From Correlation to Entanglement

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In this writeup, I'm going to show the relation between reduced density matrix and the correlation function of fermion modes.

First of all, I need to show that the correlation $A_{mn} = \left\langle a_m^\dagger a_n \right\rangle$ within a block of L sites has nothing to do with its environment part of density matrix. This is explained in the appendix. As a result, the correlation matrix can be expressed as

$$A_{mn} = \mathrm{Tr}\left(a_m^\dagger a_n \rho_L\right) \tag{1}$$

Our goal is to invert this equation, i.e. to compute the RDM ρ_L by correlation matrix $A_{mn} = \left\langle a_m^\dagger a_n \right\rangle$.

The matrix A_{mn} is neccessarily Hermitian, since $A^\dagger \equiv A_{nm}^* = \left\langle a_n^\dagger a_m \right\rangle^* = \left\langle (a_n^\dagger a_m)^\dagger \right\rangle = \left\langle a_m^\dagger a_n \right\rangle = A_{mn}$. So A_{mn} can be diagonalized by a unitary transformation $G = UAU^\dagger$:

$$\begin{aligned} G_{pq} &= \sum_{m,n} U_{pm} A_{mn} U_{nq}^* = \sum_{m,n} U_{pm} \left\langle a_m^\dagger a_n \right\rangle U_{nq}^* \\ &= \left\langle \left(\sum_m U_{pm} a_m^\dagger \right) \left(\sum_n a_n U_{nq}^* \right) \right\rangle \\ &\equiv \left\langle g_p^\dagger g_q \right\rangle \delta_{pq} \end{aligned} \tag{2}$$

where the δ_{pq} comes from the fact that G_{pq} is diagonal. Now if we point to some element (m, n) of A_{mn}, the element G_{mn} corresponding to the same index must satisfy

$$G_{mn} = \sum_{m,n} U_{mm} \, \mathrm{Tr}\left(a_m^\dagger a_n \rho_L\right) U_{nn}^* = \mathrm{Tr}\left(g_m^\dagger g_n \rho_L\right) \tag{3}$$

It's readily to see that g_m satisfies fermionic anti-commuatation: $\{g_n, g_m^\dagger\} = \{\sum_i U_{ni} a_i,\ \sum_j a_j^\dagger U_{jm}^*\} = \sum_{ij} U_{ni} U_{jm}^* \{a_i, a_j^\dagger\} = \delta_{nm}$. This amounts to

$$G_{mn} = \nu_m \delta_{mn} \tag{4}$$

where $\nu_m \equiv \left\langle g_m^\dagger g_m \right\rangle$ is the m-th eigen value of correlation matrix. It's worth pointing out that g_m This implies that ρ_L is uncorrelated in the occupation number basis of $g_m^\dagger$. Hence ρ_L can be described by the following:

Theorem 1. *In a fermionic lattice model, the block (reduced) density matrix can be factorized under the basis that diagonalizes the correlation matrix* $\left\langle a_m^\dagger a_n \right\rangle$*:*

$$\rho_L = \varrho_1 \otimes \varrho_2 \otimes \ldots \otimes \varrho_L \tag{5}$$

where ϱ_m *is the single-mode density matrix corresponding to the* m*-th fermionic mode, and all* ϱ_m *are neccessarily diagonal.*

Let us represent g_m and $g_m^\dagger$ in their matrix representation.

Proof. We've shown that $G_{mn} = \mathrm{Tr}\Big(a_m^\dagger a_n \rho_L\Big) = 0$ if $m \neq n$. Since $g^\dagger$ creates fermion, we can denote the set of single-mode basis as $\{|1\rangle_m, |0\rangle_m\}$, the 1 fermion and 0-fermion respectively. Now we inspect modes m and n, the relevant part of RDM is

$$\rho_L = \sum_{j,j'} c_{jj'} |j\rangle \langle j'| \tag{6}$$

where $|j\rangle \in \{|1_m 1_n\rangle, |10\rangle, |01\rangle, |00\rangle\}$. The two-point correlation of modes m and n is

$$\begin{aligned} G_{mn} &= \mathrm{Tr}\Big(a_m^\dagger a_n \rho_L\Big) = \mathrm{Tr}\Big(a_n \rho_L a_m^\dagger\Big) \\ &= \sum_i \langle i| g_n \rho_L g_m^\dagger |i\rangle = \langle 00| g_n \rho_L g_m^\dagger |00\rangle \\ &= \sum_{jj'} c_{jj'} \langle 0_m 1_n | j\rangle \langle j' | 1_m 0_n\rangle \stackrel{!}{=} 0 \end{aligned} \tag{7}$$

Now let's pick out matrix elements that do not annihilate the brakets, whose corresponding $c_{jj'}$ has to vanish. These are:

$$|j\rangle \langle j'| \sim |0_m 1_n\rangle \langle 1_m 0_n|$$

so the matrix element at $|0_m\rangle \langle 1_m|$ of single-mode RDM ρ_m, and the element at $|1_n\rangle \langle 0_n|$ of local RDM ρ_n have to vanish. Also since G_{mn} is diagonal, the other off-diagonal also vanishes. Therefore the only elements that survives are $c_{jj'}$ corresponding to

$$\{|0_m\rangle \langle 0_m|, |1_m\rangle \langle 1_m|\} \otimes \{|0_n\rangle \langle 0_n|, |1_n\rangle \langle 1_n|\}$$

Hence all single-mode RDMs are neccessarily diagonal. □

In the aforesaid basis, $g_m^\dagger$ and g_m can be written as

$$g_m = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad g_m^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{8}$$

and note that the off-diagonal parts of single-mode RDM vanishes according to Theorem.1, we can parameterized ϱ_m by a undetermined variable α_m:

$$\varrho_m = \begin{pmatrix} \alpha_m & 0 \\ 0 & 1-\alpha_m \end{pmatrix} \tag{9}$$

which satisfies $\mathrm{Tr}(\varrho_m) = 1$. Then eigen value of correlation matrix ν_m and that of single-mode RDM α_m can be related by:

$$\nu_m = \mathrm{Tr}\Big(g_m^\dagger g_m \varrho_m\Big) = \mathrm{Tr}\left[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha_m & 0 \\ 0 & 1-\alpha_m \end{pmatrix}\right] = \alpha_m \tag{10}$$

where all the rest ϱ_n with $n \neq m$ have only trival contribution to the trace. So we have

$$\nu_m = \alpha_m \tag{11}$$

Therefore the total entanglement of this block of L sites is given by blocks ϱ_m (Theorem.**??**):

$$S_L = \sum_{l=1}^{L} H_2(\nu_l) \tag{12}$$

where

$$H_2(\nu_l) = -\nu_l \log \nu_l - (1-\nu_l) \log(1-\nu_l) \tag{13}$$

is the binary entropy.