Reduced Density Matrix Through Correlation Functions

Robert McKay

15 September 2018

Introduction

I will keep some notes and derivations in this section about the Reduced Density Matrix.

Calculations

Reduced Density Matrix

0.0.1 Definition

The Reduced Density Matrix is written as $\rho = \sum_j P_1 |\Psi_j\rangle\langle\Psi_i|$, where p_j add up to 1 (so think of as probability).

0.0.2 Expectation

Let $\hat{A}$ be some observable. We say the expectation is given as:

$$\langle A \rangle = \mathrm{tr}(\rho \hat{A}) \tag{1}$$

0.0.3 Entropy as a Real Life Example

Let S be entropy. We have:

$$S = -\sum_i \lambda_i \ln \lambda_i = -\,\mathrm{tr}(\rho \ln \rho) \tag{2}$$

Correlation Function

We now consider the correlation function. Since a correlation function is an expectation value, it can be written in terms of a reduced density matrix. Let our Hamiltonain be: $\hat{H} = -\sum_{n,m} \hat{t}_{n,m} c_n^\dagger c_m$. Then we define the correlation function as:

$$C_{i,j} \equiv < c_i^\dagger c_j >= \mathrm{tr}\left(\rho c_i^\dagger c_j\right) \tag{3}$$

However, by Wick's Theorem, we can represent our density matrix as:

$$\rho = \mathcal{K} \exp(-\hat{\mathcal{H}}) \tag{4}$$

Where $\mathcal{K}$ is a normalization constant and $\hat{H}$ is given according to $\hat{H} = -\sum_{n,m} \hat{t}_{n,m} c_n^\dagger c_m$

We now initiate a transform of the creation and annihilation operators such that $\hat{H}$ will be diagonalized. We introduce $c_i = \sum_k \phi_k(i)a_k$ where a_k is an annihilation operator and $\phi_k(i)$ is the eigenstate of $\hat{H}$ corresponding to eigenvalue ε_k. So, that in the diagonalized form, we obtain:

$$\rho = \mathcal{K}\exp\left(-\sum_{k=1}^{M}\varepsilon_k a_k^\dagger a_k\right) \tag{5}$$

We can now plug this into Equation (3) and use the stipulation that $tr(\rho) = 1$. We also use the transformation, $c_i = \sum_k \phi_k(i)a_k$, in plugging into (3). We end up with:

$$C_{i,j} = \sum_k \phi_k^*(i)\phi_k(j)\frac{1}{e^{\varepsilon_k}+1} \tag{6}$$

The important note is that the factor that relates the Eigenvalue of $\hat{H}$ to that of Equation (6). We see that the factor that relates the eigenvalues of these two matrices is:

$$\zeta_k = \left(e^{\varepsilon_k}+1\right)^{-1} \tag{7}$$

Or

$$\epsilon_k = \ln[(1-\zeta_k)/\zeta_k] \tag{8}$$

If we assign a matrix,C , to the eigenvalue ζ_k from Equation (7), then we can establish another matrix $H' = \ln[(1-C)/C]$.

Extension to Pair Creation and Annihilation Operators

0.2.1 *ASIDE: Bogoliubov Transformation

In order to diagonalize a system of pair creation and annihilation operators, one must utilize the Bogoliubov transformation. This is a transformation that takes a creation and annihilation pair, and maps it to a new operator that is either a creation or annihilation operator. So, for example the Bosonic operators, $\hat{a}^\dagger$ and $\hat{a}$, the Bogoliubov transform takes the form, $\hat{b} = u\hat{a} + v\hat{a}^\dagger$ and $\hat{b}^\dagger = u^*\hat{a}^\dagger + v^*\hat{a}$. u and v are found via the following condition: $[\hat{b},\hat{b}^\dagger] = (|u|^2 - |v|^2)[\hat{a},\hat{a}^\dagger]$. Hence, the price we pay is that $[\hat{b}_i,\hat{b}_j^\dagger] \neq \delta_{i,j}$.

Pair Correlation Function

We now apply a Bogoliubov transform to diagonalize our Hamiltonian. Denote $\hat{F}_{n,m} =< c_n^\dagger c_m^\dagger >$. We now acknowledge the caveat that the correlation function will be separated as

$< c_n^\dagger c_m^\dagger c_k c_l > = < c_n^\dagger c_l >< c_m^\dagger c_k > - < c_n^\dagger c_k >< c_m^\dagger c_l > + < c_n^\dagger c_m^\dagger >< c_k c_l >$ and,

$$\mathcal{H} = \sum_{i,j} \left[c_i^\dagger A_{ij} c_j + \frac{1}{2} \left(c_i^\dagger B_{ij} c_j^\dagger + h.c. \right) \right] \tag{9}$$

We now follow a similar prescription as the result of diagonalizing to go from Equations (5) to (8). In doing so, we now find