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* $\hat{n}_{j\sigma} = c^{\dagger}_{j\sigma}c_{j\sigma}$ *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* $H_{D,N\sigma}$ *and off-diagonal blocks* $H_{X,N\sigma}$ *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* $\hat{U}_{N\sigma}\hat{H}_{2N}\hat{U}^{\dagger}_{N\sigma}$ *where* $\hat{U}_{N\sigma}\hat{U}^{\dagger}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\hat{U}_{N\sigma} = I$*, such that the below given decoupling condition between states* $1_{N\sigma}$ *and* $0_{N\sigma}$ *holds,*

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

This statement is equivalent to stating $[\hat{U}_{N\sigma}\hat{H}_{2N}\hat{U}^{\dagger}_{N\sigma}, \hat{n}_{N\sigma}] = 0$.
Statement-2: *Form of the Unitary operator is given by,*

$$\hat{U}_{N\sigma} = \exp(\mathrm{arctan}h(\hat{\eta}_{N\sigma} - \hat{\eta}^{\dagger}_{N\sigma})) \ ,$$

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

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

having the following properties,

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

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,

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

where,

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

where the form of $\hat{T}^{\dagger}_{N\sigma,e-h}$ 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,

$$HP_{N\sigma} = H'P_{N\sigma} \tag{2}$$

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,

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

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 ,

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

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

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

and $\eta^2_{N\sigma} = 0$. 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 $\eta^{\dagger}_{N\sigma}$ follows from above. Using the definition eq(34) and the block diagonalization equation eq(33) we can write down the following matrix equations,

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

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

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

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 $N\sigma$,

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

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

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

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

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

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

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

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

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

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 $1 - P_{N\sigma}$,

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

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,

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

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

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

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

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

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 $N\sigma$,

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

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,

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

This proves that there exist a unitary operation $\hat{U}_{N\sigma}$ which puts the matrix into a block diagonal form i.e. $\hat{U}_{N\sigma}\hat{H}\hat{U}^\dagger_{N\sigma} = \hat{H}'$, 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,

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

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 ,

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

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

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

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

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

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

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

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

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

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

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

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,

$$U_{N\sigma}\hat{H}_{2N}U^\dagger_{N\sigma} = \begin{pmatrix} \hat{E}_{[N\sigma]} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} \ . \tag{21}$$

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

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

This entire block diagonalization procedure leads to the following corollaries ,
Corollaries:

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

2.
$$\begin{aligned} &\begin{pmatrix} 0 & 1 \end{pmatrix}\hat{E}_{N\sigma}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \implies \begin{pmatrix} 1 & 0 \end{pmatrix}U^\dagger_{N\sigma}\hat{E}_{N\sigma}U_{N\sigma}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hat{E}_{N\sigma} \\ &\implies \begin{pmatrix} \eta_{N\sigma} & 1 \end{pmatrix}\hat{E}_{N\sigma}\begin{pmatrix} 1 \\ -\eta_{N\sigma} \end{pmatrix} = \hat{E}_{N\sigma} \to [\hat{E}_{[N\sigma]}, \eta_{N\sigma}] = 0 \end{aligned} \tag{24}$$

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,

$$\begin{aligned} \hat{E}_{N\sigma}\eta_{N\sigma} &= \hat{E}_{N\sigma}\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h}c_{N\sigma} \\ &= \Big(1 + Tr_{N\sigma}(H(1-\hat{n}_{N\sigma}))\hat{G}_h(\hat{E}_{N\sigma})\Big) \\ &\quad \times T^\dagger_{N\sigma,e-h}c_{N\sigma} \ . \end{aligned} \tag{25}$$

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

$$\begin{aligned} &Tr_{N\sigma}(H(1-\hat{n}_{N\sigma}))\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h}c_{N\sigma} \\ &= T^\dagger_{N\sigma,e-h}c_{N\sigma}Tr_{N\sigma}(H\hat{n}_{N\sigma})\hat{G}_e(\hat{E}_{N\sigma}) \ . \end{aligned} \tag{26}$$

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

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

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

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

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

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

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 $\hat{n}_{1,2}=c^\dagger_{1,2}c_{1,2}$. 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 $I_1=\hat{P}_1+1-P_1$ corresponding to a new basis in which this matrix attains a block diagonal form i.e.,

$$\begin{aligned} P_1H(1-P_1) &= (1-P_1)HP_1=0 \; , \; P_1HP_1=P_1H'P_1 \; , \\ (1-P_1)H(1-P_1) &= (1-P_1)H''(1-P_1) \; , \end{aligned}$$

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,

$$HP_1=H'P_1 \tag{32}$$

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 , $\eta_1^\dagger$ are the electron to hole and hole to electron transition operators having the following properties,

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

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,

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

The form of the transition operators η_1 , $\eta_1^\dagger$ that satisfies the matrix equations are,

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

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,

$$U_1HU_1^\dagger = \begin{pmatrix} \hat{\omega} & 0 \\ 0 & \hat{\omega}' \end{pmatrix} \quad (41)$$

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) $|1_11_2\rangle, |0_10_2\rangle, |1_10_2\rangle, |0_11_2\rangle$ in the number occupancy basis.