed, using an **entanglement criterion** found in the literature, that the atoms are **entangled** for ***g*≥*1***.



But does it hold in the thermodynamic limit?

The **Concurrence** (**entanglement for N=2**) **vanishes** for **large *g***.

For larger systems, we thus conjecture that entanglement also **vanishes for large *g*** and **converges to a finite value** at ***g*=*1***.

A. Vesperini, M. Cini, and R. Franzosi, *"Entanglement signature of the Superradiant Quantum Phase Transition"*, Manuscript in preparation
N. Yu, "*Separability of a mixture of Dicke states*", en, Phys. Rev. A, 2016

Part II:

Metastability and Phase Transitions in Classical Systems

1) The Bicluster: a Metastable State in the HMF Model

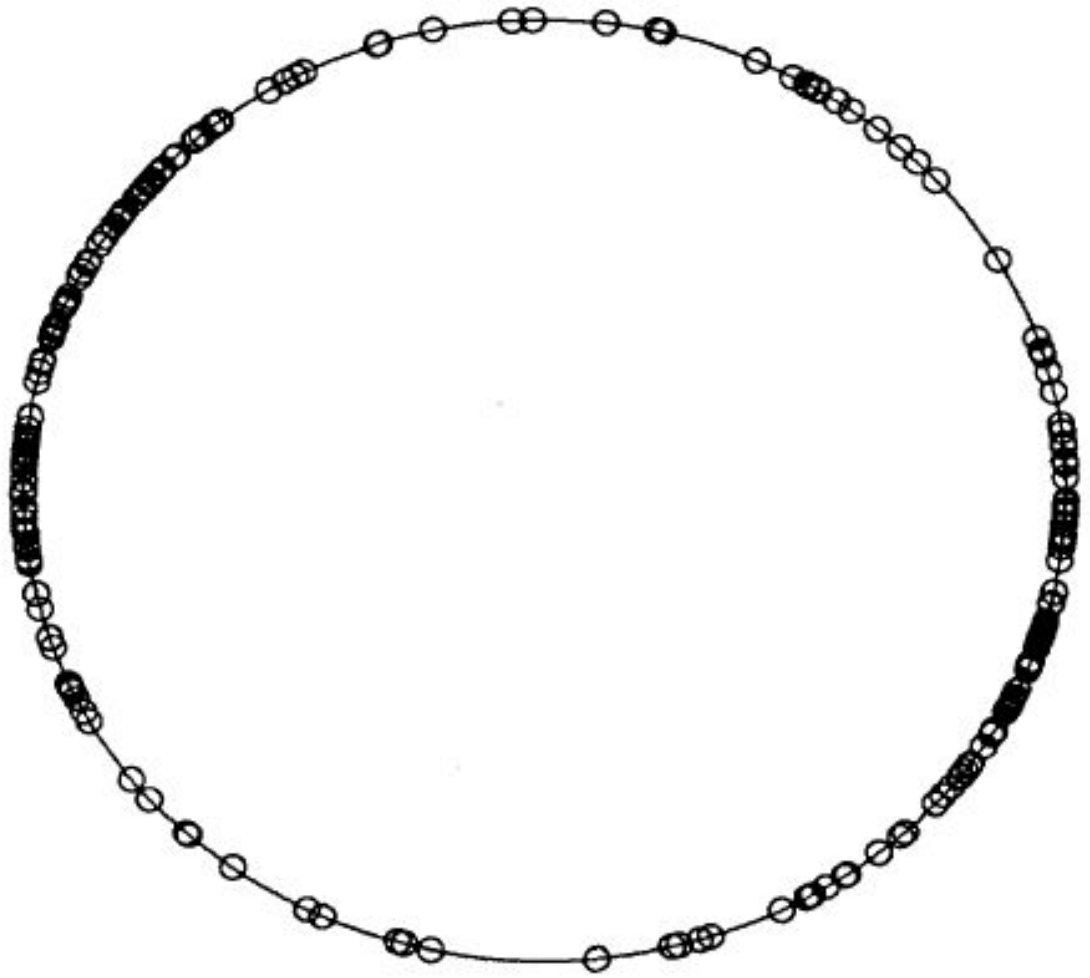
1) The Bicluster: a Metastable State in the HMF Model

The Antiferromagnetic Hamiltonian Mean-Field Model:

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + V(\{\theta_i\})$$

$$V(\{\theta_i\}) = \frac{1}{2N} \sum_{i,j=1}^{N} \cos(\theta_i - \theta_j) = \frac{N\mathbf{m}^2}{2}$$

$$\mathbf{m} = \frac{1}{N} \sum_{j=1}^{N} \begin{pmatrix} \cos(\theta_j) \\ \sin(\theta_j) \end{pmatrix}$$



At low energy, a **long-lived metastable structure** is forming: **the *bicluster***.

A. Vesperini, R. Franzosi, S. Ruffo, A. Trombettoni, and X. Leoncini, *"Fast collective oscillations and clustering phenomena in an antiferromagnetic mean-field model,"* Chaos, Solitons & Fractals,2021

1) The Bicluster: a Metastable State in the HMF Model

Mean-field-induced self-consistency of the potential

$$\frac{d^2}{dt^2}\mathbf{m}(t) = \mathbf{A}(\{\theta_j\})\mathbf{m}(t) \quad \Rightarrow \quad \textbf{Spectrum:} \left\{ \mathbf{m}_\pm(\phi_2), \;\; -\omega_\pm^2 = -\frac{1 \pm |\mathbf{m}^{(2)}|}{2} \right\}$$

$$\mathbf{m}^{(2)} = \frac{1}{N}\sum_{j=1}^{N} \begin{pmatrix} \cos(2\theta_j) \\ \sin(2\theta_j) \end{pmatrix}$$

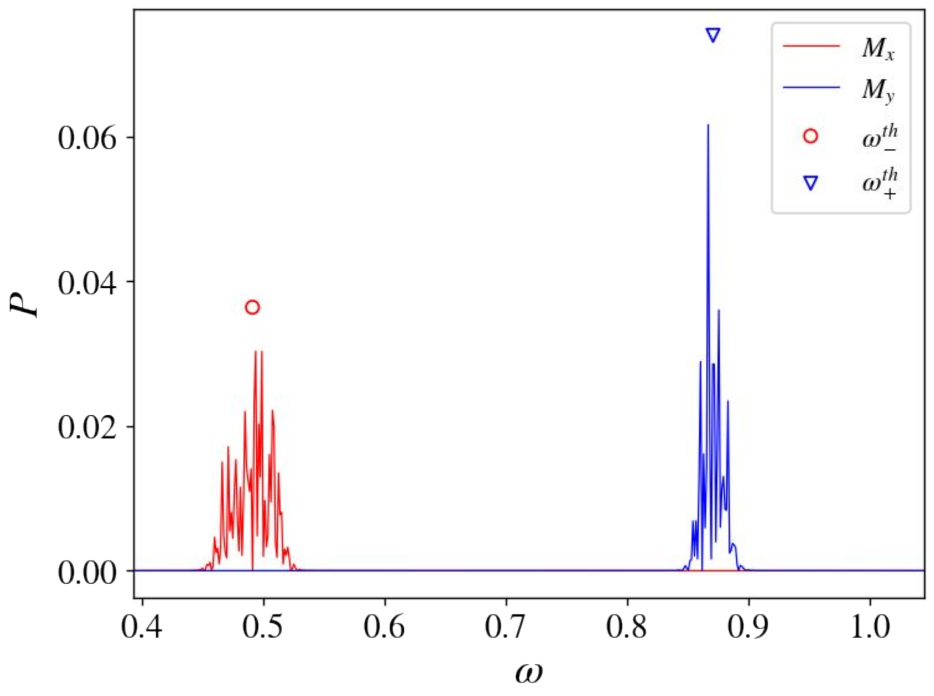
- ➔ pseudo order parameter measuring the degree of ***biclustering***
- ➔ its **phase** defines the **center of mass**
- ➔ its **magnitude** determines the **frequencies** (hence the overall shape) of **m.**

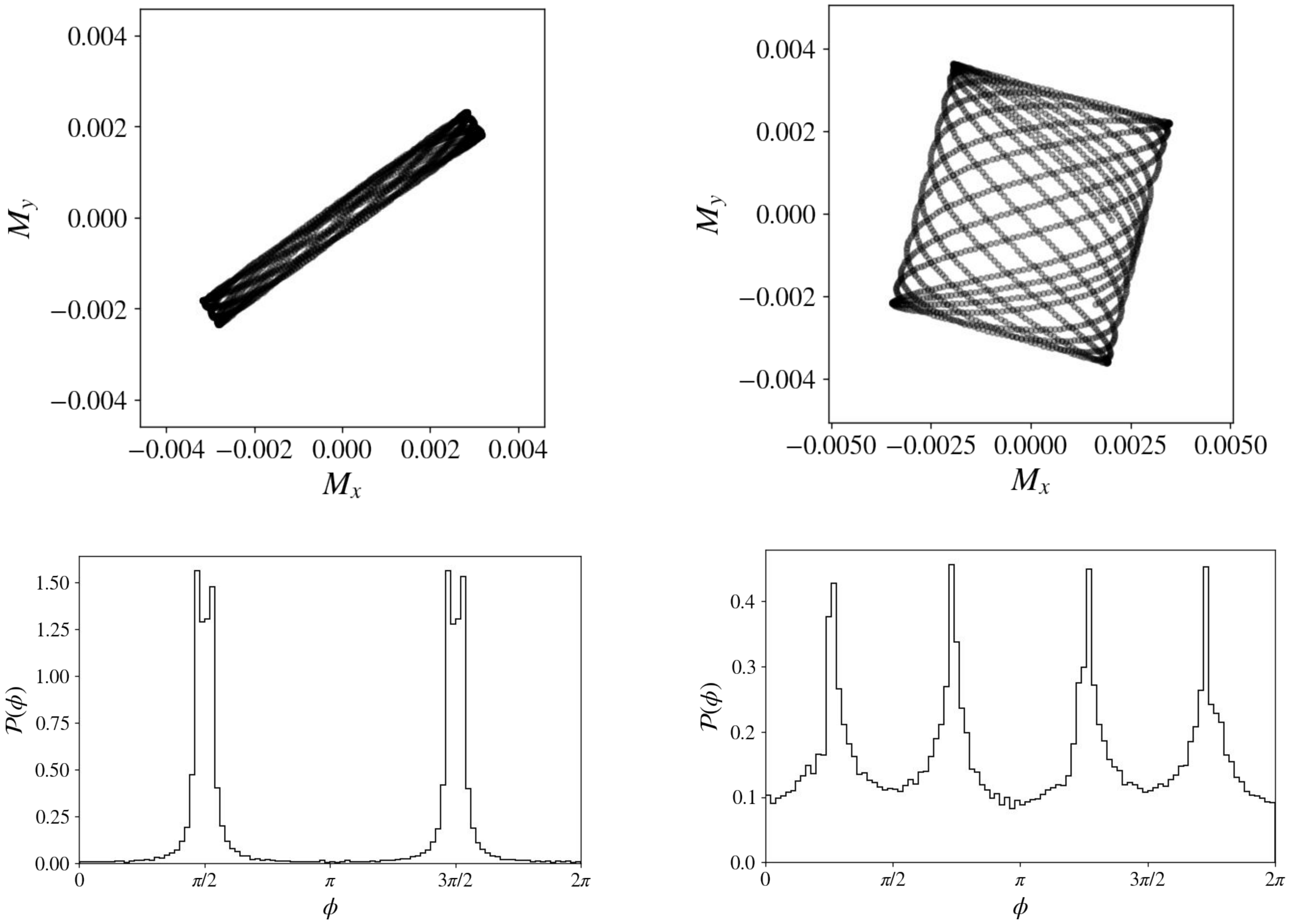
A. Vesperini, R. Franzosi, S. Ruffo, A. Trombettoni, and X. Leoncini, *"Fast collective oscillations and clustering phenomena in an antiferromagnetic mean-field model,"* Chaos, Solitons & Fractals,2021

1) The Bicluster: a Metastable State in the HMF Model

Lissajous-like time-dependent potential,
“running from its own shadow”

$$\mathbf{m}(t) = \begin{pmatrix} m_- \cos\left(\omega_- t + \phi_-\right) \\ m_+ \cos\left(\omega_+ t + \phi_+\right) \end{pmatrix}$$





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1) The Bicluster: a Metastable State in the HMF Model

"***Stroboscopic***" time-dependent potential force: ***the ponderomotive effect.***

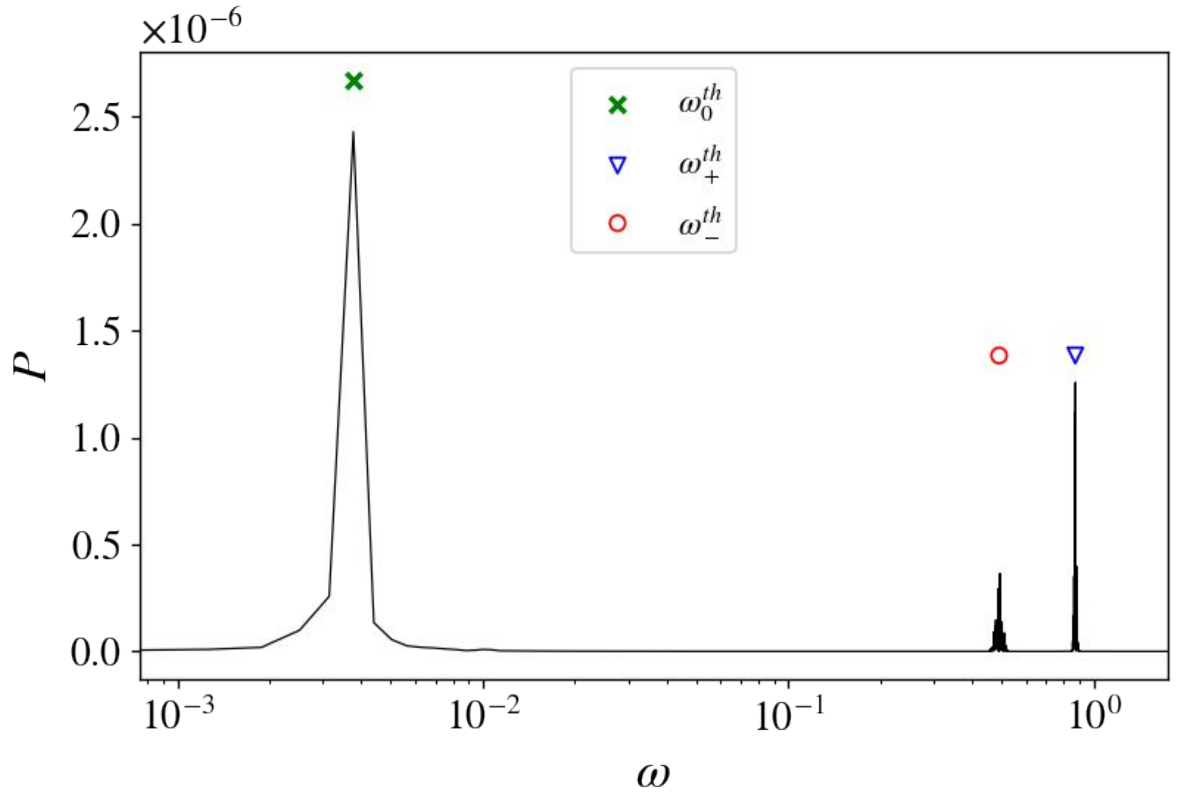
$$\dot{p}_j(t) = m_- \cos(\omega_- t) \sin(\theta_j) - m_+ \cos(\omega_+ t) \cos(\theta_j)$$

Time scale separation:

$$\theta_j(t) = \theta_j^0(\tau, t) + \epsilon f_j(t)$$

Leading to an expression for the **low frequency**:

$$\omega_0 = \frac{1}{\sqrt{2}} \sqrt{\frac{m_-^2}{\omega_-^2} - \frac{m_-^2}{\omega_+^2}}$$

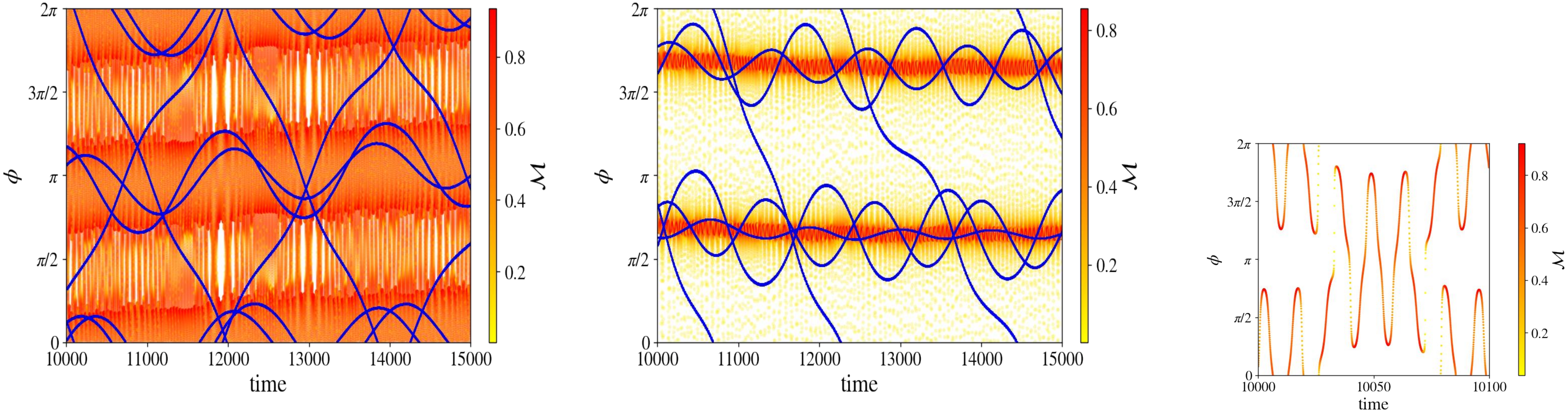


Power spectrum of a single trapped rotator, in a system with well-formed biclusters ($|\mathbf{m}^{(2)}| \approx 0.5$), at low energy ($e \approx 10^{-5}$).

A. Vesperini, R. Franzosi, S. Ruffo, A. Trombettoni, and X. Leoncini, *"Fast collective oscillations and clustering phenomena in an antiferromagnetic mean-field model,"* Chaos, Solitons & Fractals,2021

1) The Bicluster: a Metastable State in the HMF Model

Overall bimodal dynamic picture



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2) The Glass Transition:

a Topological Point of View

2) The Glass Transition: a Topological Point of View

The conventional **theories of phase transitions** lack generality.

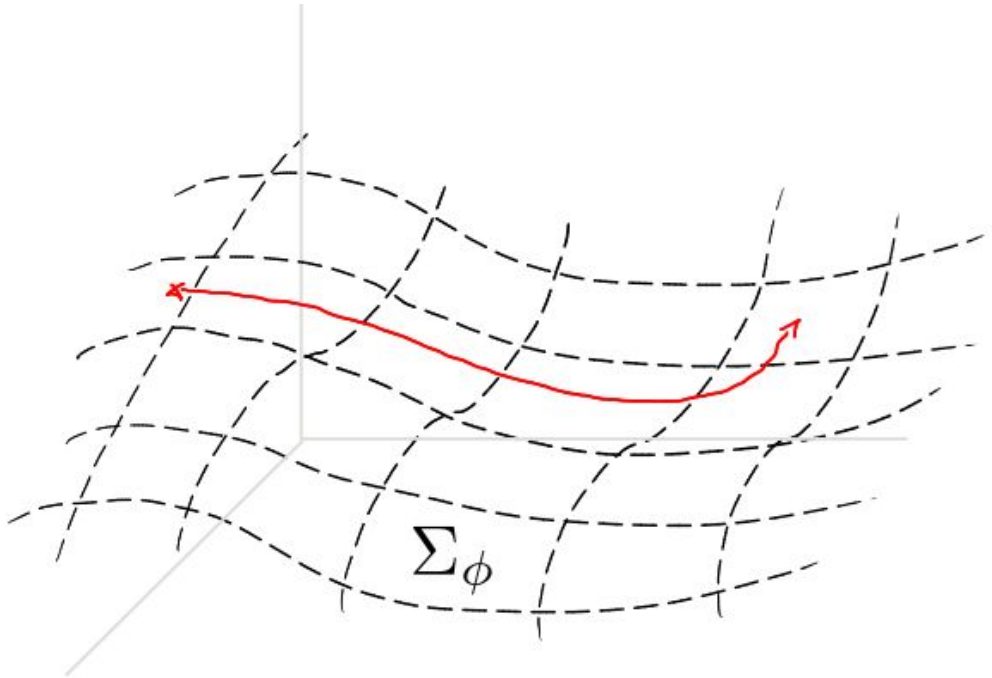
Many **phase transitions** are in fact poorly described by the conventional theories:

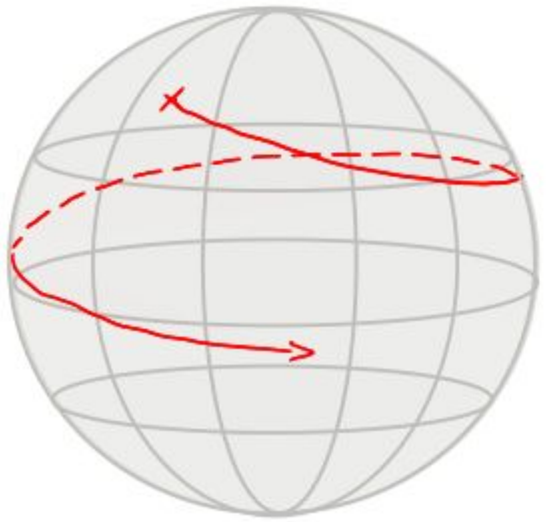
- The **Yang-Lee theory** relies on the thermodynamic limit, thus does not apply to transitions in **small systems** (e.g. **protein folding**).
- The heuristic **theory of Landau** fails in the absence of ***order parameter*** and ***symmetry breaking*** (e.g. **Kosterlitz–Thouless transition**).

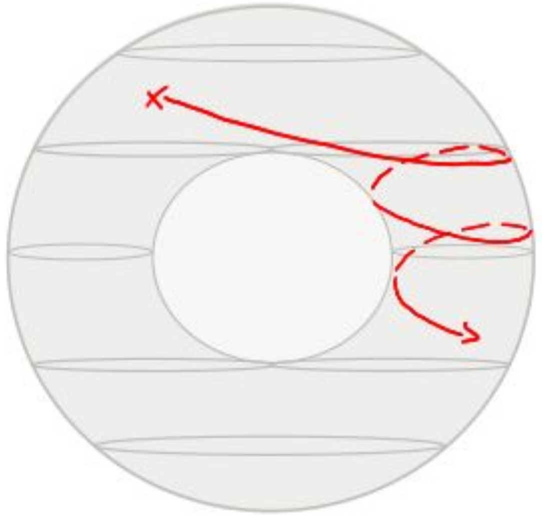
M. Pettini, *Geometry and Topology in Hamiltonian Dynamics and Statistical Mechanics*, Springer New York, 2007
M. Gori et al., *“Topological origin of phase transitions in the absence of critical points of the energy landscape”*, J. Stat. Mech., 2018
L. Di Cairano et al., *“Topology and Phase Transitions: A First Analytical Step towards the Definition of Sufficient Conditions”*, Entropy, 2021

2) The Glass Transition: a Topological Point of View

An **isolated N-body system** can be represented as a point in a **6N-dimensional space**, with its **dynamics constrained** on **hypersurface of constant E**.







Topological theory of phase transitions: ***Phase transitions*** *are accompanied by a* ***change of the topology*** *of the* ***potential level sets (PLS****, i.e.* iso-potential hypersurfaces***)***.

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2) The Glass Transition: a Topological Point of View

Glass transition : from **liquid** to **amorphous solid**.
No *order parameter* nor *symmetry breaking*, thus **Landau theory** fails.

Dynamical freezing comes from a large number of **deep potential wells** in the low energy phase.

It has been shown that, at the transition, the **instability index density** of the **critical points** of the potential energy vanishes.

Morse theory shows that changes of **stability indices** are accompanied by **changes of topology**.

G. Parisi, *"Physics of the glass transition"*, Physica A, 2000
Grigera et al., *"Geometric Approach to the Dynamic Glass Transition"*, PRL, 2002

2) The Glass Transition: a Topological Point of View

Model of glass-former: a frustrated Lennard-Jones binary mixture

$$\Phi(\boldsymbol{\Gamma}) = \underbrace{\sum_{i,j\in\Lambda_1} 4\epsilon_{11}\left(\frac{\sigma_{11}}{r_{ij}}\right)^{12}}_{\text{Intra-species, Repulsive}} + \underbrace{\sum_{i,j\in\Lambda_2} 4\epsilon_{22}\left(\frac{\sigma_{22}}{r_{ij}}\right)^{12}}_{\text{Intra-species, Repulsive}} + \underbrace{\sum_{i\in\Lambda_1, j\in\Lambda_2} 4\epsilon_{12}\left[\left(\frac{\sigma_{12}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{12}}{r_{ij}}\right)^{6}\right]}_{\text{Inter-species}}$$

Intra-species
Repulsive

Intra-species
Repulsive

Inter-species
Short-range repulsive,
long-range attractive

D. Coslovich and G. Pastore, *“Dynamics and energy landscape in a tetrahedral network glass-former: Direct comparison with models of fragile liquids”*, J. Phys.: Condens. Matter, 2009

2) The Glass Transition: a Topological Point of View

Because of the phenomenon of **dynamical freezing**, **glass-formers** are notoriously hard to simulate: **thermodynamic equilibrium** is very difficult to achieve.

We used a **Microcanonical Monte-Carlo (MC) algorithm**, implementing various techniques (**particle swapping, replica exchange**) to speedup the simulation by ***jumping over the potential barriers***.

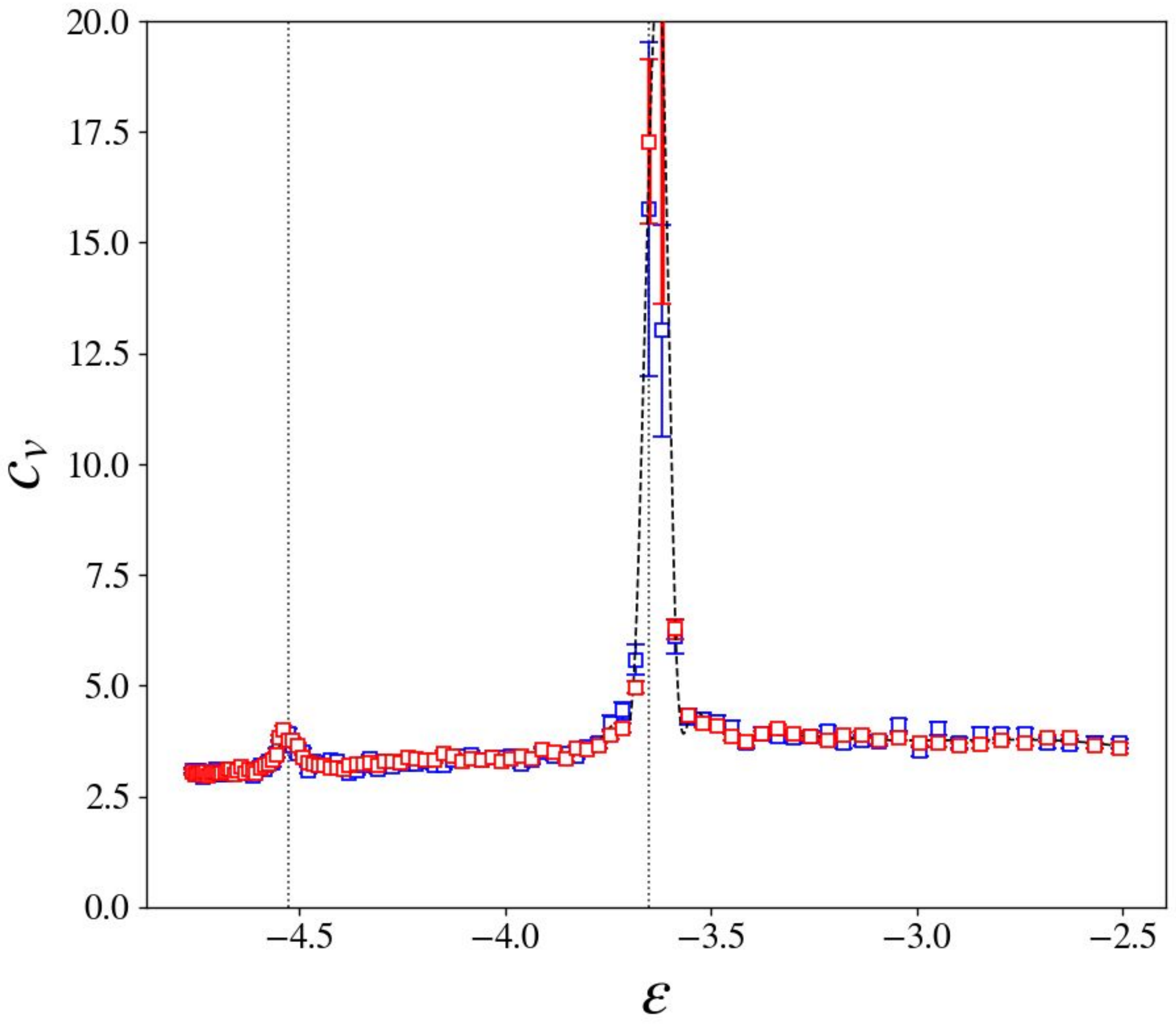
2) The Glass Transition: a Topological Point of View

Specific heat computed:

- from **fluctuations of kinetic energy** (in blue)
- from **derivative of *T* with respect to *E*** (in red)

The agreement of both methods suggest (quasi) **equilibrium**.

Two-step 2nd order transition, with clear **divergence** of **high E** peak.



2) The Glass Transition: a Topological Point of View

We are looking for a **signature of topological changes**, and thus need relations between **computable geometric quantities** (e.g. *mean curvature of the PLS*, …) and **topological invariants**.

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G. Bel-Hadj-Aissa, M. Gori, R. Franzosi, and M. Pettini, "*Geometrical and topological study of the Kosterlitz–Thouless phase transition in the XY model in two dimensions*", J. Stat. Mech., 2021

2) The Glass Transition: a Topological Point of View

We are looking for a **signature of topological changes**, and thus need relations between **computable geometric quantities** (e.g. *mean curvature of the PLS*, …) and **topological invariants**.

Pinkall's theorem (abridged): a link between the average **dispersion of the principal curvatures**, and a weighted sum of the **Betti numbers b_i** .

$$\langle \sigma_\kappa^2 \rangle_{\Sigma_\phi} \sim \left[\sum_{i=1}^{3N} w_i b_i(\Sigma_\phi) \right]^{2/3N}$$

An abrupt change of the LHS corresponds to a change of the RHS, i.e. most likely to a change of the **Betti numbers**, thus of **the topology of the PLS**.

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Di Cairano, R. Capelli, G. Bel-Hadj-Aissa, and M. Pettini, "*Topological origin of the protein folding transition*", Phys. Rev. E, 2022
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2) The Glass Transition: a Topological Point of View

We are looking for a **signature of topological changes**, and thus need relations between **computable geometric quantities** (e.g. *mean curvature of the PLS*, …) and **topological invariants**.

Overholt's theorem (abridged): yet another link, between the **variance of the scalar curvature**, and the sum of the **Betti numbers** b_i .

$$\langle R_\Sigma^2 \rangle - \langle R_\Sigma \rangle^2 \gtrsim C_{\Sigma_\phi} \left[\sum_{i=0}^{3N} b_i(\Sigma_\phi) \right]^{2/3N}$$

Again, an abrupt change of the LHS most likely corresponds to a change of the **Betti numbers**, i.e. a **change of the topology of the PLS**.

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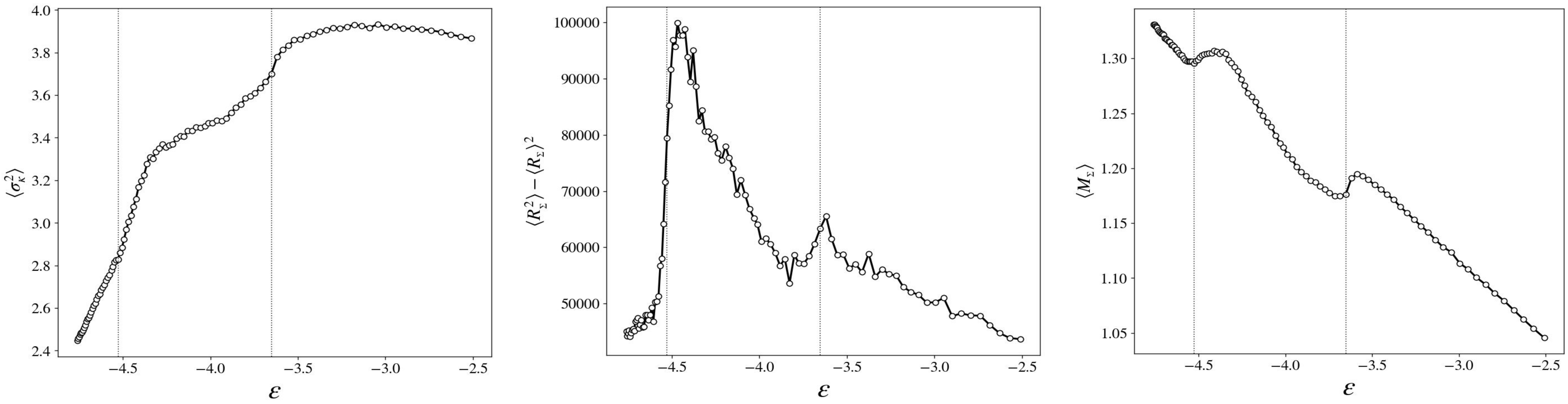
II. Metastability and Phase Transitions in Classical Systems

2) The Glass Transition: a Topological Point of View



As expected, we found that these quantities exhibit sharp **inflexion points** in correspondence with the **peaks of specific heat**, indicating a **topological change** at the transition.

FUTURE PERSPECTIVES

To apply the **topological theory of phase transitions** to a **quantum phase transition**, possibly with a link to **entanglement** and **quantum correlations.**

To connect a **quantum** (or **effectively classical**) **dynamics** in the **quantum state space** with the **metric properties** we exposed here.

Thank you.