

Fermion Block diagonalization, Example: A two site system

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1 Block diagonalization of a Fermionic Hamiltonian in single Fermion number occupancy basis-The main theorem

Theorem 1 *A fermionic Hamiltonian describing a system of $2N$ fermionic single particle degrees of freedom defined in the number occupancy basis of $\hat{n}_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$ for all $[j\sigma] \in [1, N] \times [\sigma, -\sigma]$ can be resolved with respect to the fermionic state $N\sigma$ into a sum of diagonal $\hat{H}_{D,N\sigma}$ and off-diagonal blocks $\hat{H}_{X,N\sigma}$ that is a block matrix as,*

$$\begin{aligned}\hat{H}_{2N} &= (\hat{n}_{N\sigma} + 1 - \hat{n}_{N\sigma})\hat{H}_{2N}(\hat{n}_{N\sigma} + 1 - \hat{n}_{N\sigma}) \\ &= \begin{pmatrix} \hat{n}_{N\sigma}\hat{H}_{2N}\hat{n}_{N\sigma} & \hat{n}_{N\sigma}\hat{H}_{2N}(1 - \hat{n}_{N\sigma}) \\ (1 - \hat{n}_{N\sigma})\hat{H}_{2N}\hat{n}_{N\sigma} & (1 - \hat{n}_{N\sigma})\hat{H}_{2N}(1 - \hat{n}_{N\sigma}) \end{pmatrix}\end{aligned}\quad (1)$$

where $\hat{H}_{D,N\sigma} = \hat{n}_{N\sigma}\hat{H}_{2N}\hat{n}_{N\sigma} + (1 - \hat{n}_{N\sigma})\hat{H}_{2N}(1 - \hat{n}_{N\sigma})$ and $\hat{H}_{X,N\sigma} = \hat{n}_{N\sigma}\hat{H}_{2N}(1 - \hat{n}_{N\sigma}) + (1 - \hat{n}_{N\sigma})\hat{H}_{2N}\hat{n}_{N\sigma}$.
Statement-1: *There exist a unitarily equivalent representation $\hat{U}_{N\sigma}\hat{H}_{2N}\hat{U}_{N\sigma}^\dagger$ where $\hat{U}_{N\sigma}\hat{U}_{N\sigma}^\dagger = \hat{U}_{N\sigma}^\dagger\hat{U}_{N\sigma} = I$, such that the below given decoupling condition between states $1_{N\sigma}$ and $0_{N\sigma}$ holds,*

$$\begin{aligned}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\hat{H}_{2N}\hat{U}_{N\sigma}^\dagger(1 - \hat{n}_{N\sigma}) &= (1 - \hat{n}_{N\sigma})\hat{U}_{N\sigma}\hat{H}_{2N}\hat{U}_{N\sigma}^\dagger\hat{n}_{N\sigma} \\ &= 0.\end{aligned}$$

This statement is equivalent to stating $[\hat{U}_{N\sigma}\hat{H}_{2N}\hat{U}_{N\sigma}^\dagger, \hat{n}_{N\sigma}] = 0$.

Statement-2: *Form of the Unitary operator is given by,*

$$\hat{U}_{N\sigma} = \exp(\text{arctanh}(\hat{\eta}_{N\sigma} - \hat{\eta}_{N\sigma}^\dagger)) ,$$

where $\hat{\eta}_{N\sigma}$ is a non-hermitian operator given by,

$$\begin{aligned}\hat{\eta}_{N\sigma}^\dagger &= \frac{1}{\hat{E}_{[N\sigma]} - \hat{n}_{N\sigma}\hat{H}_{2N}\hat{n}_{N\sigma}}\hat{n}_{N\sigma}\hat{H}_{2N}(1 - \hat{n}_{N\sigma}) \\ &= \hat{n}_{N\sigma}\hat{H}_{2N}(1 - \hat{n}_{N\sigma})\frac{1}{\hat{E}_{[N\sigma]} - (1 - \hat{n}_{N\sigma})\hat{H}_{2N}(1 - \hat{n}_{N\sigma})} ,\end{aligned}$$

having the following properties,

$$\{\hat{\eta}_{N\sigma}^\dagger, \hat{\eta}_{N\sigma}\} = 1 , \quad [\hat{\eta}_{N\sigma}^\dagger, \hat{\eta}_{N\sigma}] = 2\hat{n}_{N\sigma} - 1 .$$

Proof:

Case-1 Hamiltonian composed of operators containing even number of c^\dagger 's and c 's.

A Fermionic Hamiltonian of the size $2^{2N} \times 2^{2N}$ can be written as a block matrix constituting diagonal and off-diagonal blocks of size $2^{2N-1} \times 2^{2N-1}$ in the resolution of the identity $\hat{I}_{N\sigma} = \hat{n}_{N\sigma} + \hat{I}_{N\sigma} - \hat{n}_{N\sigma}$ as,

$$\hat{H}_{2N} = H_{N\sigma,e}\hat{n}_{N\sigma} + H_{N\sigma,h}(1 - \hat{n}_{N\sigma}) + \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} + c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h}$$

where,

$$\begin{aligned}\hat{H}_{N\sigma,e} &= Tr_{N\sigma}(\hat{H}_{2N}\hat{n}_{N\sigma}) , \quad H_{N\sigma,h} = Tr_{N\sigma}(\hat{H}_{2N}(1 - \hat{n}_{N\sigma})) \\ \hat{T}_{N\sigma,e-h}^\dagger &= Tr_{N\sigma}(c_{N\sigma}^\dagger \hat{H}_{2N}) , \quad \hat{T}_{N\sigma,e-h} = Tr_{N\sigma}(\hat{H}_{2N}c_{N\sigma}) ,\end{aligned}$$

where the form of $\hat{T}_{N\sigma,e-h}^\dagger$ operator holds true when H contains even number of Fermion operators (see eq(??)). We ask for a new resolution of the identity $I_{N\sigma} = \hat{P}_{N\sigma} + 1 - P_{N\sigma}$ corresponding to a new basis in which this matrix attains a block diagonal form i.e.,

$$\begin{aligned}P_{N\sigma}H(1 - P_{N\sigma}) &= (1 - P_{N\sigma})HP_{N\sigma} = 0 , \\ P_{N\sigma}HP_{N\sigma} &= P_{N\sigma}H'P_{N\sigma} , \\ (1 - P_{N\sigma})H(1 - P_{N\sigma}) &= (1 - P_{N\sigma})H''(1 - P_{N\sigma}) ,\end{aligned}$$

where $[H', \hat{n}_{N\sigma}] = 0$, $[H'', \hat{n}_{N\sigma}] = 0$. From the above the block diagonal form equation for the subspace projection operator $P_{N\sigma}$ can be also written as,

$$HP_{N\sigma} = H'P_{N\sigma} \quad (2)$$

using $HP_{N\sigma} = P_{N\sigma}HP_{N\sigma}$ as $(1 - P_{N\sigma})HP_{N\sigma} = 0$. A form of $\hat{H}' = I_{N\sigma} \otimes \hat{E}_{[N\sigma]}$ satisfies the block diagonal equation,

$$\begin{pmatrix} H_{N\sigma,e}\hat{n}_{N\sigma} & c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} \\ \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} & H_{N\sigma,h}(1 - \hat{n}_{N\sigma}) \end{pmatrix} P_{N\sigma} = I_{N\sigma} \otimes \hat{E}_{[N\sigma]} P_{N\sigma} \quad (3)$$

where $\hat{E}_{[N\sigma]}$ is a matrix of size $2^{2N-1} \times 2^{2N-1}$ and $I_{N\sigma}$ is the 2×2 identity . For this equation we will now implement the Gauss Jordan Block diagonalization procedure as follows, firstly we write a ansatz for $P_{N\sigma}$ as ,

$$\begin{aligned}P_{N\sigma} &= \mathcal{N}(1 + \eta_{N\sigma} + \eta_{N\sigma}^\dagger) , \\ &= \mathcal{N}(1 + \eta_{N\sigma})\hat{n}_{N\sigma} + \mathcal{N}(1 + \eta_{N\sigma}^\dagger)(1 - \hat{n}_{N\sigma}) , \\ &= \mathcal{N} \begin{pmatrix} 1 & 0 \\ \eta_{N\sigma} & 0 \end{pmatrix} + \mathcal{N} \begin{pmatrix} 0 & \eta_{N\sigma}^\dagger \\ 0 & 1 \end{pmatrix} ,\end{aligned} \quad (4)$$

where $\eta_{N\sigma}$, $\eta_{N\sigma}^\dagger$ are the electron to hole and hole to electron transition operators having the following properties,

$$(1 - \hat{n}_{N\sigma})\eta_{N\sigma}\hat{n}_{N\sigma} = \eta_{N\sigma} , \quad \hat{n}_{N\sigma}\eta_{N\sigma}(1 - \hat{n}_{N\sigma}) = 0 ,$$

and $\eta_{N\sigma}^2 = 0$. In eq(34) quantity \mathcal{N} is a normalization factor which maintains the idempotent nature of the new projection operator $P_{N\sigma}$, below we will show \mathcal{N} is determined as an outcome of our analysis. The properties of $\eta_{N\sigma}^\dagger$ follows from above. Using the definition eq(34) and the block diagonalization equation eq(33) we can write down the following matrix equations,

$$\begin{aligned}\begin{pmatrix} H_{N\sigma,e}\hat{n}_{N\sigma} & c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} \\ \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} & H_{N\sigma,h}(1 - \hat{n}_{N\sigma}) \end{pmatrix} \begin{pmatrix} 1 \\ \eta_{N\sigma} \end{pmatrix} &= \hat{E}_{[N\sigma]} \begin{pmatrix} 1 \\ \eta_{N\sigma} \end{pmatrix} , \\ \begin{pmatrix} H_{N\sigma,e}\hat{n}_{N\sigma} & c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} \\ \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} & H_{N\sigma,h}(1 - \hat{n}_{N\sigma}) \end{pmatrix} \begin{pmatrix} \eta_{N\sigma}^\dagger \\ 1 \end{pmatrix} &= \hat{E}_{[N\sigma]} \begin{pmatrix} \eta_{N\sigma}^\dagger \\ 1 \end{pmatrix} .\end{aligned} \quad (5)$$

The form of the transition operators $\eta_{N\sigma}$, $\eta_{N\sigma}^\dagger$ that satisfies the matrix equations are,

$$\begin{aligned}\hat{\eta}_{N\sigma} &= \hat{G}_h(\hat{E}_{[N\sigma]})\hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} , \\ \hat{\eta}_{N\sigma}^\dagger &= \hat{G}_e(\hat{E}_{[N\sigma]})c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} ,\end{aligned} \quad (6)$$

where $\hat{G}_{(h,e)}(\hat{E}_{[N\sigma]}) = (\hat{E}_{[N\sigma]} - H_{N\sigma,(h,e)})^{-1}$. The following transition operators lead to the following block diagonal representation of the operator $\hat{E}_{[N\sigma]}$ in the projected space of electron/hole occupancy operator corresponding to state $N\sigma$,

$$\begin{aligned} \left[H_{N\sigma,e} \hat{n}_{N\sigma} + c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} \hat{G}_h(\hat{E}_{[N\sigma]}) \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} \right] &= \hat{E}_{[N\sigma]} \hat{n}_{N\sigma}, \\ \left[H_{N\sigma,h} (1 - \hat{n}_{N\sigma}) + \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} \hat{G}_e(\hat{E}_{[N\sigma]}) c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} \right] &= \hat{E}_{[N\sigma]} (1 - \hat{n}_{N\sigma}). \end{aligned} \quad (7)$$

From the two equations of the transition operators eq(36) we have the following identity,

$$\hat{G}_h(\hat{E}_{[N\sigma]}) \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} = \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} \hat{G}_e(\hat{E}_{[N\sigma]}) . \quad (8)$$

The above operator ordering relation eq(8) and form of the block diagonal operators eq(37) we have,

$$\begin{aligned} \eta_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} &= \hat{n}_{N\sigma} \hat{G}_e^{-1}(\hat{E}_{[N\sigma]}) \implies \eta_{N\sigma}^\dagger \eta_{N\sigma} = \hat{n}_{N\sigma} \\ \eta_{N\sigma} c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} &= (1 - \hat{n}_{N\sigma}) \hat{G}_h^{-1}(\hat{E}_{[N\sigma]}) \\ \implies \eta_{N\sigma} \eta_{N\sigma}^\dagger &= 1 - \hat{n}_{N\sigma} . \end{aligned}$$

This leads to a canonical commutation and anticommutation relation for the $\eta_{N\sigma}$ operators ,

$$[\eta_{N\sigma}^\dagger, \eta_{N\sigma}] = 2\hat{n}_{N\sigma} - 1, \quad \{\eta_{N\sigma}^\dagger, \eta_{N\sigma}\} = 1 . \quad (9)$$

With this constraints eq(9) on the $\eta_{N\sigma}$ and $\eta_{N\sigma}^\dagger$ operators one can check that the idempotent nature of the projection operator $P_{N\sigma}^2 = P_{N\sigma}$ is satisfied for a specific normalization factor,

$$\mathcal{N}^{-1} = (1 + \eta_{N\sigma}^\dagger \eta_{N\sigma} + \eta_{N\sigma} \eta_{N\sigma}^\dagger) = 2 . \quad (10)$$

The number $\mathcal{N}^{-1} = 2$ can then be seen to be associated with the block matrix dimension of the identity matrix $I_{N\sigma}$ or can be equivalently seen as the number of choices for the single electronic state configuration, i.e. it is either occupied or unoccupied. There is a orthogonal subspace projection operator $1 - P_{N\sigma}$,

$$\begin{aligned} 1 - P_{N\sigma} &= \mathcal{N}(1 - \eta_{N\sigma} - \eta_{N\sigma}^\dagger) , \\ &= \mathcal{N}(1 - \eta_{N\sigma}^\dagger)(1 - \hat{n}_{N\sigma}) + \mathcal{N}(1 - \eta_{N\sigma})\hat{n}_{N\sigma} , \end{aligned}$$

from the algebra of the $\eta_{N\sigma}$ operators one can check that the above form is consistent with the requirement $P_{N\sigma}(1 - P_{N\sigma}) = 0$. To get the other blocks of the final block diagonal form we start with the block diagonal equation satisfied by $(1 - P_{N\sigma})$ which is given by,

$$\begin{aligned} \begin{pmatrix} H_{N\sigma,e} \hat{n}_{N\sigma} & c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} \\ \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} & H_{N\sigma,h} (1 - \hat{n}_{N\sigma}) \end{pmatrix} \begin{pmatrix} 1 \\ -\eta_{N\sigma} \end{pmatrix} &= \hat{E}'_{[N\sigma]} \begin{pmatrix} 1 \\ -\eta_{N\sigma} \end{pmatrix} \\ \begin{pmatrix} H_{N\sigma,e} \hat{n}_{N\sigma} & c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} \\ \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} & H_{N\sigma,h} (1 - \hat{n}_{N\sigma}) \end{pmatrix} \begin{pmatrix} -\eta_{N\sigma}^\dagger \\ 1 \end{pmatrix} &= \hat{E}'_{[N\sigma]} \begin{pmatrix} -\eta_{N\sigma}^\dagger \\ 1 \end{pmatrix} . \end{aligned} \quad (11)$$

As above by solving the simultaneous set of equations we have the form of the transition operators,

$$\begin{aligned} \hat{\eta}_{N\sigma} &= -\hat{G}_h(\hat{E}'_{[N\sigma]}) \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} , \\ \hat{\eta}_{N\sigma}^\dagger &= -\hat{G}_e(\hat{E}'_{[N\sigma]}) c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} , \end{aligned}$$

which leads to a further consistency condition using eq(36),

$$\begin{aligned} -\hat{G}_h(\hat{E}'_{[N\sigma]}) \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} &= \hat{G}_h(\hat{E}_{[N\sigma]}) \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} , \\ -\hat{G}_e(\hat{E}'_{[N\sigma]}) \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} &= \hat{G}_e(\hat{E}_{[N\sigma]}) \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} . \end{aligned} \quad (12)$$

Again replacing this transition operators in the simultaneous equation for both sets we have the following block diagonal representation of the operator $\hat{E}'_{[N\sigma]}$ in the projected space of electron/hole occupancy operator corresponding to state $N\sigma$,

$$\begin{aligned}
& c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} \hat{G}_h(\hat{E}_{[N\sigma]}) \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} |\Psi_{N\sigma}^1, 1_{N\sigma}\rangle \\
&= (H_{N\sigma,e} - \hat{E}'_{[N\sigma]}) \hat{n}_{N\sigma} |\Psi_{N\sigma}^1, 1_{N\sigma}\rangle, \\
& \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} \hat{G}_e(\hat{E}_{[N\sigma]}) c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} |\Psi_{N\sigma}^0, 0_{N\sigma}\rangle \\
&= (H_{N\sigma,h} - \hat{E}'_{[N\sigma]})(1 - \hat{n}_{N\sigma}) |\Psi_{N\sigma}^0, 0_{N\sigma}\rangle.
\end{aligned} \tag{13}$$

The block diagonal equation can be reconstructed now as,

$$\begin{pmatrix} \hat{E}_{N\sigma} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hat{E}_{[N\sigma]} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} \hat{E}_{N\sigma} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hat{E}'_{[N\sigma]} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{14}$$

By identifying the two blocks $\hat{E}_{[N\sigma]}$ and $\hat{E}'_{[N\sigma]}$ using eq(37) and eq(13) the block diagonalized Hamiltonian is given by,

$$\begin{aligned}
\hat{H}' &= \hat{E}_{[N\sigma]} \hat{n}_{N\sigma} + \hat{E}'_{[N\sigma]}(1 - \hat{n}_{N\sigma}) \\
&= \frac{1}{2} Tr_{N\sigma}(\hat{H}_{2N}) + \left(\hat{n}_{N\sigma} - \frac{1}{2} \right) \{ c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h}, \eta_{N\sigma} \}
\end{aligned} \tag{15}$$

This proves that there exist a unitary operation $\hat{U}_{N\sigma}$ which puts the matrix into a block diagonal form i.e. $\hat{U}_{N\sigma} \hat{H} \hat{U}_{N\sigma}^\dagger = \hat{H}'$, such that $[\hat{H}', \hat{n}_{N\sigma}] = 0$, i.e. proof of **statement-1**.

To find the Unitary operator we write down the block matrix equation as follows,

$$\begin{aligned}
& \frac{1}{\sqrt{2}} \begin{pmatrix} H_{N\sigma,e} \hat{n}_{N\sigma} & c_{N\sigma}^\dagger \hat{T}_{N\sigma,e-h} \\ \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} & H_{N\sigma,h} \end{pmatrix} \begin{pmatrix} 1 & \eta_{N\sigma}^\dagger \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
&= \frac{1}{\sqrt{2}} \hat{E}_{[N\sigma]} \begin{pmatrix} 1 & \eta_{N\sigma}^\dagger \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}.
\end{aligned} \tag{16}$$

Using the proof of statement-1 we know that there exist some $\hat{U}_{N\sigma}$ such that the above block matrix equation becomes equivalent to ,

$$\begin{aligned}
& \begin{pmatrix} \hat{E}_{[N\sigma]} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} \hat{U}_{N\sigma} \begin{pmatrix} 1 & \eta_{N\sigma}^\dagger \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
&= \hat{U}_{N\sigma} \hat{E}_{[N\sigma]} U_{[N\sigma]}^\dagger U_{[N\sigma]} \begin{pmatrix} 1 & \eta_{N\sigma}^\dagger \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}.
\end{aligned} \tag{17}$$

The requirement of the block diagonal equation eq(14) is,

$$\hat{U}_{N\sigma} \begin{pmatrix} 1 & \eta_{N\sigma}^\dagger \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = c \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{18}$$

where c is some constant. The Unitary operator $\hat{U}_{N\sigma}$ that fulfills the requirement is uniquely determined and has the form,

$$\hat{U}_{N\sigma} = \frac{1}{\sqrt{2}}(1 + \eta_{N\sigma}^\dagger - \eta_{N\sigma}). \tag{19}$$

That this matrix is unitary $\hat{U}_{N\sigma} \hat{U}_{N\sigma}^\dagger = \hat{U}_{N\sigma}^\dagger \hat{U}_{N\sigma} = 1$ can be checked using eq(9). Below we show the fulfillment of the requirement eq(18) ,

$$\begin{pmatrix} 1 & \eta_{N\sigma}^\dagger \\ -\eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 & \eta_{N\sigma}^\dagger \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 2 \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{20}$$

The Unitary operator $\hat{U}_{N\sigma}$ can be written in an exponential form as,

$$\hat{U}_{N\sigma} = \exp(\text{arctanh}(\eta_{N\sigma}^\dagger - \eta_{N\sigma})) = \frac{1 + \eta_{N\sigma}^\dagger - \eta_{N\sigma}}{\sqrt{1 + \eta_{N\sigma} \eta_{N\sigma}^\dagger + \eta_{N\sigma}^\dagger \eta_{N\sigma}}} = \frac{1}{\sqrt{2}}(1 + \eta_{N\sigma}^\dagger - \eta_{N\sigma}) ,$$

where $\eta_{N\sigma}$ is given by,

$$\eta_{N\sigma}^\dagger = \hat{G}_e(\hat{E}_{[N\sigma]})c_{N\sigma}^\dagger T_{N\sigma, e-h} = c_{N\sigma}^\dagger T_{N\sigma, e-h} \hat{G}_h(\hat{E}_{[N\sigma]}) .$$

This proves **statement-2**.

Case 2 Hamiltonian constituted of operators containing arbitrary number of c 's and c^\dagger 's .

In this case due to Fermion signature issues the partial trace decomposed block form Hamiltonian might have non trivial pre-factors to take into account, so it is better suited to write the block diagonalized Hamiltonian and the Unitary operator in the following fashion,

$$U_{N\sigma} \hat{H}_{2N} U_{N\sigma}^\dagger = \begin{pmatrix} \hat{E}_{[N\sigma]} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} . \quad (21)$$

where $\hat{U}_{N\sigma}$ and $\hat{E}_{[N\sigma]}, \hat{E}'_{[N\sigma]}$ are defined as ,

$$\begin{aligned} \eta_{N\sigma}^\dagger &= \hat{n}_{N\sigma} \hat{H}(1 - \hat{n}_{N\sigma}) \frac{1}{\hat{E}_{[N\sigma]} - (1 - \hat{n}_{N\sigma}) \hat{H}_{2N} (1 - \hat{n}_{N\sigma})} , \\ \hat{U}_{N\sigma} &= \frac{1}{\sqrt{2}} \left[1 + \hat{\eta}_{N\sigma} - \hat{\eta}_{N\sigma}^\dagger \right] , \\ \hat{E}_{[N\sigma]} &= \hat{n}_{N\sigma} \hat{H}_{2N} \hat{n}_{N\sigma} + \eta_{N\sigma}^\dagger (1 - \hat{n}_{N\sigma}) \hat{H}_{2N} \hat{n}_{N\sigma} . \end{aligned} \quad (22)$$

This entire block diagonalization procedure leads to the following corollaries ,

Corollaries:

1.

$$\begin{aligned} \begin{pmatrix} \hat{E}_{[N\sigma]} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \hat{U}_{N\sigma} \hat{E}_{[N\sigma]} \hat{U}_{N\sigma}^\dagger \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \implies \hat{U}_{N\sigma} \hat{E}_{[N\sigma]} \hat{U}_{N\sigma}^\dagger &= \hat{E}_{[N\sigma]} . \end{aligned} \quad (23)$$

2.

$$\begin{aligned} (0 \ 1) \hat{E}_{N\sigma} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 &\implies (1 \ 0) U_{N\sigma}^\dagger \hat{E}_{N\sigma} U_{N\sigma} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hat{E}_{N\sigma} \\ \implies (\eta_{N\sigma} \ 1) \hat{E}_{N\sigma} \begin{pmatrix} 1 \\ -\eta_{N\sigma} \end{pmatrix} &= \hat{E}_{N\sigma} \rightarrow [\hat{E}_{[N\sigma]}, \eta_{N\sigma}] = 0 \end{aligned} \quad (24)$$

3. **Prove:** $[\hat{E}_{N\sigma}, \hat{G}_e(\hat{E}_{N\sigma})] = 0$

Let us first rewrite $\hat{E}_{N\sigma} \eta_{N\sigma}$ as,

$$\begin{aligned} \hat{E}_{N\sigma} \eta_{N\sigma} &= \hat{E}_{N\sigma} \hat{G}_h(\hat{E}_{N\sigma}) T_{N\sigma, e-h}^\dagger c_{N\sigma} \\ &= \left(1 + \text{Tr}_{N\sigma}(H(1 - \hat{n}_{N\sigma})) \hat{G}_h(\hat{E}_{N\sigma}) \right) \\ &\quad \times T_{N\sigma, e-h}^\dagger c_{N\sigma} . \end{aligned} \quad (25)$$

As eq(8) i.e. $\hat{G}_h(\hat{E}_{[N\sigma]}) \hat{T}_{N\sigma, e-h}^\dagger c_{N\sigma} = \hat{T}_{N\sigma, e-h}^\dagger c_{N\sigma} \hat{G}_e(\hat{E}_{[N\sigma]})$ for all $\hat{E}_{N\sigma}$ satisfying the block equation eq(33) therefore,

$$\begin{aligned} \text{Tr}_{N\sigma}(H(1 - \hat{n}_{N\sigma})) \hat{G}_h(\hat{E}_{N\sigma}) T_{N\sigma, e-h}^\dagger c_{N\sigma} \\ = T_{N\sigma, e-h}^\dagger c_{N\sigma} \text{Tr}_{N\sigma}(H \hat{n}_{N\sigma}) \hat{G}_e(\hat{E}_{N\sigma}) . \end{aligned} \quad (26)$$

Using eq(26) we have the transition operator rearrangement relation,

$$\begin{aligned}
& \left(1 + \text{Tr}_{N\sigma}(H(1 - \hat{n}_{N\sigma}))\hat{G}_h(\hat{E}_{N\sigma})\right) T_{N\sigma,e-h}^\dagger c_{N\sigma} \\
&= T_{N\sigma,e-h}^\dagger c_{N\sigma} \left(1 + \text{Tr}_{N\sigma}(H\hat{n}_{N\sigma})\hat{G}_e(\hat{E}_{N\sigma})\right), \\
\hat{E}_{N\sigma}\eta_{N\sigma} &= T_{N\sigma,e-h}^\dagger c_{N\sigma} \hat{E}_{N\sigma} G_e(\hat{E}_{N\sigma}).
\end{aligned} \tag{27}$$

From eq(24) we have $[\hat{E}_{[N\sigma]}, \eta_{N\sigma}] = 0$ this implies,

$$\begin{aligned}
T_{N\sigma,e-h}^\dagger c_{N\sigma} \hat{E}_{N\sigma} G_e(\hat{E}_{N\sigma}) &= \eta_{N\sigma} \hat{E}_{N\sigma} \\
T_{N\sigma,e-h}^\dagger c_{N\sigma} [\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] &= 0.
\end{aligned} \tag{28}$$

Using the form of the electron-hole transition operator $\eta_{N\sigma} = T_{N\sigma,e-h}^\dagger c_{N\sigma} G_e(\hat{E}_{N\sigma})$ and eq(28) we prove our assertion,

$$\begin{aligned}
T_{N\sigma,e-h}^\dagger c_{N\sigma} [\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] &= 0, \\
c_{N\sigma}^\dagger T_{N\sigma,e-h} G_h(\hat{E}_{N\sigma}) T_{N\sigma,e-h}^\dagger c_{N\sigma} [\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] &= 0 \\
\hat{G}_e^{-1}(\hat{E}_{N\sigma}) \eta_{N\sigma}^\dagger \eta_{N\sigma} [\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] &= 0 \\
\implies [\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] &= 0.
\end{aligned} \tag{29}$$

2 An example

Let us consider a two site Hamiltonian,

$$\hat{H} = -t(c_1^\dagger c_2 + h.c.) + V\hat{n}_1\hat{n}_2 - \mu(n_1 + n_2), \tag{30}$$

where $\hat{n}_{1,2} = c_{1,2}^\dagger c_{1,2}$. First step is to represent this Hamiltonian in a block form in the occupancy basis of site 1 which are eigenstates of number operator \hat{n}_1 ,

$$\hat{H} = \begin{pmatrix} (V - \mu)\hat{n}_1\hat{n}_2 - \mu\hat{n}_1 & -tc_1^\dagger c_2 \\ -tc_2^\dagger c_1 & -\mu\hat{n}_2(1 - \hat{n}_1) \end{pmatrix} \tag{31}$$

Let us note that the quantum fluctuations in the number occupancy basis has its source in the off-diagonal blocks of the above matrix leading to $[\hat{H}, \hat{n}_1] \neq 0$. We ask for a new resolution of the identity $I_1 = \hat{P}_1 + 1 - \hat{P}_1$ corresponding to a new basis in which this matrix attains a block diagonal form i.e.,

$$\begin{aligned}
P_1 H (1 - P_1) &= (1 - P_1) H P_1 = 0, \quad P_1 H P_1 = P_1 H' P_1, \\
(1 - P_1) H (1 - P_1) &= (1 - P_1) H'' (1 - P_1),
\end{aligned}$$

where $[H', \hat{n}_1] = 0$, $[H'', \hat{n}_1] = 0$. From the above the block diagonal form equation for the subspace projection operator P_1 can be also written as,

$$H P_1 = H' P_1 \tag{32}$$

A form of $\hat{H}' = I_1 \otimes \hat{E}_{[1]}$ satisfies the above block diagonal equation,

$$\begin{pmatrix} (V - \mu)\hat{n}_1\hat{n}_2 - \mu\hat{n}_1 & -tc_1^\dagger c_2 \\ -tc_2^\dagger c_1 & -\mu\hat{n}_2(1 - \hat{n}_1) \end{pmatrix} P_1 = I_1 \otimes \hat{E}_{[1]} P_1 \tag{33}$$

where $\hat{E}_{[1]}$ is a matrix of size 2×2 and I_1 is the 2×2 identity. For this equation we will now implement the Gauss Jordan Block diagonalization procedure as follows, firstly we write a ansatz for P_1 as ,

$$\begin{aligned}
P_1 &= \mathcal{N}(1 + \eta_1 + \eta_1^\dagger), \\
&= \mathcal{N}(1 + \eta_1)\hat{n}_1 + \mathcal{N}(1 + \eta_1^\dagger)(1 - \hat{n}_1), \\
&= \mathcal{N} \begin{pmatrix} 1 & 0 \\ \eta_1 & 0 \end{pmatrix} + \mathcal{N} \begin{pmatrix} 0 & \eta_1^\dagger \\ 0 & 1 \end{pmatrix},
\end{aligned} \tag{34}$$

where η_1 , η_1^\dagger are the electron to hole and hole to electron transition operators having the following properties,

$$(1 - \hat{n}_1)\eta_1\hat{n}_1 = \eta_1 , \quad \hat{n}_1\eta_1(1 - \hat{n}_1) = 0 ,$$

and $\eta_1^2 = 0$. In eq(34) quantity \mathcal{N} is a normalization factor which maintains the idempotent nature of the new projection operator P_1 , below we will show \mathcal{N} is determined as an outcome of our analysis. The properties of $\eta_{N\sigma}^\dagger$ follows from above. Using the definition eq(34) and the block diagonalization equation eq(33) we can write down the following matrix equations,

$$\begin{pmatrix} (V - \mu)\hat{n}_1\hat{n}_2 - \mu\hat{n}_1 & -tc_1^\dagger c_2 \\ -tc_2^\dagger c_1 & -\mu\hat{n}_2 \end{pmatrix} \begin{pmatrix} 1 \\ \eta_1 \end{pmatrix} = \hat{E}_{[1]} \begin{pmatrix} 1 \\ \eta_1 \end{pmatrix} , \quad \begin{pmatrix} (V - \mu)\hat{n}_1\hat{n}_2 - \mu\hat{n}_1 & -tc_1^\dagger c_2 \\ -tc_2^\dagger c_1 & -\mu\hat{n}_2 \end{pmatrix} \begin{pmatrix} \eta_1^\dagger \\ 1 \end{pmatrix} = \hat{E}_{[1]} \begin{pmatrix} \eta_1^\dagger \\ 1 \end{pmatrix} . \quad (35)$$

The form of the transition operators η_1 , η_1^\dagger that satisfies the matrix equations are,

$$\hat{\eta}_1^\dagger = -\frac{t}{\hat{\omega} - (V - \mu)\hat{n}_1\hat{n}_2 + \mu\hat{n}_1} c_1^\dagger c_2 , \quad \hat{\eta}_1 = -\frac{t}{\hat{\omega} - (V - \mu)\hat{n}_1\hat{n}_2 + \mu\hat{n}_2} c_2^\dagger c_1 . \quad (36)$$

The following transition operators lead to the following block diagonal representation of the operator $\hat{E}_{[N\sigma]}$ in the projected space of electron/hole occupancy operator corresponding to state $N\sigma$,

$$\left[(V - \mu)\hat{n}_1\hat{n}_2 - \mu\hat{n}_1 + c_1^\dagger c_2 \frac{t^2}{\hat{\omega} - (V - \mu)\hat{n}_1\hat{n}_2 + \mu\hat{n}_2} c_2^\dagger c_1 \right] = \hat{E}_{[1]}\hat{n}_1 , \quad (37)$$

From the block diagonal operators eq(37) and the transition operator definitions eq(36) we have

$$\eta_1^\dagger \eta_1 = \hat{n}_1 , \quad (38)$$

similarly using the block equations eq(35) one can arrive at $\eta_1 \eta_1^\dagger = 1 - \hat{n}_1$. The relation eq(38) is equivalent to,

$$\hat{n}_1(\hat{\omega} - (\mu + V)\hat{n}_1\hat{n}_2 + \mu\hat{n}_1) = t^2\hat{n}_1(1 - \hat{n}_2) , \quad (39)$$

satisfied by the form of $\hat{\omega}$,

$$\hat{\omega}\hat{n}_1 = (t - \mu)(1 - \hat{n}_2)\hat{n}_1 + (V - 2\mu)\hat{n}_1\hat{n}_2 . \quad (40)$$

The block diagonal form of the Hamiltonian H is given by,

$$U_1 H U_1^\dagger = \begin{pmatrix} \hat{\omega} & 0 \\ 0 & \hat{\omega}' \end{pmatrix} \quad (41)$$

where the form of the block $\hat{\omega}'$ is constrained from the partial trace preservation condition seen in equation eq(15),

$$\begin{aligned} \hat{\omega}\hat{n}_1 + \hat{\omega}'(1 - \hat{n}_1) &= (V - 2\mu)\hat{n}_1\hat{n}_2 + (t - \mu)\hat{n}_1(1 - \hat{n}_2) + (-t - \mu)\hat{n}_2(1 - \hat{n}_1) \\ \hat{\omega}' &= (-t - \mu)\hat{n}_2(1 - \hat{n}_1) , \end{aligned} \quad (42)$$

and U_1 is the unitary operator that takes the matrix to a block diagonal form. The form of the unitary operator is given by, $U_1 = \frac{1}{\sqrt{2}}[1 + \eta_1 - \eta_1^\dagger]$. If one directly diagonalizes the 4×4 matrix then the eigen values obtained are,

$$U_1 \begin{pmatrix} V - 2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -\mu & -t \\ 0 & 0 & -t & -\mu \end{pmatrix} U_1^\dagger \rightarrow \begin{pmatrix} V - 2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & t - \mu & 0 \\ 0 & 0 & 0 & -t - \mu \end{pmatrix} \quad (43)$$

where this matrix is represented in the basis (starting from top row) $|1_1 1_2\rangle, |0_1 0_2\rangle, |1_1 0_2\rangle, |0_1 1_2\rangle$ in the number occupancy basis.