Two-orbital quantum discord in fermion systems

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A simple expression to compute the quantum discord between two orbitals in fermion systems is derived using the parity superselection rule. As the correlation between orbitals depends on the basis chosen, we discuss a special orbital basis, the natural one. We show that quantum correlations between orbitals disappear when the pairing tensor is zero. The Hartree-Fock orbital within a Slater determinant state is a Hartree-Fock-Bogoliubov quasiparticle orbital in a quasiparticle vacuum, or the ground state of a Hamiltonian with particle symmetry and their corresponding natural orbitals are some relevant examples of natural basis and corresponding states. Since natural orbitals have a special property, we seek for the quantum discord in non-natural orbital basis. We analyze our findings in the context of the Lipkin-Meshkov-Glick and Agassi models.

I. INTRODUCTION

Quantum correlations have been a central field of research since the inception of quantum mechanics [1, 2]. They are a fundamental feature of the quantum theory and give rise to many interesting phenomena like those observed in the fields of quantum cryptography [3–6], quantum teleportation [7–9], quantum phase transitions [10–12], etc.

They can be studied from different points of view. For instance, from a many body perspective, it is known that, if we solve a many body Hamiltonian through mean field techniques, such as the Hartree-Fock or Hartree-Fock-Bogoliubov method, the ground state will, in general, not preserve the symmetries of the Hamiltonian [13] (Bogoliubov quasiparticle orbitals in a quasiparticle vacuum, or the ground state of a Hamiltonian with particle symmetry and their corresponding natural orbitals are some relevant examples of natural basis and corresponding states). Since natural orbitals have a special property, we seek for the quantum discord in non-natural orbital basis. We analyze our findings in the context of the Lipkin-Meshkov-Glick and Agassi models.

II. QUANTUM DISCORD

Given the Hilbert space $\mathcal{H}$ of a quantum system, let us assume there exists a bi-partition $\mathcal{H} = \mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)}$. The quantum discord, introduced by Ollivier and Zurek [17], is a measure of the purely-quantum correlations beyond entanglement between both parts $A$ and $B$. It is defined as the discrepancy between two classically equivalent measures $I(A, B)$ and $J(A, B)$ of the mutual infor-
While $I(A, B)$ is a measure of all kind of correlations, $J(A, B)$ quantifies the classical part. The measurement-based conditional entropy entering the definition of $J(A, B)$ is defined as
\[ S(\rho^{(A,B)}|\{\Pi^k_B\}) = \sum_k p_k S(\rho_k^{(A,B)}) \]
where $\rho_k^{(A,B)} = \frac{1}{p_k} \Pi_k^B \rho^{(A,B)} \Pi_k^B$ is the measured-projected state and $p_k = \text{tr}(\Pi_k^B \rho^{(A,B)} \Pi_k^B)$ is the associated probability. The measurement and the associated projector $\Pi_k^B$ are defined only in the sector $B$ of the bi-partition.

Due to the variational process involved in Eq. (2) the quantum discord is hard to compute in general either analytically [18] or numerically [19]. Some results exist for two qubit systems [20, 21], and there is also some work related to the quantum discord in fermionic systems [12, 22–24]. The calculation is enormously simplified if there exist in the model considered some kind of selection rule that reduces the variational space (i.e., the set of valid projective measurements in $B$). In this work, we derive a very simple expression for the two orbital quantum discord in a general fermionic system by using a number-parity selection rule, and we apply it under the context of the Agassi model. This approach is a novelty and has not been used in studies just mentioned.

## III. TWO-ORBITAL FERMIONIC SYSTEM

Consider a system formed by $\Omega$ orbitals occupied by fermions where number-parity symmetry [25] is preserved and can be considered as a selection rule (NPSR) [1]. Since we are dealing with fermions, the single-orbital occupation may be 0 (if there is no fermion in the orbital) or 1 (if there is a single fermion in the orbital). We divide the system in three subsystems: $A$, $B$ and $C$. $A(B)$ corresponds to the $i(j)$-th orbital, and $C$ corresponds to the orthogonal complement of $AB$. Since all pure and mixed states must fulfill the NPSR, the density matrix corresponding to the $AB$ subsystem will have the following structure in the occupation basis:
\[ \rho^{(A,B)} = \begin{pmatrix} \rho_1 & 0 & 0 & \alpha^* \\ 0 & \rho_2 & \gamma & 0 \\ 0 & \gamma^* & \rho_3 & 0 \\ \alpha & 0 & 0 & \rho_4 \end{pmatrix} \]
with $\sum_{i=1}^4 \rho_i = 1$. Now we must find a complete set of projectors in the $B$ subspace. For this purpose, one would be tempted to follow the path as in [20], this is, performing $U(2)$ rotations on the two “computational” local projectors. Nonetheless, as the NPSR must be fulfilled a projective measurement that mix the occupied and non-occupied state of just one orbital would be unphysical. In fact, a self-adjoint operator must commute with the super-selection rule in order to be an observable. A measurement that do not respect the super-selection rule can not be related to any observable, so it would be unrealizable. Then, the only possible projectors in the $j$-th orbital’s occupation space are
\[ \Pi_0 = a_j a_j^\dagger \]
\[ \Pi_1 = a_j^\dagger a_j \]
Since the set of possible projective measurements for part $B$ has just one pair of elements instead of infinite, no optimization process is involved in Eq. (2) and quantum discord can be easily computed. The measured-projected states will be
\[ \rho_0^{(A,B)} = \frac{1}{\rho_1 + \rho_3} \begin{pmatrix} \rho_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \rho_3 & 0 \\ 0 & 0 & 0 & \rho_4 \end{pmatrix} \]
\[ \rho_1^{(A,B)} = \frac{1}{\rho_2 + \rho_4} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \rho_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \rho_4 \end{pmatrix} \]
and, straightforwardly, the conditional entropy can be written as
\[ S(\rho^{(A,B)}|\{\Pi_k^B\}) = S(\mathcal{Z}(\rho^{(A,B)})) - S(\rho^{(B)}) \]
where $\mathcal{Z}(\rho)$ is the de-phasing channel, i.e, the quantum channel that destroys the off-diagonal elements of $\rho$. Finally the quantum discord can be written as
\[ \delta(A, B) = S(\mathcal{Z}(\rho^{(A,B)})) - S(\rho^{(A,B)}) \]
or, more explicitly, in terms of the two-orbital reduced matrix elements:
\[ \delta(A, B) = \sum_k \lambda_k \ln \lambda_k - \rho_k \ln \rho_k \]
\footnote{Wave functions mixing configurations with an even and odd number of fermions are not allowed.}
with

\[
\begin{align*}
\lambda_0 &= \frac{\rho_1 + \rho_4}{2} + \sqrt{\frac{(\rho_1 - \rho_4)}{2}^2 + |\alpha|^2} \\
\lambda_1 &= \frac{\rho_1 + \rho_4}{2} - \sqrt{\frac{(\rho_1 - \rho_4)}{2}^2 + |\alpha|^2} \\
\lambda_2 &= \frac{\rho_2 + \rho_3}{2} + \sqrt{\frac{(\rho_2 - \rho_4)}{2}^2 + |\gamma|^2} \\
\lambda_3 &= \frac{\rho_2 + \rho_3}{2} - \sqrt{\frac{(\rho_2 - \rho_4)}{2}^2 + |\gamma|^2}
\end{align*}
\]

(6)

The quantum discord between the $i$ and $j$ orbitals grows with the off-diagonal matrix elements of $\rho^{(A,B)}$ in Eq 3, whose value reflects the amount of quantum coherence of the state. This fact can be easily seen if we write a pair of diagonal elements, i.e, $\rho_1$ and $\rho_4$ (the same discussion applies to $\rho_2$ and $\rho_3$) as $\rho_1 = \frac{1}{2} + \epsilon$ and $\rho_4 = \frac{1}{2} - \epsilon$ with $\epsilon \in [0, \frac{1}{2}]$. This corresponds to the case in which $S(\mathcal{Z}(\rho^{(A,B)}))$ is maximum, and we perturb it via the parameter $\epsilon$. The eigenvalues are, in this case, $\lambda_0 = \frac{1}{2} + \sqrt{\epsilon^2 + |\alpha|^2}$ and $\lambda_1 = \frac{1}{2} - \sqrt{\epsilon^2 + |\alpha|^2}$. For all allowed values of $\epsilon$, $S(\rho^{(A,B)}) \leq S(\mathcal{Z}(\rho^{(A,B)}))$ with equality when the off-diagonal elements are zero (in this case, $\alpha = 0$). If $\alpha$ increases, then the quantum discord increases too, revealing that the exclusively quantum correlations increase as the coherence grows, which is an expected and intuitive result.

IV. QUANTUM DISCORD AND NATURAL ORBITALS

The two-orbital reduced density matrix $\rho^{(A,B)}$ can be written in terms of three well known quantities in many-body theory: the one-body density matrix, the two-body density matrix and the pairing tensor, defined as $\gamma_{i,j} = \langle a_i^\dagger a_j \rangle$, $\gamma_{i,j,i,j} = \langle a_i^\dagger a_j^\dagger a_j a_i \rangle$ and $\kappa_{i,j} = \langle a_i a_j \rangle$, respectively. It has the same structure as Eq. 3, with:

\[
\begin{align*}
\rho_1 &= 1 - \gamma_{i,i} - \gamma_{j,j} + \gamma_{i,j,i,j} \\
\rho_2 &= \gamma_{j,j} - \gamma_{i,j,i,j} \\
\rho_3 &= \gamma_{i,i} - \gamma_{i,j,i,j} \\
\rho_4 &= \gamma_{i,i,j,j} \\
\alpha &= \kappa_{j,i} \gamma_{i,j,i,j} \\
\gamma_{j,i,i,j} &= 0
\end{align*}
\]

Together with Eq. 3, we see that the off-diagonal elements of the one-body density matrix and the pairing tensor are directly related with the quantum discord between $i$ and $j$ orbitals: if at least one of them is non-zero, there exist quantum correlations between $i$ and $j$. Inversely, it can be easily seen that there are two conditions for the quantum discord to be zero for all pairs of orbitals: $\gamma_{j,i} = 0$ and $\kappa_{j,i} = 0$. The first condition, $\gamma_{j,i} = 0$, is fulfilled for all $i,j$ if and only if the orbitals are the natural ones, i.e, those who diagonalize the one-body density matrix. Additionally, if the state has a well defined number of particles, then $\kappa_{j,i} = 0$ for all $i,j$. Thus, the two conditions for the vanishing of quantum discord between orbital pairs are:

1. The orbital basis is the natural one
2. The state has a well defined particle number

Additionally, it is known that the natural orbitals are the ones that minimize the overall entropy, defined as the sum of all the one-orbital entropies [26]. Since this quantity is used to quantify the amount of total correlation in a state (the total entanglement if the state is pure) [27], then, if the number of particles is well defined and the state is pure, a non-zero overall entropy implies that all correlations between pairs of natural orbitals will be purely classical (if they exists) and the entanglement must be manifested between three orbitals or more.

V. GENERAL ORBITAL BASIS

It is important to remark that the quantum discord is measured between orbitals, and not between particles. For this reason, a change in the orbital basis may induce a change in the correlations between them. So, in order to study the quantum discord of a state, it is fundamental to specify properly the orbital basis. The natural orbital basis in a state with well defined number of particles implies that those orbitals are constructed so that they can keep the intrinsic quantum correlation of the state without needing quantum correlation by pairs between them (this will be clearer in Sec. 11B). Therefore the following question arises: which is the value of the quantum discord of a given state in a general orbital basis?

Suppose that we have a general orbital basis and the natural orbital basis (of the given state), related by the most general linear canonical transformation between creation/annihilation operators (Bogoliubov transformation [18]):

\[
\beta_k^\dagger = \sum_i U_{i,k} c_i^\dagger + V_{l,k} c_l
\]

where $\{\beta_k^\dagger\}$ are the fermionic creation operators for the general basis, $\{c_i^\dagger\}$ are the fermionic creation operators for the natural basis. The following relations among the Bogoliubov amplitudes $U$ and $V$

\[
\begin{align*}
U^\dagger U + V^\dagger V &= UU^\dagger + V^*V^T = I \\
U^T V + V^T U &= UV^\dagger + V^*U^T = 0
\end{align*}
\]

hold. Then, the one-body matrix and the pairing tensor
elements read [13]:

$$\gamma_{k,k'} = \sum_l V_{k,l}^d V_{l,k'} + (U_{k,l}^d U_{l,k'} - V_{k,l}^d V_{l,k'}) p_l$$

$$\kappa_{k,k'} = \sum_l V_{k,l}^a U_{l,k'}^a + (U_{k,l}^a V_{l,k'}^a - V_{k,l}^a U_{l,k'}^a) p_l$$

where $p_l = \langle c_{l}^\dagger c_{l} \rangle$. In this general case, the quantum discord will be nonzero and orbital dependent except for the case $p_l = \frac{1}{N}$ $\forall l$. This can be checked using the relations in [10]. Since $\sum_l p_l = N$ where $N$ is the number of particles, this case can only exist when the number of particles is exactly half the number of orbitals. Less restrictive is the case of a transformation among particles, i.e., $V = 0$. Again, the quantum discord will be nonzero except for the case $p_l = \frac{N}{\Omega}$ $\forall l$ where $\Omega$ is the number of orbitals. In both cases, the quantum discord will be zero and orbital independent if the occupation of the system in the natural orbital basis is equally distributed.

A common measure of entanglement among particles is the entanglement entropy of the one-body density matrix, defined as $S(\gamma) = -\log \gamma = -\sum_l p_l \log p_l$ [10]. It is interesting to note that the orbital-independent zero discord case in general corresponds with the maximum $S(\gamma)$, which is indeed related to the overall entropy in the natural orbital basis since $S_{\text{nat}} = -\sum_l p_l \ln p_l + \sum_l (1 - p_l) \ln (1 - p_l)$ [20], and it reaches its maximum value when $p_l = \frac{1}{2}$. In other words, for a pure system with half filling, i.e., $\Omega = 2N$, if the particles are equally distributed between all natural orbitals, the entanglement is maximum but there is no quantum correlations between orbital pairs.

VI. RESULTS

As an example of how the quantum discord between pairs of fermionic orbitals can be used to characterize the correlations in the system, we apply the previous concepts to the HFB ground state of the Agassi model and the exact ground state of the Lipkin-Meshkov-Glick (LMG) model. Both models are composed by a two-level fermionic system, each having a $\Omega$-fold degeneracy. The difference between them lies in the interaction terms of their respective Hamiltonians.

The LMG model [28] has been widely used over the years as a benchmark in the characterization of different approximations to the many-body problem. The model is simple enough to be exactly solvable and at the same time is sufficiently rich to catch some non-trivial properties of many-body systems, mainly, the quantum phase transition to a ‘deformed’ state through a spontaneous symmetry breaking of the mean field approximation. As we will see, its Hamiltonian is composed by two terms: the non-interacting one, and the so-called monopole-monopole interaction, which mixes the high and low-lying orbitals of the same degeneracy. The model is very well known in the nuclear physics literature – see Ref [29] for a study of the model adequate for the present purposes.

The Agassi model [30], is an extension of the LMG one where a separable pairing interaction has been added. The pairing interaction induces the creation and annihilation of particles by pairs with the same (and different) energies. When treated at the mean field level, the Agassi model contains a superfluid phase (treated using the Bardeen-Cooper-Schrieffer theory of superconductivity) as well as a deformed one where the broken symmetry is parity (see [29] for a thorough discussion). The model can also be solved exactly using group theory techniques and it is also often used as a benchmark of different approximations in the context of nuclear physics.

A. The HFB ground state of the Agassi model as a benchmark

The Agassi model [30] is a two-level system, each of them with a degeneracy $\Omega$ (even). The system is filled with $N = \Omega$ fermions, and the Hamiltonian is given by

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

with

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

$$J_+ = (J_-)^\dagger = \sum_m c_{1,m}^\dagger c_{-1,m}$$

$$A_{\sigma} = \sum_{m>0} c_{\sigma,-m} c_{\sigma,m}$$

where $\sigma = \pm 1$ labels the upper/lower level, $m = \pm 1, \pm 2, \ldots, \pm \Omega$ labels the states within a level, and $c_{\sigma,m}$ is the fermionic creation operator of the single particle state labelled by $(\sigma, m)$. This model is exactly solvable using group theory methods [31], and the HFB ground state solution can be easily obtained. For this reason, we are going to analyze the quantum correlation properties of the HFB ground state as a benchmark of the proposed measure of quantum discord between pairs of fermionic orbitals (Eq. (5)).

Following reference [31], the one body density matrix and the pairing tensor of the HFB ground state can be written as

$$\gamma_{\sigma m, \sigma' m'} = \gamma_{\sigma, \sigma'} \delta_{m, m'}$$

$$\kappa_{\sigma m, \sigma' m'} = \text{sgn}(m) \frac{1}{2} \sin \alpha \delta_{\sigma, \sigma'} \delta_{m, -m'}$$

with

$$\gamma_{\sigma, \sigma} = \frac{1}{2} (1 - \sigma \cos \phi \cos \alpha)$$

$$\gamma_{\sigma, -\sigma} = -\frac{1}{2} \sin \phi \cos \alpha$$

(10)
The values of $\phi$ and $\alpha$ depend on the parameters of the Hamiltonian, that is:

$$
\begin{align*}
\phi = \alpha = 0 & \quad \text{if } \chi, \Sigma_0 < 1 \\
\cos \phi = \frac{1}{\chi}, \alpha = 0 & \quad \text{if } \chi > \Sigma_0 \\
\phi = 0, \cos \alpha = \frac{1}{\Sigma_0} & \quad \text{if } \chi < \Sigma_0
\end{align*}
$$

with $\chi = \frac{(\Omega - 1) V}{\epsilon}$, $\Sigma = \frac{(\Omega - 1) g}{\epsilon}$ and $\Sigma_0 = \Sigma + \frac{V}{\epsilon}$. As can be seen, there are three differentiated regions in the parameters space: the HF spherical phase, the HF deformed phase and the BCS phase. The first one corresponds to the conditions $\chi, \Sigma_0 < 1$, and the HFB ground state is the non interacting exact ground state, i.e., all the lower levels occupied. The second one corresponds to the conditions $\chi > \Sigma_0$ and $\chi > 1$. In this case the HFB ground state breaks the parity symmetry (that’s why it’s called ‘deformed’). The last region corresponds to $\chi < \Sigma_0$ and $\Sigma_0 > 1$. It preserves the parity symmetry but breaks the particle number symmetry and represents a superfluid system described by the BCS approximation. Since in all regions the ground state is defined as a quasi-particle vacuum, the two body density is separable and the diagonal elements can be written as

$$
\gamma_{i,j,i,j} = \gamma_{i,i} \gamma_{j,j} + \Delta_{i,j}
$$

with $\Delta_{i,j} = |\kappa_{i,j}|^2 - |\gamma_{i,j}|^2$ and, using Eq. (7) and (3), we can write the two orbital reduced density matrix as

$$
\begin{align*}
\rho_1 &= (1 - \gamma_{i,i})(1 - \gamma_{j,j}) + \Delta_{i,j} \\
\rho_2 &= (1 - \gamma_{i,i})\gamma_{j,j} - \Delta_{i,j} \\
\rho_3 &= \gamma_{i,i}(1 - \gamma_{j,j}) - \Delta_{i,j} \\
\rho_4 &= \gamma_{i,i}\gamma_{j,j} + \Delta_{i,j} \\
\alpha &= \kappa_{i,i}^* \\
\gamma &= \gamma_{j,j}
\end{align*}
$$

With those results and using Eq. (8) we can easily compute the quantum discord between a pair of orbitals in the HFB ground state solution, which is

$$
\delta(m,\sigma; m', -\sigma') = h(\chi)
$$

in the deformed HF region

$$
\delta(m,\sigma; -m, \sigma') = h(\Sigma_0)
$$

in the BCS region

$$
\delta(m,\sigma; m', \sigma') = 0
$$

otherwise

with $h(x) = -\frac{1}{2}(1 - \frac{1}{x}) \ln \frac{1}{2}(1 - \frac{1}{x}) - \frac{1}{2}(1 + \frac{1}{x}) \ln \frac{1}{2}(1 + \frac{1}{x})$. This solution is shown in Figs. 1 and 2.

The structure of the quantum discord is the same as the phase diagram [31]. In the deformed HF phase, there are quantum correlations only between orbitals with the same $m$ and opposite $\sigma$ due to the monopole-monopole interaction. In the same way, there are quantum correlations in the BCS phase only between orbitals

FIG. 1. Quantum discord between an orbital pair with $m = m'$ and $\sigma = -\sigma'$ as a function of the two Hamiltonian parameters $\chi$ and $\Sigma$. The quantum correlations in this case are zero for the spherical HF and BCS regions, while is non-zero only in the deformed HF region. $\Omega = 20$.

FIG. 2. Quantum discord between an orbital pair with $m = -m'$ and $\sigma = \sigma'$ as a function of the two Hamiltonian parameters $\chi$ and $\Sigma$. The quantum correlations in this case are zero for the spherical HF and BCS regions, while is non-zero only in the deformed HF region. $\Omega = 20$.

2 In the context of the Agassi model, particles in the upper (lower) level are assumed to have positive (negative) parity.

3 It can be checked that the eigenvalues of the two-body density matrix, i.e., $\lambda_i$ in Eq. (5) acquire the values $\lambda_i = 0, 1$. 

\[\Delta \]
obtained in Sec. III. Moreover, we note that the quantum discord between a transition from a spherical HF state to a deformed HF or BCS state is continuous, while the quantum discord between a transition from a deformed HF state to a BCS one is discontinuous. Since the quantities $\rho = \frac{1}{2} \sin \phi \cos \alpha$ and $\kappa = \frac{1}{2} \sin \alpha$ from Eqs. (10) and (11) can be considered as order parameters of the model [31], the quantum discord shows the behaviour of a combined order parameter.

B. The exact ground state of the LMG model

Finally, we analyze the quantum discord between orbital pairs within the exact ground state of the LMG model. The LMG Hamiltonian is the same as Eq. (9), with $g = 0$, i.e., there are only monopole-monopole interaction. For this reason, we only consider the quantum discord between orbitals with same $m$ and opposite $\sigma$.

Since the Hamiltonian commutes with the particle number and parity operators, the Hamiltonian orbitals, represented by the creation/annihilation operators ($c_{\sigma,m}^\dagger$ and $c_{\sigma,m}$ respectively) in Eq. (10) are the natural ones ($\gamma_{i,j} = 0$ for $i \neq j$), and the pairing tensor is zero. Thus, as explained in Sec. IV, the quantum discord is zero for all pairs.

But this is not true if we change the orbital basis. In general, a low quantum discord implies a better adaptation of the orbitals in order to describe the exact ground state, while a high quantum discord reflects the contrary case. If we compute the quantum discord between an up-down pair of HF orbitals, we obtain the result shown in Fig. 3. It is interesting to analyze the behaviour of the quantum discord of the exact ground state between those orbitals since they are defined in order to catch the maximum correlations as possible within a mean field scenario.

For $\chi < 1$ the quantum discord is zero, since the HF orbitals in this region coincide with the natural ones. For $\chi > 1$ there are two different regimes. First, as $\chi$ is big enough and it grows, the quantum discord decreases. This decrease is more drastic if the particle number is bigger, in coherence with the mean field description, in which more accuracy is obtained when the number of particles is big enough. The other regime is manifested when $\chi > 1$ acquires intermediate values, this is, near the quantum phase transition point ($\chi = 1$) and far from the asymptotic limit. In this region, the quantum discord grows fast until reaching the maximum. Then, it decreases exponentially until the asymptotic regime. This intermediate region is where the Hartree-Fock approximation becomes less accurate, and this is reflected as a high quantum discord between the HF orbitals: since the orbitals are less optimum in order to encode the exact ground state, more quantum correlation is needed between them for that task. In this intermediate region it is necessary to consider linear combinations of mean field Slater determinants to catch the physics of the exact ground state [29].

VII. CONCLUSIONS

The quantum discord is a measure of quantum correlations in a given state. It is defined as the minimum difference between two classically equivalent but quantumly different versions of the mutual information. This definition is based in the fact that, given a bi-partition $A|B$ of a system, a measurement on $A$ may break the quantum correlations between $A$ and $B$. In this manner, a projective measurement may be performed in one of the subsystems. Nonetheless, a fermion system must satisfy the parity super-selection rule, so not all the projective measurements are physical.

In this work, we use this property and we propose a simple expression (see Eq (5)) in order to compute the quantum discord between two orbitals in a general fermionic pure or mixed state. This expression does not require an optimization procedure and is directly related to two central many-body quantities: the one body density matrix and the pairing tensor. Thus, we have shown that the natural orbital basis, which is defined as the one that diagonalize the one body density matrix and the pairing tensor, reduces the quantum discord between any pair of orbitals to zero when the state has a well defined number of particles. Moreover, when the system’s orbitals are half filled, there is no quantum correlations between pairs for any arbitrary orbital basis. Finally, we compute and discuss the quantum discord between pairs of orbitals in the HFB ground state of the Agassi model, and in the exact ground state of the LMG model. Our results may be useful in order to analyze quantum correlations in more compli-
cated many body fermionic systems, for instance, the exact ground state of the Agassi model and more realistic models.

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Appendix A: Relation between two orbital fermionic quantum discord, variational diagonalization and measurement induced disturbance

In this appendix we briefly comment some connections between the proposed measure of quantum discord and the literature.

Following Eq. (5), and taking into account that \( \delta(A, B) = 0 \Leftrightarrow Z(\rho^{A,B}) = \rho^{A,B} \), the quantum discord can be used as a cost function for a variational quantum state diagonalization algorithm \[32\]. Indeed, following the inverse argument, the difference of purities between \( Z(\rho^{A,B}) \) and \( \rho^{A,B} \), which is used as a cost function in \[32\], could be interpreted as a measure of the quantum correlations, at least, in the case of a two fermionic orbital state.

On the other hand, Shunlong Luo proposed in \[33\] an alternative way to characterize the quantum correlations of a state. He defined classical states as the ones that fulfill the condition \( \Pi(\rho) = \rho \) with \( \Pi(\rho) = \sum_{k,l} \Pi_k^{(A)} \otimes \Pi_l^{(B)} \rho \Pi_k^{(A)} \otimes \Pi_l^{(B)} \) and \( \Pi_k^{(A)}, \Pi_k^{(B)} \) general projective measurements into the \( A \) and \( B \) systems, respectively. As explained in Sec. III, the only possible projectors are those of Eq. (4). Thus, we have

\[ \Pi(\rho^{A,B}) = Z(\rho^{A,B}) \]

and therefore, Eq. (5) could be interpreted as a distance between the dephased density matrix and the original one, and therefore, the quantum discord and the measurement-induced disturbance coincide.

Appendix B: Multipartite generalization of quantum discord

Until now, we have only taken into account quantum correlations among pairs of orbitals. In this appendix, we discuss the quantum discord beyond the bipartite case and derive an expression for a measure of the total quantum correlation of a state which, indeed, matches with the proposed generalization of the multipartite quantum discord in \[34\].

As explained in Sec. IV, the overall entropy is a measure of the total entanglement in a pure state (the total correlation if the state is mixed) \[27\]. With the definition in Eq. (1), we can write the overall entropy as

\[ S_{ov} = I(\Omega - 1; \Omega) + I(\Omega - 2; \Omega - 1, \Omega) + I(\Omega - 3; \Omega - 2, \Omega - 1, \Omega) + \ldots + S(\rho) \]

where \( I(i; j, k, ..., l) \) is the mutual information (Eq. (1)) with \( A \) as the \( i \)-th orbital and \( B \) as the system composed by the \( j, k, ..., l \)-th orbitals. \( S(\rho) \) is the von Neumann entropy of the system’s density matrix. Naturally, if the system is pure, \( S(\rho) = 0 \). Since the mutual information quantifies the total correlation, both classical and quantum, between parties, and the overall entropy measures the total correlation encoded in a state \[27\], then we propose the following quantity

\[ S'_{ov} = J(\Omega - 1; \Omega) + J(\Omega - 2; \Omega - 1, \Omega) + J(\Omega - 3; \Omega - 2, \Omega - 1, \Omega) + \ldots + S(\rho) \]

as a measure of the total classical correlation encoded in a state. Then, the total quantum correlation, i.e., the multipartite generalization of the quantum discord of a state will be the difference between \( S_{ov} \) and \( S'_{ov} \). Since

\[ J(i; j, k, ..., l) = \max_{\{\Pi_{\alpha}^{(j,k,...,l)}\}} \left( S(i) - S(i, j, k, ..., l|\{\Pi_{\alpha}^{(j,k,...,l)}\}) \right) \]

where \( \Pi_{\alpha}^{(j,k,...,l)} \) are the \( \alpha \)-th projector living in the space formed by the \( j, k, ..., l \) orbitals, then we have

\[ \delta(i, ..., l) = S_{ov} - S'_{ov} = \min_{\{\Pi_{\alpha}\}} S(m, l|\{\Pi_{\alpha}^{(j)}\}) + S(k, m, l|\{\Pi_{\alpha}^{(j)}\}) + \ldots - S(i, ..., k, m, l) \]

as an expression for the multipartite quantum discord. This proposal coincides with the one in Ref. \[34\]. This alternative derivation justifies the validity of the result and, since it is related to the overall entropy, may be interesting in future work to study its relationship with the orbital basis used. Of special interest would be to study the connection with the natural basis, which is the one that minimizes \( S_{ov} \) \[26\].

\[4\] It is assumed here that \( \rho \in \mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)} \)
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