Annales Univ. Sci. Budapest., Sect. Comp. 39 (2013) 149–159

ON THE CORRELATION ENTROPY OF DISCRETE NANOELECTRONIC SYSTEMS

Klaus Michael Indlekofer (Rüsselsheim, Germany)
José María Castelo Ares (Rüsselsheim, Germany)

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

Communicated by Imre Kátai

(Received December 18, 2012; accepted December 29, 2012)

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.

Key words and phrases: Correlation entropy, nanoelectronic systems.
The research leading to these results has received funding from the European Union Seventh Framework Programme under grant agreement no. 265073.

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

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

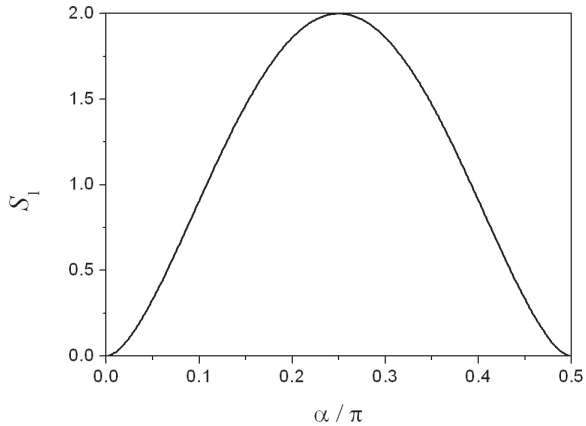

Figure 1: Correlation entropy $S_1(\alpha)$ for the considered two-electron model system.

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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Klaus Michael Indlekofer
Institute of Microtechnologies (IMtech),
RheinMain University of Applied Sciences
Am Brückweg 26
D-65428 Rüsselsheim, Germany
michael.indlekofer@hs-rm.de

José María Castelo Ares
RheinMain University of Applied Sciences
Am Brückweg 26
D-65428 Rüsselsheim, Germany
jose.casteloares@hs-rm.de