Quantum information meets nuclear structure

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Motivation

Nuclear physics

- Deals with a system of non-relativistic **fermions** Schrodinger Equation and symmetrization principle
- In typical processes the number of fermions is neither small nor too large: **Mesoscopic system**
- The **interaction** is not well characterized/understood
- **In medium effects** are very important

Various approximate many body methods required to cover all possible nuclear structure scenarios

Comparison with experiment cannot be used to tell the goodness of the (variational) many body method used

It is important to **quantify correlations** at each level of approximation

Approximations

There is a hierarchy (ladder) of approximations in nuclear structure

- Mean field with symmetry breaking (HFB)
- Symmetry restoration
- Fluctuation in ”collective variables” (the canonical conjugate of orientations)

One can add additional steps to the ladder by considering

- elementary two quasiparticle excitations $\beta_k^+ \beta_l^+ |\Phi\rangle$
- elementary four quasiparticle excitations $\beta_{k_1}^+ \beta_{k_2}^+ \beta_{k_3}^+ \beta_{k_4}^+ |\Phi\rangle$
- etc ...

to eventually reach (QC language) full CI.

Full CI impossible except in small configuration spaces

Tools beyond gs correlation energy required to quantify correlations

Quantum information

By using quantum information tools we would like to quantify how much correlations are incorporated into the different wf of the different approaches considered. The non-correlated symmetry restricted Hartree Fock (HF) is used as a baseline

- Spontaneous symmetry breaking
- Symmetry restoration
- GCM
- Restricted CI

Assumption: Correlations are connected with the degree of entanglement in the system

Quantities like **quantum discord** or the **von Neuman entropy** of the one body density matrix are explored.

Our focus it to understand also how the QI quantities evolve across **quantum phase transitions**, typically as a function of force strength parameters.

Quantum information tools

- **Symmetrization principle** for fermions poses a problem
- Instead of particles (Hilbert spaces) one uses **orbitals (algebras)**
- **Quantum discord**
  Measures quantum correlations between two partitions A and B of the whole set of orbitals as the difference between the quantum conditional entropy and its classical counterpart
- **Entropy one body density matrix**
  The relative entropy of each single orbital with respect to the remaining ones is summed up to define the entropy. Orbital dependent. Uses the natural orbital basis as a reference.

Our work

We have studied several variants of the **Lipkin model** with various tools of quantum information

- Entropies
- Discord

In those models parity symmetry and particle number symmetries could be broken.

II. SINGLE-J SHELL

We consider the $(2j+1)$-fold degenerate single shell of angular momentum j filled with an even number N of identical particles, which without the interaction, is assumed to be at zero energy. The Hamiltonian is composed of the PPQ interaction,

$$\hat{H} = -G\hat{P}^{+}\hat{P} - \chi\hat{Q}\cdot\hat{Q}\ , \tag{2.1}$$

where $\hat{P}^{+}$ is the pair transfer operator and $\hat{Q}$ is the quadrupole moment operator,

$$\hat{P}^{+} = \sum_{mm'}(jmjm'|00)a^{+}_{m}a^{+}_{m'}\ , \tag{2.2a}$$

$$\hat{Q}^{+}_{\mu} = \sum_{mm'}(jmjm'|2\mu)a^{+}_{m}\tilde{a}_{m'}\ , \tag{2.2b}$$

while G and χ are pairing and quadrupole coupling constants, respectively. Hamiltonian (2.1) describes basic collective correlations between nucleons [6,7] and it has been used by many authors [8–11,20,21]. In the mean-

Can be solved exactly
Breaks rotational invariance

Phys. Rev. A 104, 032428; Phys. Rev. A 103, 032426; Phys. Rev. A 105, 062449

Quantum information tools: Entropy

- **Symmetrization principle** for fermions induces correlations
- Slater determinant as the base line (uncorrelated) state
- **Entropy one body density matrix**
  The relative entropy of each single orbital with respect to the remaining ones is summed up to define the entropy.
  Orbital dependent.
  Uses the natural orbital basis of the one body density ρ

$$S = -\sum_k n_k \log n_k$$

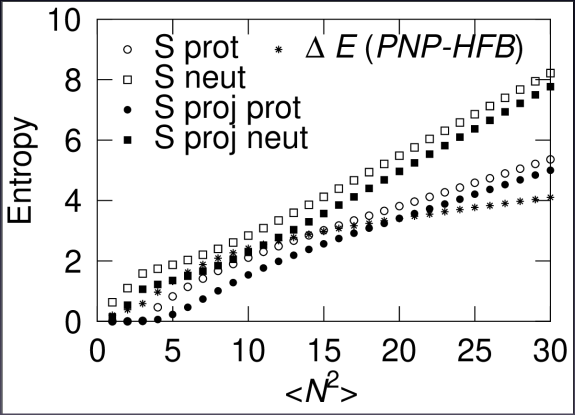
n_k eigenvalues of the density matrix

Slater: $n_k = 0$ or $1 \longrightarrow S = 0$

BCS and HFB

- Eigenvalues of the density ρ are the occupancies v_k^2
- $S \neq 0$ reflects the correlations gained by the BCS (HFB) canonical transformation with respect to Slater
- S grows with ΔN^2 as expected

^{238}U $\beta_2 = 0.3$ Proj means PNP



Collective fluctuation

Collective fluctuations in the GCM scheme

$$|\Psi_\sigma\rangle = \int dq f_\sigma(q)|\Phi(q)\rangle$$

Generating wf $|\Phi(q)\rangle$ is in general of HFB type

To remove BCS (HFB) correlations use the generalized density matrix

$$\mathcal{R}_q = \langle\Phi(q)|\hat{\mathcal{R}}|\Phi(q)\rangle = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}$$

Eigenvalues 0 or 1 $\longrightarrow S(\mathcal{R}) = 0$

Consider now

$$\mathcal{R}_\sigma = \int dq dq' f^*_\sigma(q) f_\sigma(q') \mathcal{R}_{q\,q'}$$

with $\mathcal{R}_{q\,q'} = \langle\Phi(q)|\hat{\mathcal{R}}|\Phi(q')\rangle$

Entropy computed from the eigenvalues of $\mathcal{R}_\sigma$

Correlated densities

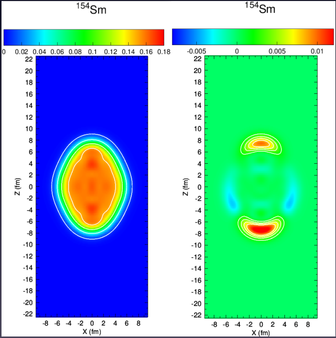
As a side product one can compute the correlated density in coordinate space

$$\rho_\sigma = \int dq dq' f_\sigma^*(q) f_\sigma(q') \rho_{q\,q'}$$

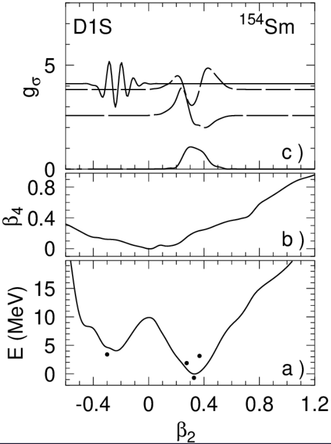
with $\rho_{q\,q'} = \langle \Phi(q) | \hat{\rho} | \Phi(q') \rangle$

$\rho_\sigma(\vec{r}) = \sum_{kl} (\rho_{q\,q'})_{kl} \varphi_k^*(\vec{r}) \varphi_l(\vec{r})$

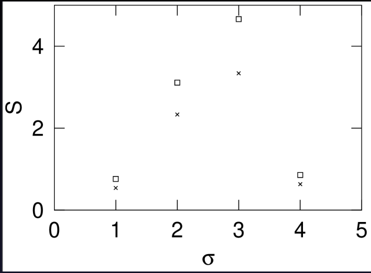
Look at $\rho_\sigma(\vec{r}) - \rho_{HFB}(\vec{r})$

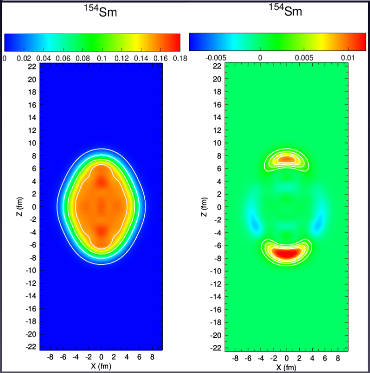


An example



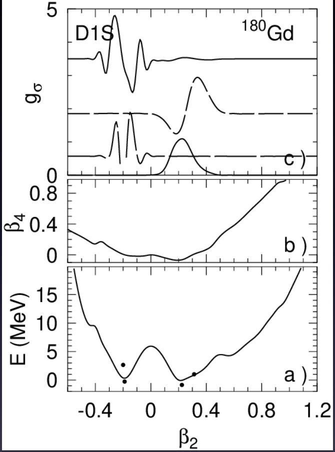
GCM study of ^{154}Sm with β_2
Ground state and two excited states shown



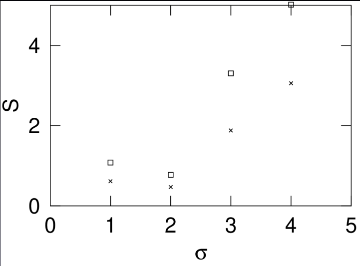


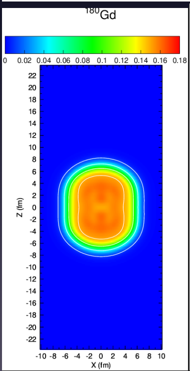
Excited states get a larger entropy !

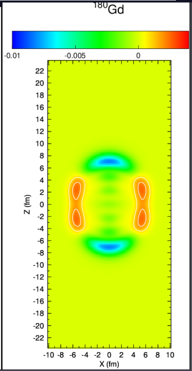
An example



GCM study of ^{180}Gd with β_2
Ground state and two excited states shown



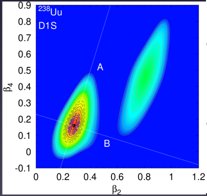


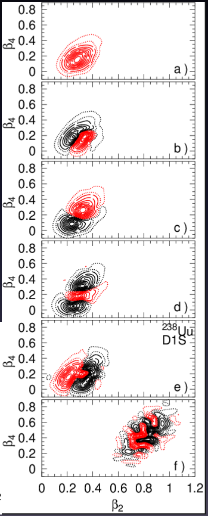


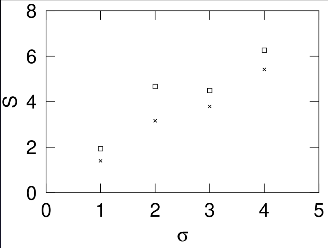
Shape coexistence: two “ground states”

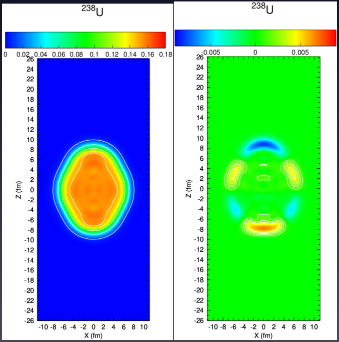
238U $\beta_2 - \beta_4$

GCM $\beta_2 - \beta_4$ in ^{238}U





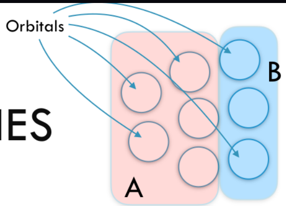




Excited states get a larger entropy !

Quantum information tools: Discord

QUANTUM DISCORD: DEFINITION AND PROPERTIES



Definition:

$$\delta(A, B) = I(A, B) - J(A, B)$$

$$I(A, B) = S(A) + S(B) - S(A, B)$$

Measurement-based conditional entropy

$$J(A, B) = \max_{\Pi_k^B} S\left(\rho^A\right) - S(\rho^{A,B} \,|\, \Pi_k^B)$$

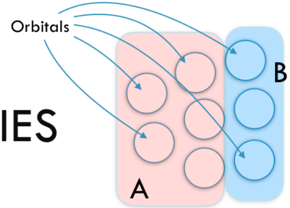
$$S\left(\rho^{A,B} \middle| \Pi_k^B\right) = \sum_k p_k S(\rho_k^{A,B})$$

$$\rho_k^{A,B} = \frac{1}{p_k} \Pi_k^B \rho^{A,B} \Pi_k^B$$

1. Represents all the purely quantum correlations, beyond entanglement.
2. For pure states, it reduces to the von Neumann entropy of a subsystem, and the classical correlations acquires the same value.
3. Hard to compute due to the maximization process.

Quantum information tools: Discord

QUANTUM DISCORD: DEFINITION AND PROPERTIES



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$$\rho_k^{A,B} = \frac{1}{p_k}\Pi_k^B \rho^{A,B} \Pi_k^B$$

How to compute it for qubits:

$$\Pi_{k=0}^B = V\,|\,0\rangle\langle 0\,|\,V^\dagger$$
$$\Pi_{k=1}^B = V\,|\,1\rangle\langle 1\,|\,V^\dagger$$

The unitary V is the 'variational parameter'

Discord for fermions

QUANTUM DISCORD IN FERMION SYSTEMS: TWO ORBITALS

The fermion systems must satisfy the Parity Superselection Rule (PSSR). Hence, not all the measurements are allowed.

Only a superposition of odd/even number of fermions is allowed

Example:

NO!

$$\Pi_+^B |00\rangle\langle 00| \Pi_+^B \propto |00\rangle\langle 00| + |00\rangle\langle 01| + |01\rangle\langle 00| + |01\rangle\langle 01|$$

PSSR allows us to compute the quantum discord: for a system of two orbitals, only two measurements are allowed

$$\Pi_0^B = a_B a_B^\dagger$$
$$\Pi_1^B = a_B^\dagger a_B$$

They are projectors since

$$a_B a_B^\dagger + a_B^\dagger a_B = I$$

Discord for fermions

QUANTUM DISCORD IN FERMION SYSTEMS: TWO ORBITALS

Result:

Dephasing channel

$$\delta(i,j) = S\Big(Z\big(\rho^{i,j}\big)\Big) - S(\rho^{i,j})$$

The two orbital reduced density can be written as

$$\rho^{ij} = \begin{pmatrix} \rho_1 & 0 & 0 & \alpha \\ 0 & \rho_2 & \gamma & 0 \\ 0 & \gamma^* & \rho_3 & 0 \\ \alpha^* & 0 & o & \rho_4 \end{pmatrix}$$

with

$$\begin{aligned} \rho_1 &= 1 - \gamma_{ii} - \gamma_{jj} + \gamma_{ijij} \\ \rho_2 &= \gamma_{jj} - \gamma_{ijij} \\ \rho_3 &= \gamma_{ii} - \gamma_{ijij} \\ \rho_4 &= \gamma_{ijij} \\ \alpha &= \kappa_{ji}^* \\ \gamma &= \gamma_{ji} \end{aligned}$$

Typical many-body variables

$$\gamma_{ji} = \langle\psi|a_i^\dagger a_j|\psi\rangle$$

$$\kappa_{ji} = \langle\psi|a_i a_j|\psi\rangle$$

$$\gamma_{ijij} = \langle\psi|a_i^\dagger a_j^\dagger a_j a_i|\psi\rangle$$

Discord for fermions

QUANTUM DISCORD IN FERMION SYSTEMS: TWO ORBITALS PAIRS

Following the qubit parametrization: $\Pi_k^{(B)} \rightarrow R^{\dagger}\Pi_k^{(B)}R$

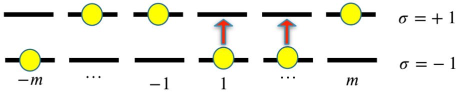
The parametrized projectors doesn't have to mix states with different parity (because of the PSSR):

$$R = e^{iH} \qquad H = \sum_{ij \in \mathcal{H}_B} h_{ij} c_i^{\dagger} c_j + \frac{1}{2}\Delta_{ij}(c_i^{\dagger} c_j^{\dagger} + c_j c_i) \Longrightarrow \text{Thouless rotation}$$

Models: Lipkin

Monopole-monopole term

THE 2-LIPKIN MODEL



The 2 level Lipkin model simulates the nuclear interaction between two shells with same angular momentum introducing a monopole-monopole interaction.

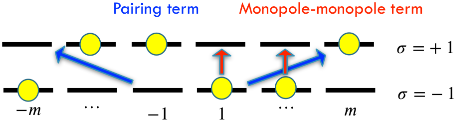
- It simulates the behaviour between degenerated energy levels between the Fermi surface
- Parity symmetry
- Number of particles symmetry

$$H = \epsilon J_0 - \frac{1}{2} V (J_+^2 + J_-^2)$$

Monopole-monopole interaction: for a given value, there is a QPT that breaks parity in the upper level

$$J_0 = \frac{1}{2} \sum_{\sigma,m} \sigma c_{\sigma,m}^{\dagger} c_{\sigma,m} \qquad J_+ = J_-^{\dagger} = \sum_{m} c_{1,m}^{\dagger} c_{-1,m}$$

Models: Agassi



THE AGASSI MODEL

Simulates a nuclear Hamiltonian introducing monopole-monopole and pairing interaction

- It simulates the behaviour between degenerated energy levels between the Fermi surface
- Parity symmetry
- Number of particles symmetry

$$H = \epsilon J_0 - \frac{1}{2}V(J_+^2 + J_-^2) - g\sum_{\sigma,\sigma'} A_\sigma^\dagger A_{\sigma'}$$

The pairing interaction adds a superconducting phase

Monopole-monopole interaction: for a given value, there is a QPT that breaks parity in the upper level

Pairing interaction: for a given value, there is a QPT that breaks particle number

V and g act as order parameters

$$J_0 = \frac{1}{2}\sum_{\sigma,m} \sigma c_{\sigma,m}^\dagger c_{\sigma,m} \qquad J_+ = J_-^\dagger = \sum_m c_{1,m}^\dagger c_{-1,m} \qquad A_\sigma = \sum_{m>0} c_{\sigma,-m} c_{\sigma,m}$$

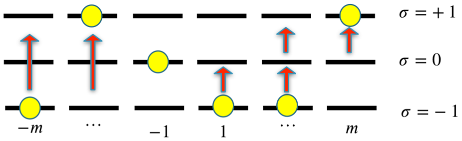
O(5) generators

SU(2) generators without pairing interaction (2-Lipkin model)

The HFB ground state has three quantum phases, corresponding to each term

Models: Lipkin 3 levels

THE 3-LIPKIN MODEL



Similar to the 2-Lipkin model, with one additional energy level.

$$H = \epsilon(K_{22} - K_{00}) - \frac{V}{2}(K_{10}^2 + K_{20}^2 + K_{21}^2 + h.c.)$$

Monopole-monopole interaction: for two given values, there is a QPT that breaks number parity in the +1 and 0 level.

$$K_{\sigma\sigma'} = \sum_m c^\dagger_{\sigma,m} c_{\sigma',m}$$

→ Monopole-monopole interaction between σ and σ' levels

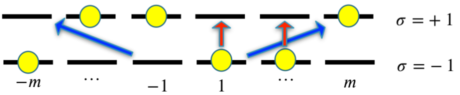
⇒ SU(3) generators

Results

Faba, Martín and Robledo, Phys. Rev. A 103, 032426, 2021

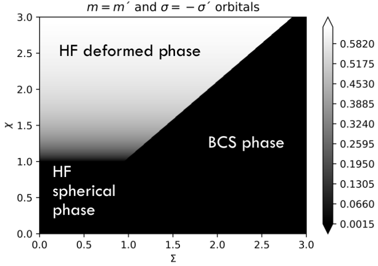
Two orbital quantum discord

THE AGASSI MODEL

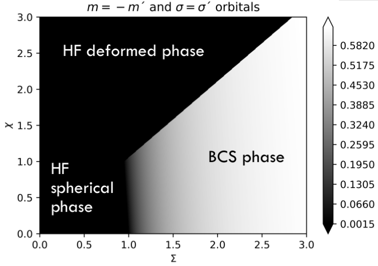


The QD acts as an order parameter

The quantum discord for the HFB ground state in the 'original' orbital basis is easy to compute:



HF deformed phase breaks parity symmetry



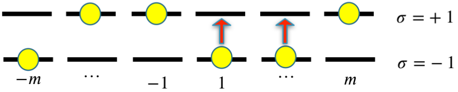
BCS phase breaks particle number symmetry

Results

Faba, Martín and Robledo, Phys. Rev. A 103, 032426, 2021

Two orbital quantum discord

THE 2-LIPKIN MODEL



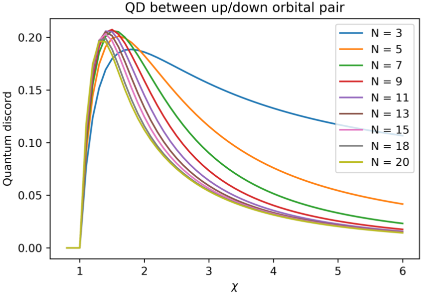
A particular case of Agassi model: only monopole-monopole interaction

$$H = \epsilon J_0 - \frac{1}{2} V (J_+^2 + J_-^2)$$

Here we have QD between HF orbitals for the exact ground state.

- If QD is high, the HF orbitals need to be very correlated in order to catch all the correlations.
- If QD is small, the HF orbitals don't need to be very correlated in order to describe the exact state.

This is in agreement with the behaviour of RCE vs OV



1. For $\chi < 1$ there is no quantum discord. The orbitals are the same as the 'original' ones.
2. For $\chi \to \infty$ the discord is low and decreases fast with the number of particles. The mean-field approx. is good.
3. For $\chi \approx 1$ and $\chi > 1$ the discord reaches a maximum. The HF approx. fails, since the orbitals need the correlate between them in order to describe the exact ground state.

Results: ϵ vs S

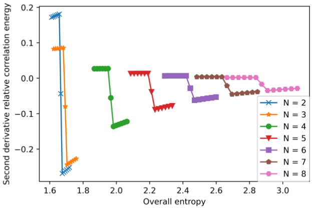
Correlation energy & overall entropy

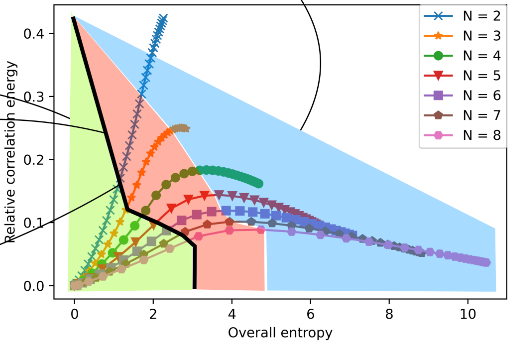
THE 2-LIPKIN MODEL

RCE starts to decrease, but the OE keeps growing until saturation ❌

RCE and OE grow quasi-linearly ✅

Due to the QPT, RCE changes the curvature ❗





Exact ground state

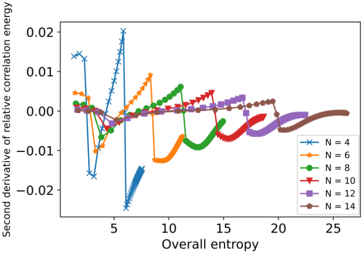
Faba, Martín and Robledo, Phys. Rev. A 104, 032428, 2021

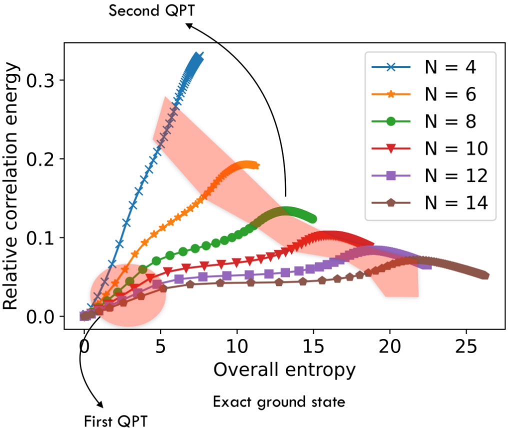
Results: ϵ vs S

Correlation energy & overall entropy

THE 3-LIPKIN MODEL

Same behaviour than 2-Lipkin model, with two QPT's





Exact ground state

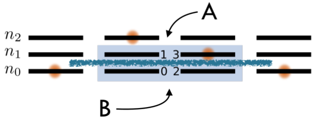
Faba, Martín and Robledo, Phys. Rev. A 104, 032428, 2021

Results: Four orbital QD

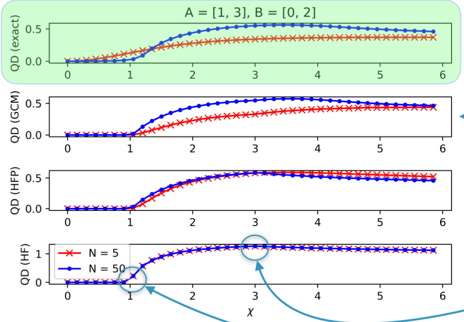
Four orbital quantum discord

THE 3-LIPKIN MODEL

$\{n_0, n_1\}$



- This partition follows the natural structure of the interaction



All the approximations reproduce more or less the exact results.

+ better fit, specially far from the first QPT point

+ particle number dependence

Change of behaviour at the QPT points

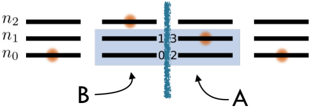
Faba, Martín and Robledo, Phys. Rev. A 105, 062449, 2022

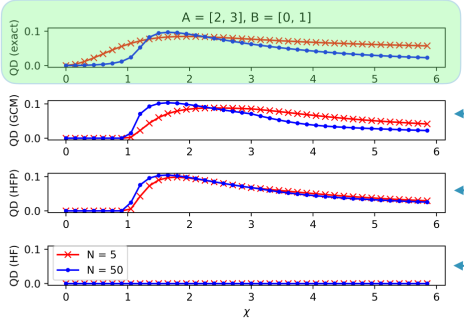
Results: Four orbital QD

Four orbital quantum discord

THE 3-LIPKIN MODEL

$\{n_0, n_1\}$





The HF approximation does not succeed catching quantum correlations, we need a symmetry restoration

Closer to the exact result

A symmetry restoration is enough to obtain quantum correlations in a similar shape with respect to the exact state + particle number dependence.

Null QD for all values!

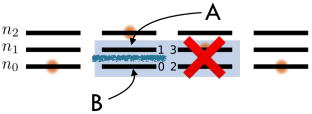
Faba, Martín and Robledo, Phys. Rev. A 105, 062449, 2022

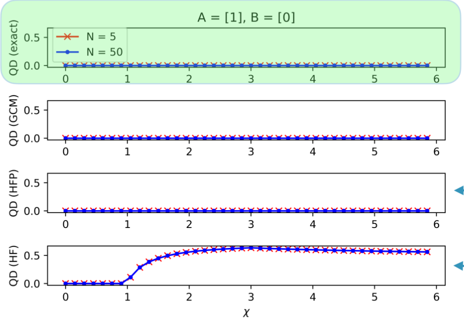
Results: Four orbital QD

Four orbital quantum discord

THE 3-LIPKIN MODEL

$\{n_0, n_1\}$





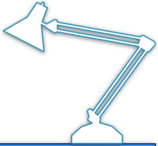
The symmetry breaking process creates ‘fake’ quantum correlations at the two orbital level

A symmetry restoration is enough to restore the true QD

‘Fake’ QD!

Faba, Martín and Robledo, Phys. Rev. A 105, 062449, 2022

CONCLUSIONS



- For fermion systems, the QD can be computed through Thouless rotations, and for the two orbital case, it is specially simple.

- QD is a good tool in order to analyze many body systems, such as QPTs. Moreover, the orbital QD is useful to understand deeply the role of the symmetries.

- In general, one needs symmetry restoration on top of HF to catch most of the correlations present in the exact ground state. The correlations are 'redistributed' with the symmetry restoration process.

- Correlation energy is not a good estimation of the correlations within a system.