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ON THE CORRELATION ENTROPY OF DISCRETE NANOELECTRONIC SYSTEMS

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Dedicated to Professor Karl-Heinz Indlekofer on the occasion of his 70th birthday

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Abstract. In this paper, we discuss the correlation entropy of discrete nanoelectronic systems, based on a quantum-statistical description in the many-body Fockspace. Considering examples of typical system preparations, mathematical properties of the correlation entropy are analyzed and interpreted in physical terms.

1. Introduction

In the following, we consider a discrete nanoelectronic system, that is, a system of spin $\frac{1}{2}$ Fermions with discrete energy spectrum. The fundamentals of a quantum-statistical many-body description of such systems, as outlined in this introdution, can be found e.g. in Refs.[1, 2].

For simplicity, we assume that all vector spaces are finite dimensional. A generalization of the discussed results to infinite dimensional spaces is possible.

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The single-particle space is isomorphic to $\mathbb{C}^n$. $n \in \mathbb{N}$ corresponds to the total number of single-electron basis states (e.g. sites with spin) in a nanoelectronic system. The resulting many-body vector space has the structure of a Fockspace, which is the direct sum of all spaces with particle numbers from 0 (vaccum) to n. The Fockspace is isomorphic to $\mathbb{C}^{2^n}$ and thus has dimension 2^n.

A special basis of the Fockspace is the set of all Slaterdeterminants, which correspond to states with well-defined occupation (0 or 1) of single-particle basis states (for a chosen single-particle basis). Therefore, a Slaterdeterminant can be uniquely identified by a bitvector of n bits $\in \{0, 1\}$. The latter corresponds to an integer number $I = 0, \ldots, 2^n - 1$ in binary representation.

In this paper, we employ the Dirac notation $|v\rangle$ for vectors. For example, $|v\rangle\langle v|$ denotes the projection operator to the subspace spanned by a normalized $|v\rangle$.

The annihilation and creation operators of an electron in single-particle state $|v_i\rangle$ are denoted by c_i and $c_i^\dagger$, respectively. The operators c_i, $c_j^\dagger$ obey anti-commutation relations for Fermions. If $|D_I\rangle$ denotes a Slaterdeterminant with respect to an ON (ortho-normalized) single-particle basis which contains $|v_i\rangle$, we obtain

$$c_i^\dagger |D_I\rangle = \begin{cases} (-1)^{N_{>i}(I)} |D_{I+2^i}\rangle & \text{for} \quad bit_i(I) = 0 \\ 0 & \text{else} \end{cases} , \tag{1.1}$$

where $bit_i(I)$ returns the i-th bit (0 or 1) of the integer I and

$$N_{>i}(I) := \sum_{j=i+1}^{n-1} bit_j(I) \tag{1.2}$$

counts the bits in I above bit position i. As a physical interpretation, $c_i^\dagger$ thus adds one particle in state i to a Slaterdeterminant. Analogously, c_i removes a particle.

A normalized Fockspace vector $|V\rangle$ describes a pure many-body state of the system. Since the set of Slaterdeterminants (built from any ON basis of single-particle states) forms an ON basis of the Fockspace, we can write

$$|V\rangle = \sum_{I=0}^{2^n-1} V_I |D_I\rangle \tag{1.3}$$

with $V_I \in \mathbb{C}$. A Fockspace vector that cannot be written as a Slaterderterminant with respect to any single-particle basis is called a "correlated" many-body state. (Please note that a Slaterdeterminant with respect to a given basis 1 may be written in terms of a superposition of multiple Slaterdeterminants with

respect to a different single-particle basis 2. Therefore, more than one Slaterdeterminant in an expansion of the form given above does not imply the property "correlated".)

The statistical preparation of the many-body system is described by the self-adjoint many-body statistical operator

$$\hat{\rho} = \sum_{J=0}^{2^n-1} w_J |\rho_J\rangle\langle\rho_J|, \tag{1.4}$$

where $|\rho_J\rangle$ is the J-th ON eigenvector of $\hat{\rho}$ with corresponding real eigenvalues $0 \leq w_J \leq 1$ and $Tr(\hat{\rho}) \equiv \sum_J w_J = 1$. (Note that $|\rho_J\rangle$ need not be a Slaterdeterminant.)

If there exists a Fockspace vector $|V\rangle$ such that $\hat{\rho} = |V\rangle\langle V|$, the preparation (or state) is called "pure", otherwise "mixed".

The expectation value of the particle number reads as

$$\bar{N} = Tr\left(\hat{\rho}\ \hat{N}\right), \tag{1.5}$$

where

$$\hat{N} = \sum_{i=0}^{n-1} c_i^\dagger c_i \tag{1.6}$$

is the self-adjoint particle number operator (with integer eigenvalues $0, 1, \ldots, n-1$).

The (von Neumann) entropy S in bit is defined as

$$S = -Tr\left(\hat{\rho}\ \mathrm{ld}\hat{\rho}\right) = -\sum_{J=0}^{2^n-1} w_J \mathrm{ld} w_J, \tag{1.7}$$

where ld is the logarithm to base 2, defined in a spectral representation of a self-adjoint operator. (Here, "0 ld 0" is interpreted as 0.) By definition, $S \geq 0$ in general. As can be seen, $S > 0$ for all mixed states, i.e. where there exists a w_J which is neither 0 nor 1. For all pure states, we have $S = 0$.

In the following sections, the so-called correlation entropy [4, 5, 6, 7, 8] is discussed with respect to its relevance for typical many-body preparations of nanoelectronic systems.

2. Correlation entropy of many-body systems

The self-adjoint "single-particle density-matrix" ρ_1 (also called "one-particle density-matrix") [1, 2, 3] for a given many-body $\hat{\rho}$ is defined as

$$\rho_{1\,ij} = Tr\left(\hat{\rho}\; c_j^\dagger c_i\right) \quad (i,j = 0,\ldots,n-1) \tag{2.1}$$

in the single-particle basis corresponding to the set of c_i operators. ρ_1 can be used to calculate expectation values of single-particle observables [1].

Single-particle eigenvectors of ρ_1 are called "natural orbitals" [2, 3]. The eigenvalues of ρ_1 are real and within the interval $[0,1]$. They need not be integers and can be interpreted as average occupation numbers of natural orbitals for the given preparation. (For the case of a single Slaterdeterminant, ρ_1 would have only eigenvalues 0 and 1.) Furthermore, the expectation value of the particle number is given by

$$\bar{N} = Tr(\rho_1). \tag{2.2}$$

In turn, the following quantity can be defined

$$S_1 := -Tr\left(\rho_1\; \mathrm{ld}\rho_1\right) \tag{2.3}$$

which is referred to as the "correlation entropy" (or "single-particle entropy") [4, 5, 6, 7, 8] in bit. As can be shown, $S_1 \geq 0$ in general. Furthermore, S_1 is invariant under unitary transformations of the chosen single-particle basis.

In the following, we consider preparation examples, comparing the two quantities S and S_1.

2.1. Pure entangled two electron system

In this section, we consider an example of a nanosystem, containing two entangled electrons. The system is assumed to be in the following pure many-body state

$$\hat{\rho}_\alpha := |V_\alpha\rangle\langle V_\alpha| \quad \text{with} \quad |V_\alpha\rangle := \left(\cos\alpha\; c_1^\dagger c_0^\dagger + \sin\alpha\; c_3^\dagger c_2^\dagger\right)|vac\rangle, \tag{2.4}$$

where $|vac\rangle$ is the vacuum state (normalized Slaterdeterminant with 0 particles) and $\alpha \in \mathbb{R}$ is a parameter. Here, we consider single-particle states with indices $0,1,2,3$. In the considered many-body state, the two electrons are entangled in the sense that finding an electron in state 0 (2) implies that the other electron must be found in state 1 (3). As can be shown, $|V_\alpha\rangle$ is normalized.

For all $\alpha = z\frac{\pi}{2}$ with $z \in \mathbb{Z}$, the state is a Slaterdeterminant. Otherwise, it is correlated.

Since the state is pure, we have an entropy $S = 0$ (see above), independent of α.

With respect to single-particle states with indices $0, 1, 2, 3$, we obtain the following single-particle density matrix

$$\rho_1 = \begin{pmatrix} \cos^2\alpha & 0 & 0 & 0 \\ 0 & \cos^2\alpha & 0 & 0 \\ 0 & 0 & \sin^2\alpha & 0 \\ 0 & 0 & 0 & \sin^2\alpha \end{pmatrix}. \tag{2.5}$$

Since ρ_1 is diagonal, the chosen single-particle basis states are also natural orbitals.

Consequently, the correlation entropy follows as

$$S_1 = -2\left[\left(\cos^2\alpha\right)\mathrm{ld}\left(\cos^2\alpha\right) + \left(\sin^2\alpha\right)\mathrm{ld}\left(\sin^2\alpha\right)\right]. \tag{2.6}$$

S_1 as a function of α has the following properties:

(i) $\forall\alpha \in \mathbb{R}: \quad 0 \le S_1(\alpha) \le 2$

(ii) $\forall\alpha \in \mathbb{R}: \quad S_1(\alpha + \frac{\pi}{2}) = S_1(\alpha)$

(iii) $\forall\alpha \in \mathbb{R}: \quad S_1(\frac{\pi}{4} + \alpha) = S_1(\frac{\pi}{4} - \alpha)$

(iv) $\forall z \in \mathbb{Z}: \quad S_1\left(z\frac{\pi}{2}\right) = 0$, corresponding to a single Slaterdeterminant

(v) $\forall z \in \mathbb{Z}: \quad S_1\left(\frac{\pi}{4} + z\frac{\pi}{2}\right) = 2$, corresponding to a fully entangled two-electron state

Figure 1. visualizes S_1 as a function of α within the first period $\left[0, \frac{\pi}{2}\right]$.

For those α, which correspond to a correlated many-body state, we have $S_1 > 0$. In this sense, S_1 can be considered as a measure of "deviation from a single Slaterdeterminant" or "degree of correlation" for a given pure many-body state.

2.2. General ensemble of Slaterdeterminants

Let us consider the case of an ensemble of Slaterdeterminants, that is, we can write

$$\hat{\rho}_{Sl} := \sum_{I=0}^{2^n-1} w_I |D_I\rangle\langle D_I|, \tag{2.7}$$

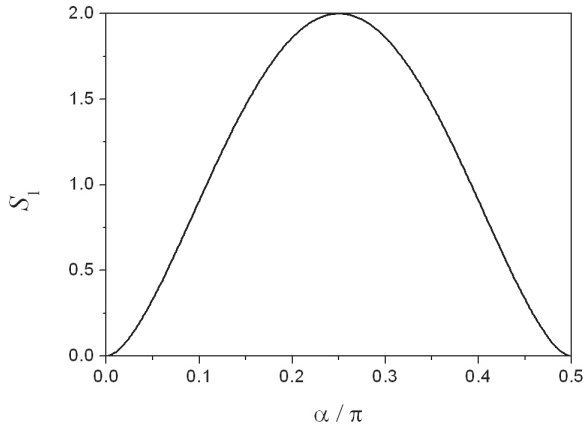

Figure 1: Correlation entropy $S_1(\alpha)$ for the considered two-electron model system.

where $|D_I\rangle$ are Slaterdeterminants with respect to a particular ON single-particle basis and $w_I \in [0,1]$ with $\sum_I w_I = 1$.

Thus, the entropy of the system reads as

$$S = -\sum_{I=0}^{2^n-1} w_I \mathrm{ld} w_I. \tag{2.8}$$

Furthermore, we obtain

$$\rho_{1\,ij} = \delta_{ij} \sum_{I=0}^{2^n-1} w_I bit_i(I), \tag{2.9}$$

where $bit_i(I)$ is the occupation number (0 or 1) of single-particle state i in Slaterdeterminant $|D_I\rangle$. Note that ρ_1 is diagonal with respect to the single-particle basis from which the Slaterdeterminants are built. Therefore, the chosen single-particle basis states are also natural orbitals.

In turn, we readily obtain for the correlation entropy

$$S_1 = -\sum_{i=0}^{n-1} \left(\sum_{I=0}^{2^n-1} w_I bit_i(I) \right) \mathrm{ld} \left(\sum_{J=0}^{2^n-1} w_J bit_i(J) \right). \tag{2.10}$$

2.3. Mixed uniform ensemble of Slaterdeterminants

As a special case, we now assume a uniform probability distribution among $M \geq 1$ Slaterdeterminants with $N \geq 1$ particles each and disjoint single-particle states (with $n \geq MN$), that is

$$\hat{\rho}_{MSl} := \frac{1}{M} \sum_{k=0}^{M-1} |D_{I_k}\rangle\langle D_{I_k}|, \tag{2.11}$$

where

$$|D_{I_k}\rangle := c^{\dagger}_{kN+N-1} c^{\dagger}_{kN+N-2} \cdots c^{\dagger}_{kN} |vac\rangle. \tag{2.12}$$

For the entropy we thus obtain

$$S = -\sum_{k=0}^{M-1} \frac{1}{M} \mathrm{ld} \frac{1}{M} = \mathrm{ld} M. \tag{2.13}$$

As can be shown, the single-particle density-matrix reads as

$$\rho_{1\,ij} = \begin{cases} \delta_{ij} \dfrac{1}{M} & \text{for} \quad i,j < MN \\ \\ 0 & \text{else} \end{cases} . \tag{2.14}$$

Consequently, the correlation entropy follows as

$$S_1 = -\sum_{i=0}^{MN-1} \frac{1}{M} \mathrm{ld} \frac{1}{M} = N \mathrm{ld} M = NS. \tag{2.15}$$

As can be seen from this example of an obviously non-correlated preparation with $S_1 > 0$, the quantity S_1 is not necessarily a measure of correlation, since it also depends on the "degree of mixture". For S_1 to be used as a measure of correlation, we must restrict ourselves to pure states.

2.4. Pure uniform amplitude state

In this section, we consider the case of a pure state of a system with $M \geq 1$ uniform amplitudes and $N \geq 1$ particles (with $n \geq MN$). The system is assumed to be in the following pure many-body state

$$\hat{\rho}_M := |V_M\rangle\langle V_M| \tag{2.16}$$

with

$$|V_M\rangle := \frac{1}{\sqrt{M}} \sum_{k=0}^{M-1} |D_{I_k}\rangle, \tag{2.17}$$

where $|D_{I_k}\rangle$ is defined in Eq.(2.12) in the example above. All amplitudes are $\frac{1}{\sqrt{M}}$, i.e. uniformly distributed. $|V_M\rangle$ is normalized.

As can be shown, the single-particle density-matrix ρ_1 is identical to Eq.(2.14) in the example above. Consequently, the correlation entropy is the same as in Eq.(2.15): $S_1 = N\mathrm{ld}M$. Since we consider a pure state, however, we now have $S = 0$. This means, that even for $S = 0$ and a fixed particle number N, the correlation entropy S_1 can grow beyond any limit (for $M \to \infty$ as a "super-correlated" state). One has to compare this result with the example of a uniform ensemble of M Slaterdeterminants above, where we obtained the same S_1 but $S = \mathrm{ld}M$.

In the considered example, the quantity $\frac{S_1}{N}$ can be interpreted as the number of bits that are required for counting the number of involved Slaterdeterminants. In other words, $2^{\frac{S_1}{N}}$ corresponds to the number of "relevant" Slaterdeterminants in the given many-body state $|V_M\rangle$.

3. Modified correlation entropy

As shown in the examples above, the correlation entropy S_1 can be used as a measure of correlation in the case of a pure state. However, S_1 can become $\neq 0$ for mixed preparations of non-correlated states (Slaterdeterminants). For a general preparation (mixed or pure), thus, a universal measure of correlation should be considered instead of S_1.

For example, one could define a quantity like (compare with Ref.[9])

$$\Delta S := \tilde{S} - S, \tag{3.1}$$

where

$$\tilde{S} := -\sum_{I=0}^{2^n-1} \tilde{w}_I \mathrm{ld}\tilde{w}_I. \tag{3.2}$$

Here, the projection weights $\tilde{w}_I$ are defined as

$$\tilde{w}_I := Tr(\hat{\rho}\, |\tilde{D}_I\rangle\langle\tilde{D}_I|) \geq 0, \tag{3.3}$$

where $|\tilde{D}_I\rangle$ are the ON Slaterdeterminants built from an "optimal" single-particle ON basis (e.g. to minimize $\tilde{S}$). In the following, we take (suitably chosen) natural orbitals, i.e. eigenvectors of ρ_1 for the given $\hat{\rho}$.

As can be readily shown, $\Delta S = 0$ for all preparations of Slaterdeterminants, and $\Delta S > 0$ for all correlated pure many-body states. As a disadvantage, however, ΔS requires the knowledge of the Fockspace operator $\hat{\rho}$, whereas S_1 can be obtained from the single-particle matrix ρ_1.

In the following, we consider ΔS for the examples which were discussed in the previous section.

3.1. Pure entangled two electron system

As shown above, single-particle states 0,1,2,3 are natural orbitals. From the resulting Slaterdeterminants $|\tilde{D}_I\rangle$, only two weights $\tilde{w}_I$ can be non-vanishing:

$$\tilde{w}_{2^0+2^1} = \cos^2\alpha \quad \text{and} \quad \tilde{w}_{2^2+2^3} = \sin^2\alpha. \tag{3.4}$$

Consequently, we obtain (with $S = 0$)

$$\Delta S = -\left[\left(\cos^2\alpha\right)\mathrm{ld}\left(\cos^2\alpha\right) + \left(\sin^2\alpha\right)\mathrm{ld}\left(\sin^2\alpha\right)\right]. \tag{3.5}$$

In comparison to Eq.(2.6), we therefore have $\Delta S = \frac{S_1}{2}$ in this example.

3.2. Mixed uniform ensemble of Slaterdeterminants

In this case, the chosen single-particle basis states are natural orbitals. The resulting Slaterdeterminants are therefore $|\tilde{D}_I\rangle = |D_I\rangle$ as defined in Eq.(2.12). Only the following M weights are non-vanishing:

$$\tilde{w}_{I_k} = w_{I_k} = \frac{1}{M} \quad \text{with} \quad I_k = \sum_{i=kN}^{kN+N-1} 2^i \quad (k = 0, \ldots, M-1). \tag{3.6}$$

Hence, we obtain $\tilde{S} = S$ and therefore $\Delta S = 0$, which is the expected result. In comparison, Eq.(2.15) yielded $S_1 > 0$ (for $N \geq 1$ and $M > 1$).

3.3. Pure uniform amplitude state

As shown above, single-particle states $i = 0, \ldots, NM-1$ are natural orbitals. From the resulting Slaterdeterminants $|\tilde{D}_I\rangle$, only the following M

weights are non-vanishing:

$$\tilde{w}_{I_k} = \left|\frac{1}{\sqrt{M}}\right|^2 = \frac{1}{M} \quad \text{with} \quad I_k = \sum_{i=kN}^{kN+N-1} 2^i \quad (k = 0, \ldots, M-1). \tag{3.7}$$

Consequently, we obtain (with $S = 0$)

$$\Delta S = -\sum_{k=0}^{M-1} \frac{1}{M} \mathrm{ld} \frac{1}{M} = \mathrm{ld} M. \tag{3.8}$$

Since $S_1 = N\mathrm{ld}M$ (see above), we therefore have $\Delta S = \frac{S_1}{N}$ in the discussed example. Due to this relation between ΔS and S_1 in this example, ΔS can be considered as a modification of S_1.

4. Conclusion

We have discussed the correlation entropy S_1 of discrete nanoelectronic systems for typical examples of quantum statistical preparations. Under certain conditions, S_1 can be interpreted as a measure for the degree of correlation in a given pure many-body state. We have shown that S_1 can grow beyond any limit, even for a pure state with fixed particle number. Finally, a modified correlation entropy has been considered which overcomes the shortcomings of S_1 for mixed preparations.

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