Quantum information tools in nuclear structure

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Nuclear energy density functional method: going beyond the minefield,

Saclay, November 2023

Authorship

The contents of the present talk mostly correspond to the thesis work of **Javier Faba** under the supervision of V. Martin and myself

Motivation

- Atomic nucleus is a strongly correlated system
- Mean field approximation is a very good starting point to describe dynamics
- As the “nuclear interaction” is not well known, comparison with experimental data cannot be used to asses the goodnes of a given many body method (like in quantum chemistry)
- Correlation energies with respect to the mean field solution have often been used to characterize the amount of correlations of a given approximation/method
- It is convenient to distinguish among classical, quantum and symmetrization principle correlations (fermions!)

Makes sense to explore other measures of correlations to characterize them

The ideas used in quantum information to characterize entanglement between subsets of the system can be very helpful here

Brief recap of nuclear physics

(low energy) Nuclear physics

- Deals with a system of non-relativistic **fermions** Schrodinger Equation and symmetrization principle
- In typical systems the number of fermions is neither small nor too large: **Mesoscopic system**

also

- The **interaction** is not well characterized/understood
- **In medium effects** are very important: *A*-body problem/correlations

Discrepancies with experimental data can be attributed either to the interaction and/or the many body method

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

The nuclear mean field

The ”**in medium**” effective nuclear interaction is soft enough to permit a mean field treatment

- Magic numbers (8,20 28, 50, 82, 126, ...) are the strongest experimental evidence supporting the existence of a mean field. Implies a strong spin-orbit (meson exchange currents)
- All ground state of even-even nuclei are 0^+ supporting the existence of short range correlations creating Cooper pairs of protons and neutrons

There is a mean field created **collaboratively** by all nucleons that must include short correlations like in the BCS theory of superfluidity
The mean field can be determined by using the standard **Hartree- Fock- Bogoliubov (HFB)** method

The HFB approach

Mean field plus pairing (Hartree Fock Bogoliubov, HFB) is based on the Bogoliubov transformation to quasi-particles

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^+ & V^+ \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} \equiv W^+ \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

The **HFB ground state** defined by the condition

$$\beta_\mu |\Phi\rangle = 0 \iff |\Phi\rangle = \prod (u_k + v_k a_k^+ a_{\bar{k}}^+ |-\rangle$$

U and V are determined by the variational principle on $\langle\Phi|\hat{H}|\Phi\rangle$

HFB **spontaneously breaks the particle number symmetry:** $|\Phi\rangle$ is not and eigenstate of the particle number operator $\hat{N}$.

The symmetry group is $U(1)$ (generated by $e^{i\varphi\hat{N}}$)

Particle number constraint $\langle\Phi|\hat{N}|\Phi\rangle = N$ and Routhian $\hat{H} - \lambda\hat{N}$

Spontaneous symmetry breaking

The nuclear interaction favors the **spontaneous breaking** of many symmetries at the mean field level

- Rotational invariance: Associated to $SO(3)$
  - Angular momentum quantum numbers no longer valid
  - Matter distribution not spherically symmetric: nuclear deformation
  - Intrinsic and laboratory frame
  - Rotational bands (ubiquitous in the nuclear chart)
- Parity: Discrete group. Parity doublets
- Traslational invariance
- Isospin (quantum number for protons and neutrons)

However, going **beyond the mean field** is required for a **proper description of quantum numbers** (very important for electromagnetic processes, to implement selection rules, etc)

Symmetry restoration

Example: Parity projection
Consider a wave function $|\Phi\rangle$ which is not eigenstate of parity.
Act with the group elements ($\mathbb{I}$ and Π) on $|\Phi\rangle$
Take linear combinations with the appropriate weights to restore parity

$$|\pi\rangle = \mathcal{N}[|\Phi\rangle + \pi|\Pi\Phi\rangle] = \mathcal{N}[\mathbb{I} + \pi\Pi]|\Phi\rangle$$

which defines the projector on good parity $P_\pi = \mathbb{I} + \pi\Pi$

- **Please note that $|\pi\rangle$ are linear combinations of $|\Phi\rangle$ and $\Pi|\Phi\rangle$ are, no longer, mean field wf**
- **Symmetry restoration incorporates additional correlations beyond mean field in the wave function**

Continuous symmetries

- Particle number, $U(1)$ symmetry group

$$P^N = \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{-i\varphi N} e^{i\varphi \hat{N}}$$

  where φ determines the orientation in "gauge space" and $\exp[-i\varphi N]$ is the symmetry dictated weight.

- Angular momentum, $SU(2)$ symmetry group

$$P^{lM} = \sum_K g_K \int d\Omega \mathcal{D}^l_{KM}(\Omega)\hat{R}(\Omega)$$

  where the Euler angles Ω determine the orientation in space and the symmetry dictated weight are the Wigner $\mathcal{D}$ matrices plus some coefficients g_K due to the non-abelian character of $SU(2)$

Order parameter

Every broken symmetry has associated order parameters

- Particle number: Pairing gap $\Delta = G\langle \sum_k c_k^+ c_{\bar{k}}^+ \rangle$
  Non zero when the symmetry is broken

  When the wf is rotated in gauge space $e^{i\varphi\hat{N}}|\Phi\rangle$ it acquires a complex phase $\Delta \rightarrow \Delta e^{2i\varphi}$
- Rotational invariance: any mean value of multipole operator $\beta_{\lambda\mu} = \langle Q_{\lambda\mu} \rangle$ proportional to the spherical harmonics $Y_{\lambda\mu}$ measuring the departure of the matter distribution from sphericity

  Quadupole moment is the lowest order and most popular

  Again the "deformation parameter" $\langle Q_{\lambda\mu} \rangle$ acquires a complex phase when the symmetry breaking mean field solution is rotated (far more involved than in the particle number case due to the non-abelian character of $SU(2)$)

Order parameters

One says that the orientation φ (phase) and the size $|\Delta|$ of the complex order parameter are **canonical conjugate variables** and therefore if one considers fluctuations in orientation

$$P^N = \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{-i\varphi N} e^{i\varphi \hat{N}}$$

one should also consider fluctuations in $|\Delta|$

$$|\Psi_\sigma\rangle = \int d|\Delta| f_\sigma(|\Delta|) P^N |\Phi(|\Delta|)\rangle$$

This is the motivation/justification of the generator coordinate method (GCM). In the rotational case

$$|\Psi_\sigma\rangle = \int d\beta_{\mu\nu} f_\sigma(\beta_{\mu\nu}) P^{IM} |\Phi(\beta_{\mu\nu})\rangle$$

The choice of the $\beta_{\mu\nu}$ depends on the physics to be described. Typically, one takes β_{20} or β_{20} and β_{30}, or β_{20} and γ etc

Approximations

The above discussed methods set up a hierarchy

- 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

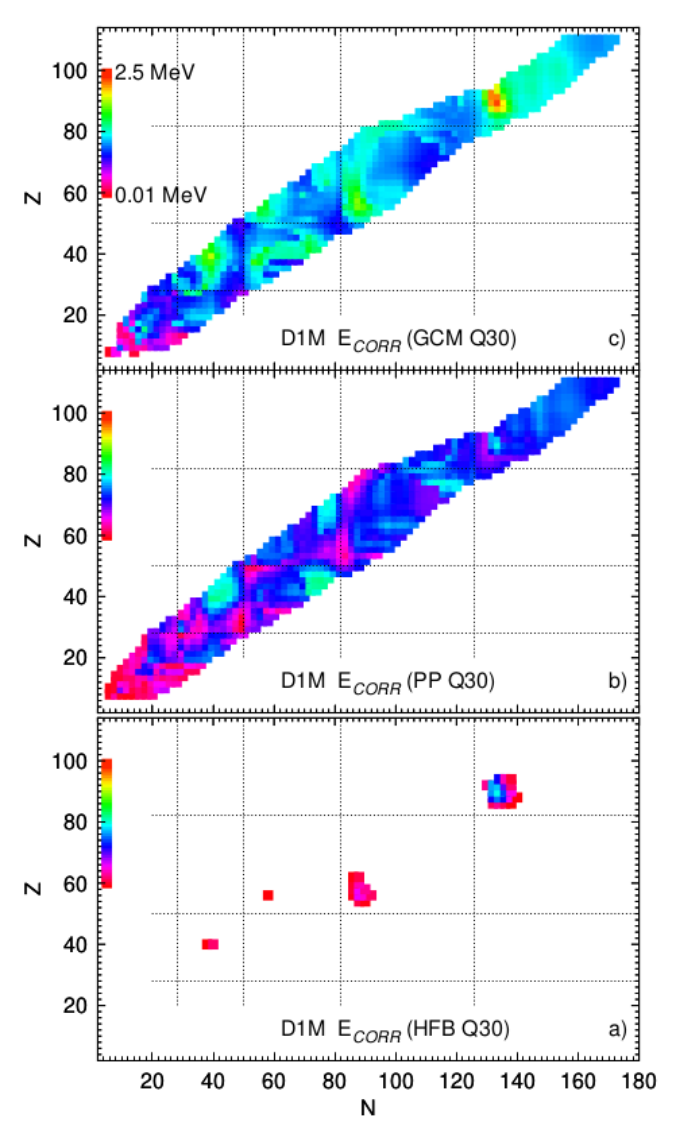
- elementary two quasiparticle excitations $\beta_k^+ \beta_l^+ |\Phi\rangle$
- elementary four quasiparticle excitations $\beta_{k_1}^+ \beta_{k_2}^+ \beta_{k_3}^+ \beta_{k_4}^+ |\Phi\rangle$
- etc ...

to eventually reach (QC language) full CI.

Full CI impossible except in small configuration spaces

Tools to quantify the amount of correlations introduced at each step are required

Correlation energy



Correlation energy with respect to a reflection symmetric HFB ground state

- Breaking reflection symmetry at the HFB level is not very effective
  A bit more correlations than RS HFB
- VAP-Parity projection brings a non-neglegible energy gain everywhere
  Lots of correlations included
- GCM-Q3 (includes VAP-Parity) brings additional correlation energy
  Even more 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) or HFB are 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.

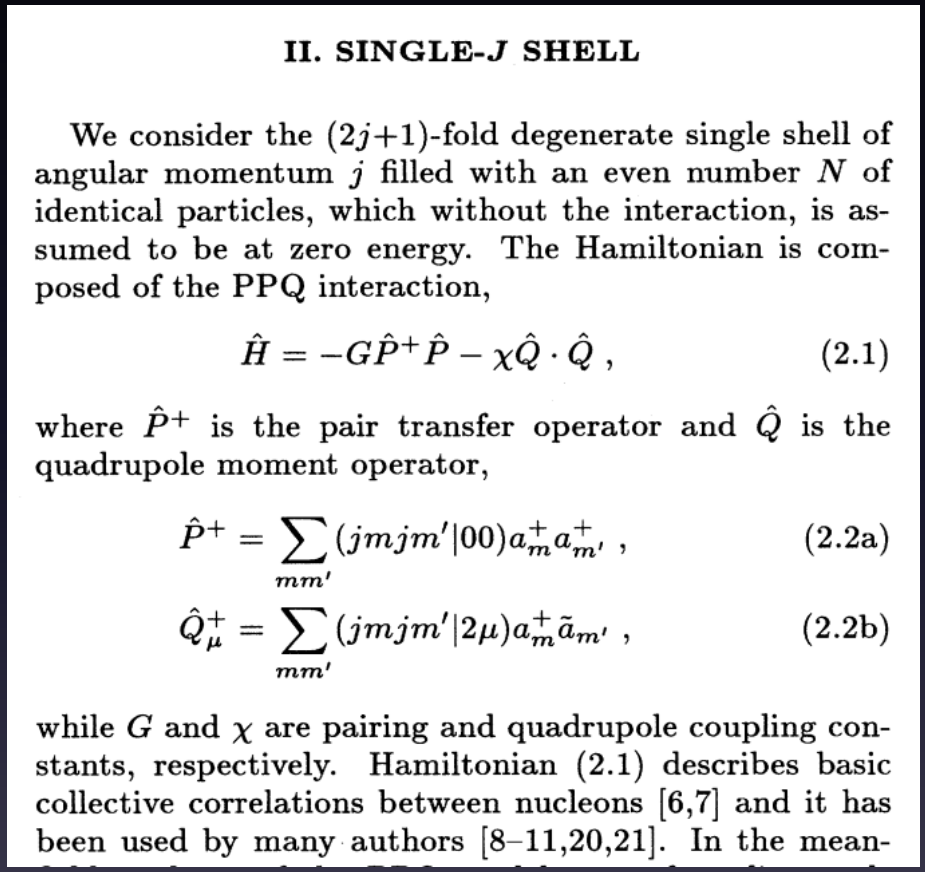
Our focus it to understand also how the QI quantities evolve across **quantum phase transitions**, typically as a function of force strength parameters.

Our work

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

- VN Entropy
- Discord

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



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-

Breaks rotational invariance

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

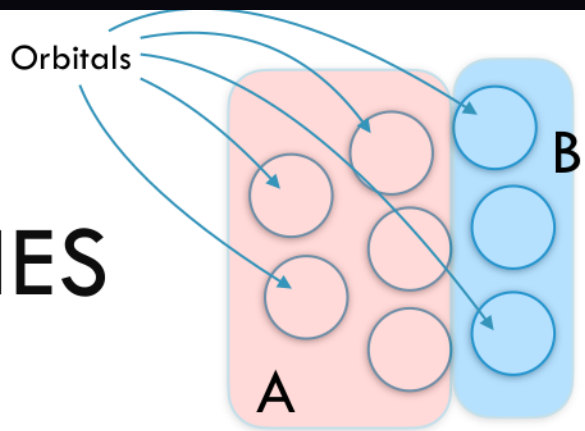
Quantum information tools

- **Symmetrization principle** for fermions poses a problem
- Instead of particles **orbitals (algebras)** are used
- **Quantum discord**
  Measures quantum correlations between partition A and B of the whole set of orbitals. Difference between the quantum conditional entropy and its classical counterpart [1]. Counts all kind of quantum correaltions, not only entanglement.
- **Overall/one body Entropy**
  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.**

[1] Classical correlations

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

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

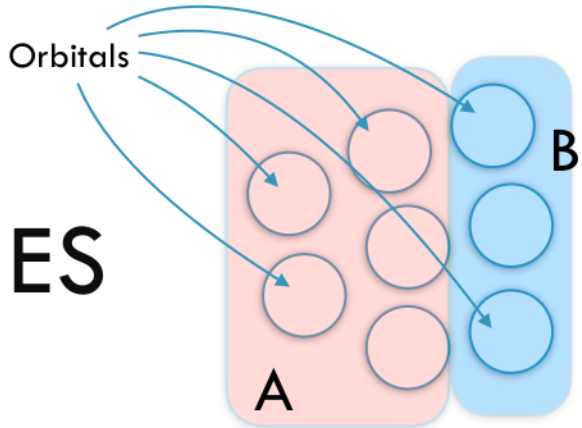
$$S(\rho^{A,B}|\Pi_k^B) = \sum_k p_k S(\rho_k^{A,B})$$

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

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

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'

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

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: $\Pi_k^{(B)} \rightarrow R^\dagger \Pi_k^{(B)} R$

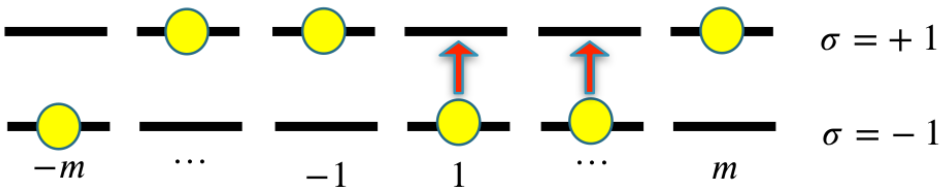
The parametrized projectors doesn't have to mix states with different parity (because of the PSSR):

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

Models: Lipkin

THE 2-LIPKIN MODEL

Monopole-monopole term



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

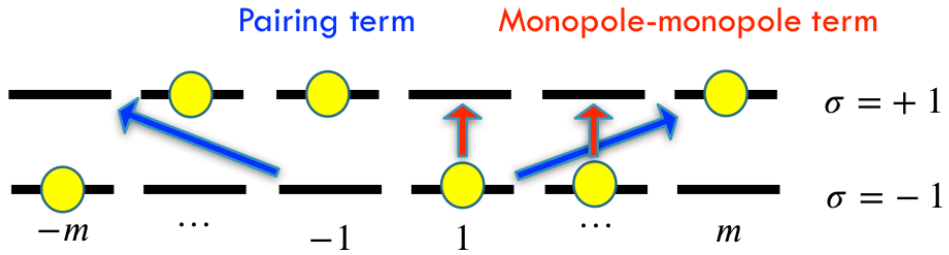
$$H = \epsilon J_0 - \frac{1}{2} V (J_+^2 + J_-^2)$$

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

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

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

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

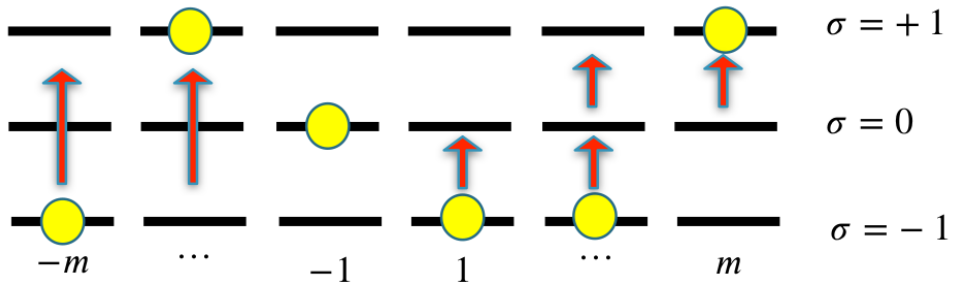
O(5) generators

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

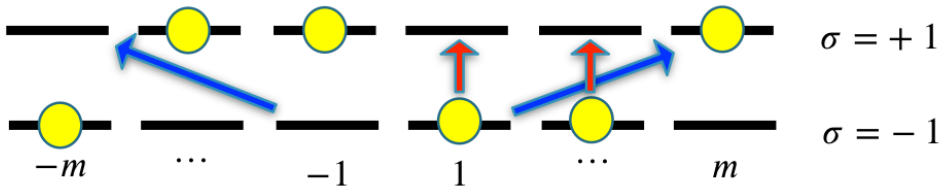
→ SU(3) generators

Results

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

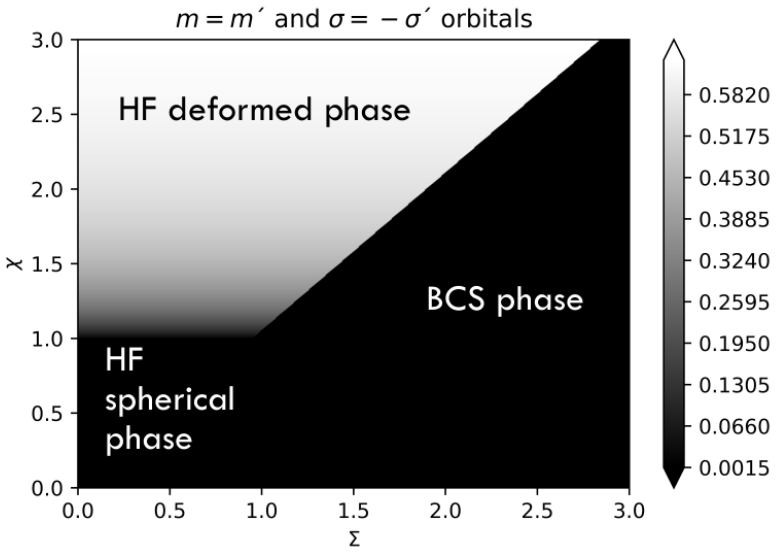
Two orbital quantum discord

THE AGASSI MODEL

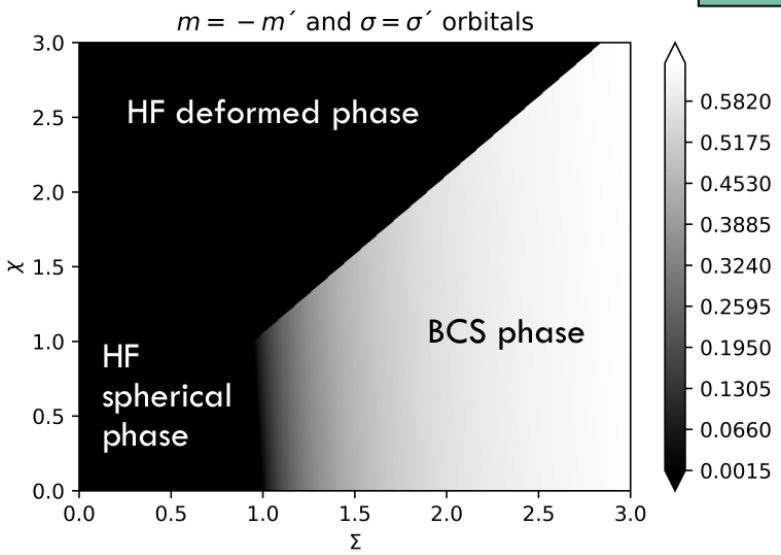


The quantum discord for the HFB ground state in the 'original' orbital basis is easy to compute:

The QD acts as an order parameter



HF deformed phase breaks parity symmetry



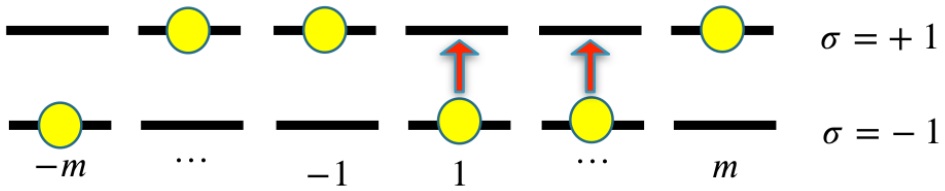
BCS phase breaks particle number symmetry

Results

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

Two orbital quantum discord

THE 2-LIPKIN MODEL



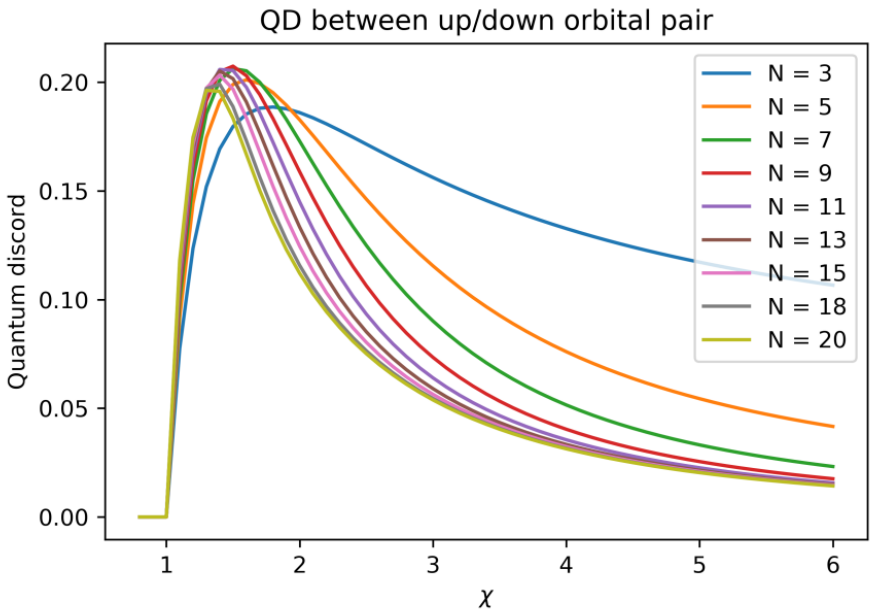
A particular case of Agassi model: only monopole-monopole interaction

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

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

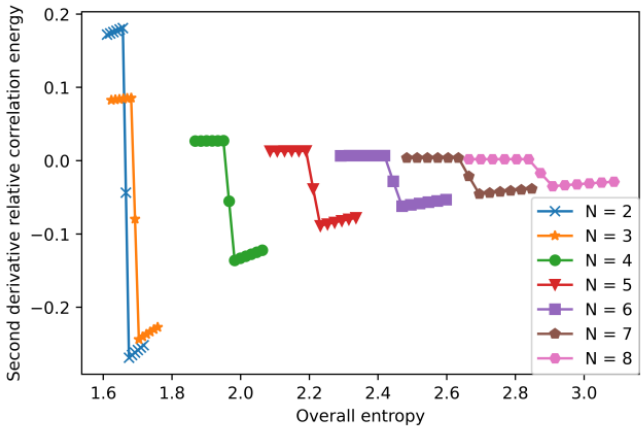
Correlation energy & overall entropy

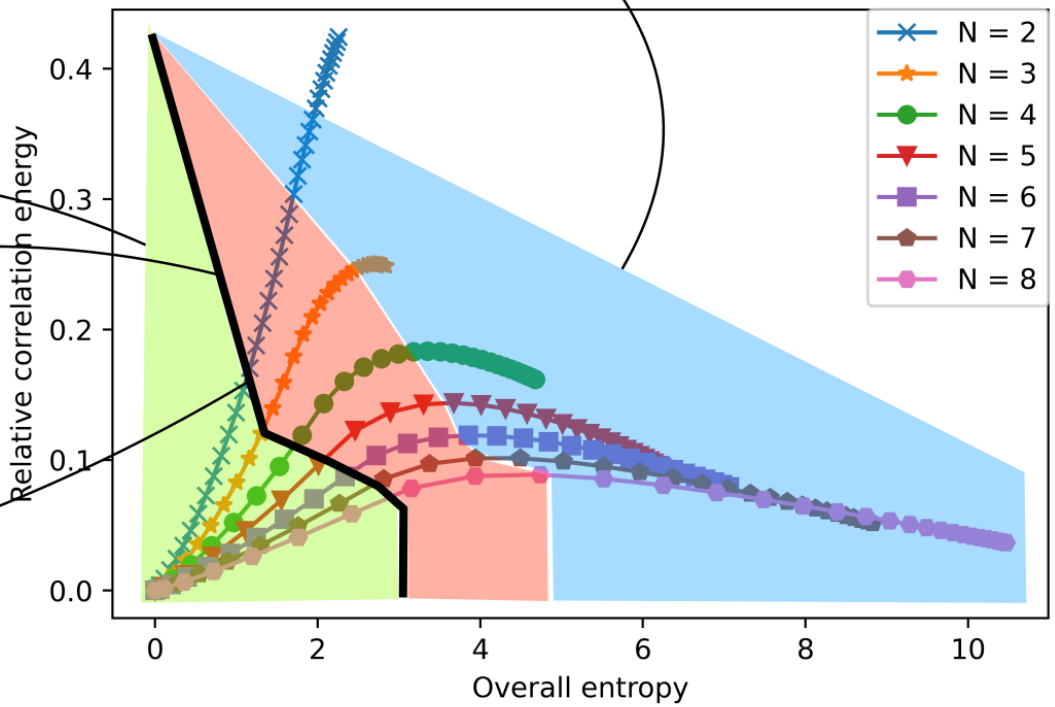
THE 2-LIPKIN MODEL

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

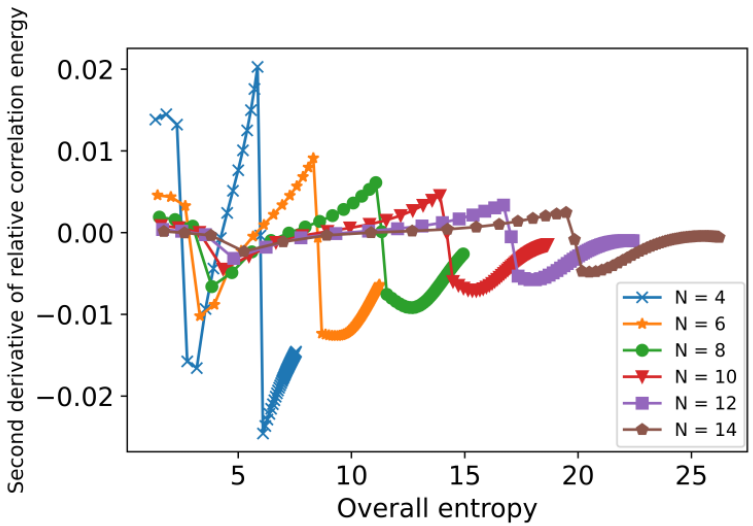
Faba, Martín and Robledo, Phys. Rev. A 104, 032428, 2021

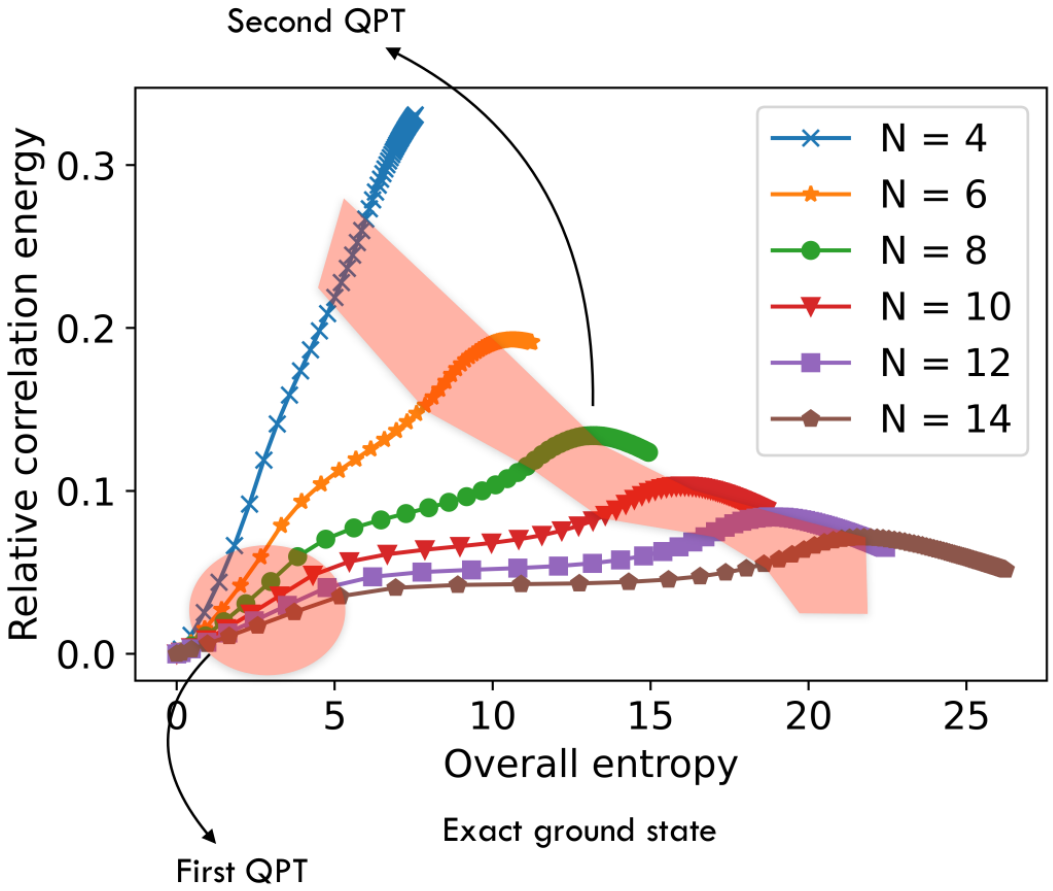
Results: ϵ vs S

Correlation energy & overall entropy

THE 3-LIPKIN MODEL

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





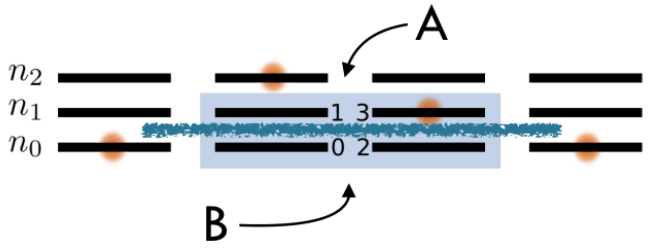
Faba, Martín and Robledo, Phys. Rev. A 104, 032428, 2021

Results: Four orbital QD

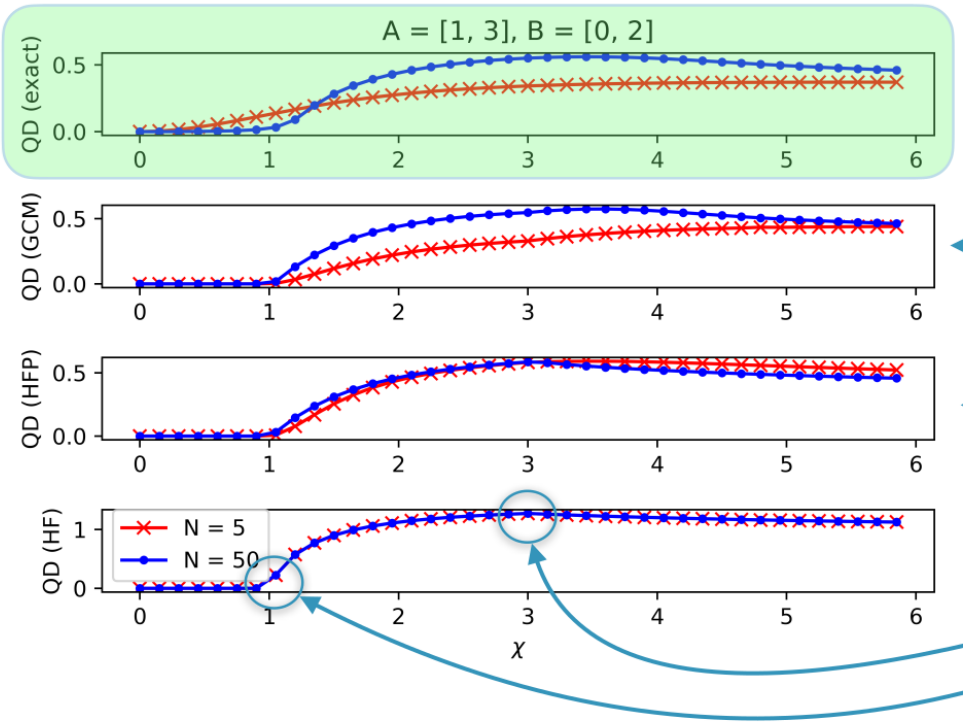
Four orbital quantum discord

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

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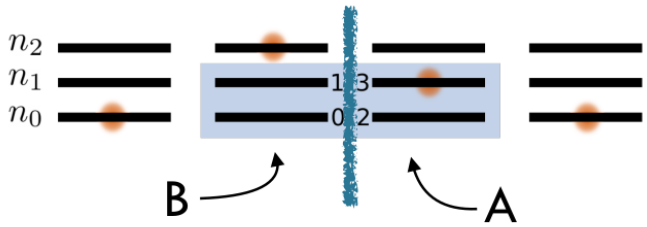
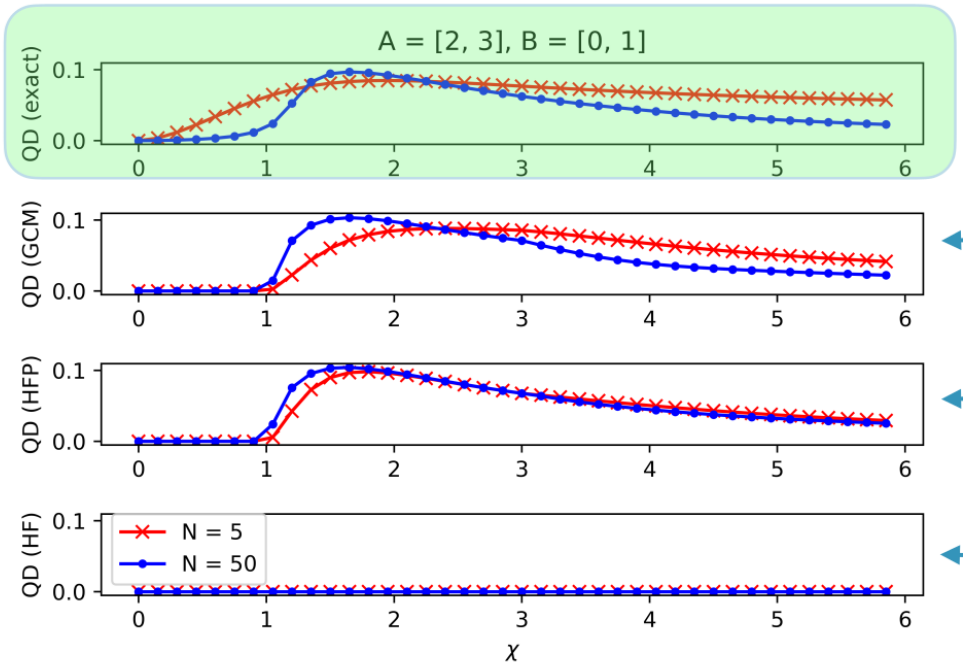




The HF approximation does not succeed catching quantum correlations, we need a symmetry restoration

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!

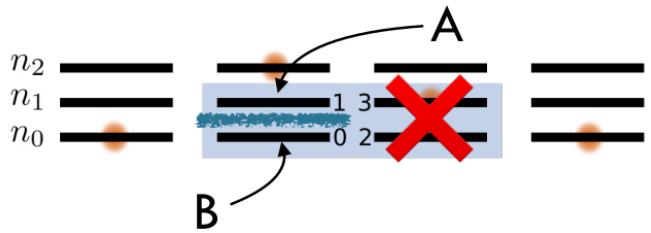
Faba, Martín and Robledo, Phys. Rev. A 105, 062449, 2022

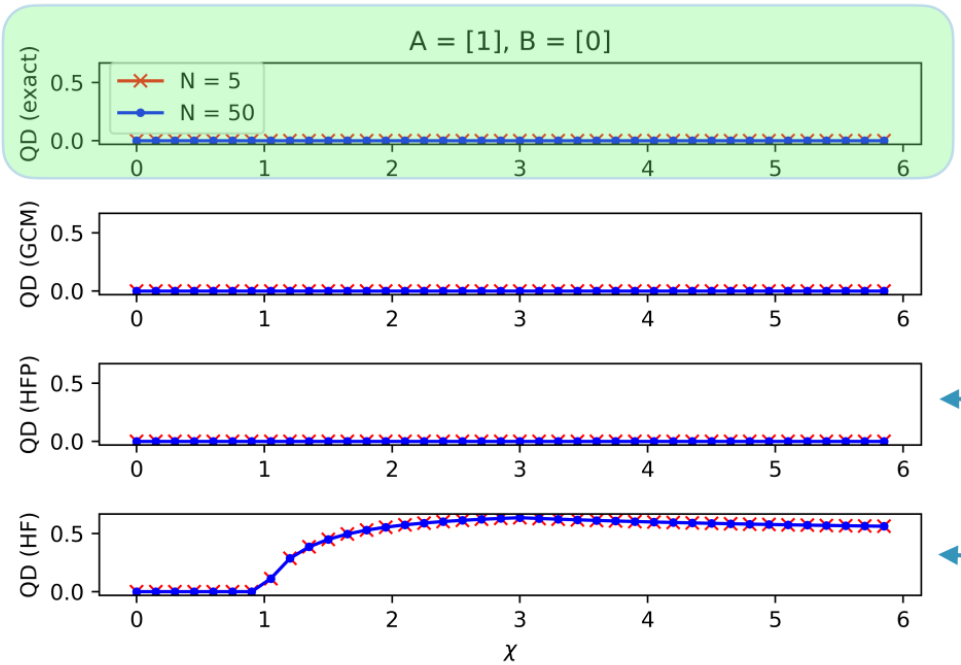
Results: Four orbital QD

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.

Single j model

- More realistic model of nuclear structure
- Pairing plus quadrupole in a reduce configuration space
- Breaks rotational invariance and particle number
- Can be solved exactly

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,

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

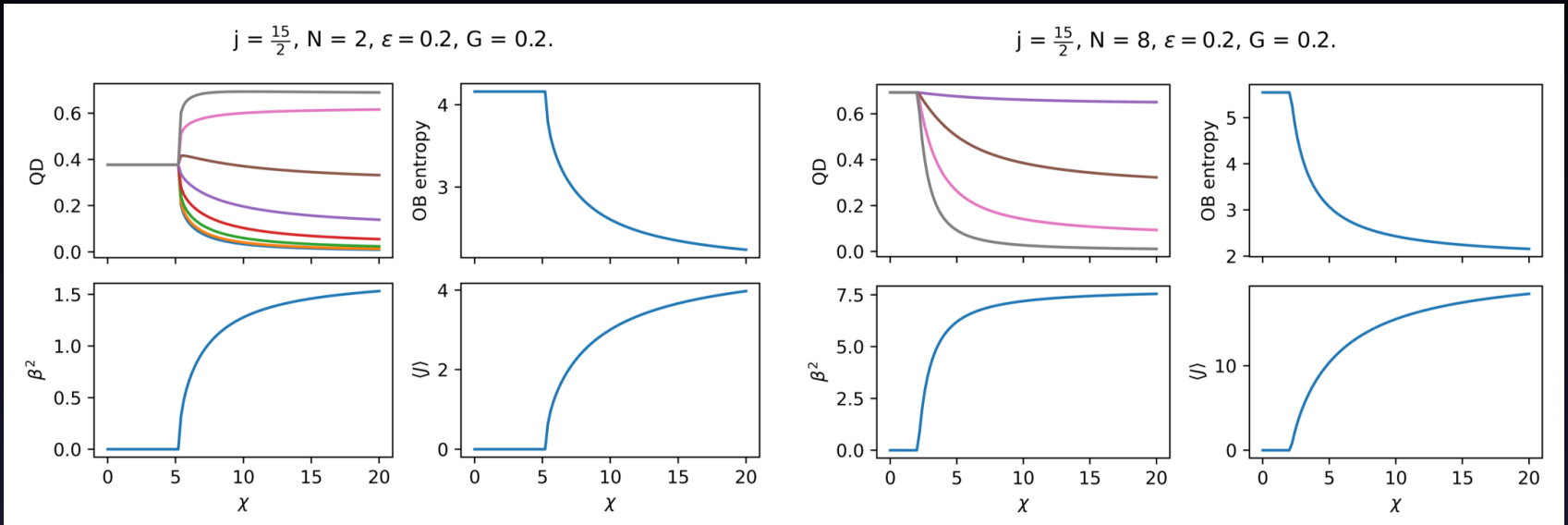
where $\hat{P}^{+}$ is the pair transfer operator and $\hat{Q}$ is the quadrupole moment operator,

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

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

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-

Single j, HFB



- N=2 and half filling
- Natural basis orbitals, pairing is the only responsible for correlations
- Transition to a deformed system as κ increases
- One body entropy decreases because the mean field approximation is better

Single j, Projection

In progress

Overall entropy in realistic GCM

I planned to present some results about overal entropies for realistic GCM wave functions and their connection with correlated spatial densities but ...

Other work in nuclear physics

- Entanglement entropy and Schmidt number as measures of delocalization of α clusters in one-dimensional nuclear systems
  Y. Kanada-En'yo, Prog. Theor. Exp. Phys. 2015, 043D04 (2015)
- Entanglement rearrangement in self-consistent nuclear structure calculations
  C. Robin et al, Phys Rev C103, 034325
- Several papers from La Plata group (Rossignoli and Gigena)
- Entanglement and correlation in two-nucleon systems
  A T Kruppa, et at J. Phys G 48, 25107
- Entanglement and seniority
  A T Kruppa et al, Phys. Rev. C 106, 024303