Formal part of the paper "Renormalization group as a iterative block diagonalization"

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A fermionic graph $\mathcal{G}_{2N}$ is defined over the configuration space $\mathcal{C}^{2N} = \mathcal{A}\mathcal{H}^{\otimes 2N}$ which is a anti-symmetrized 2N tensor power of the single particle Hilbert space $\mathcal{H}$ where $2N$ nodes are labelled as $j\sigma, j \in [1, N], \sigma \in [\uparrow, \downarrow]$. As the single particle Hilbert space dimensionality $dim(\mathcal{H}) = 2$ therefore $\dim(\mathcal{C}_{2N}) = 2^{2N}$. The Hamiltonian $\hat{H}_{2N}$ is a Hermitian operator acting on $\mathcal{C}_{2N}$ having a matrix representation of dimension $dim(\mathcal{C}_{2N}) \times dim(\mathcal{C}_{2N})$. The diagonal elements in the number occupancy basis $|1_{j\sigma}\rangle, |0_{j\sigma}\rangle \forall j \in [1, 2N]$ represents the onsite energy scale for every node in the graph, and off-diagonal elements represents the connectivities between nodes on the graph. This paper is presented in two parts part-(I) is the formalism which shows,
a)A unitarily (U) equivalent representation of the Hamiltonian $\hat{H}$ which render it block diagonal in the number occupancy basis $1_{j\sigma}, 0_{j\sigma}$ of a node $j\sigma$. The Hamiltonian of dimension $dim(\hat{H}) = 2^{2N} \times 2^{2N}$ is block diagonalized to two matrices $U[H_1 \oplus H_2]U^\dagger$ of dimension $(2^{2N-1} \times 2^{2N-1})$ each, i.e. $dim(\hat{H}) \to \dim(U[H_1 \oplus H_2]U^\dagger)$.
b)A recursion procedure of applying the unitary operators such that any individual blocks dimension scales as $2^{2N} \to 2^{2N-1} \oplus 2^{2N-1} \to (2^{2N-2} \oplus 2^{2N-2}) \oplus (2^{2N-2} \oplus 2^{2N-2})$ so on, i.e. the RG steps goes as $log_2^{2^{2N}} - log_2^{2^{2N-1}} = 1$.
Part-(II) of the paper shows the application of this formalism to a strongly correlated system , for which we obtain a set of Unitary Renormalization group generators. The flow equations in the space of coupling generated along-with this procedure leads to zooming into the low energy sector.

I. BLOCK MATRIX REPRESENTATION OF A FERMIONIC OPERATOR IN SINGLE FERMION NUMBER OCCUPANCY BASIS

A general number ordered (N.O.) operator in a 2^N dimensional Fermionic Fock space created out of N single particle number occupancy spaces labeled by $l \in [1, N]$ is represented as,

$$\hat{B} = \sum_i \hat{B}_i \ , \ \hat{B}_i = \prod_{j=1}^{p_i} c^\dagger_{l^i_{e,j}} \prod_{j=1}^{q_i} c_{l^i_{h,j}} \ ,$$
$$\prod_{j=1}^{p_i} c^\dagger_{l^i_{e,j}} := c^\dagger_{l^i_{e,1}} c^\dagger_{l^i_{e,2}} \dots c^\dagger_{l^i_{e,p_i}} \ , \quad (1)$$

here the indexing $l^i_{e,j}$ are the state labels acted upon by the electron creation operators similarly $l^i_{h,j}$ are the state labels acted upon by the electron annihilation operators, contained within the ith operator $\hat{B}_i$.

Theorem 1 *The operator $\hat{B}$ with respect to single particle number occupancy space labelled by l can be resolved into the following block form i.e.,*

$$\hat{B} = U_l \hat{n}_l + V_l c_l + c^\dagger_l W_l + X_l(1 - \hat{n}_l) = \begin{pmatrix} U_l & W_l \\ V_l & X_l \end{pmatrix} \quad (2)$$

Definition: The partial trace of $\hat{O}$ with respect to state l is defined as ,

$$Tr_l(\hat{B}) = \sum_i Tr_l(\hat{O}_i)$$

where ,

$$Tr_l(\hat{B}_i) = 2\left(1 - \sum_{j=1}^{p_i} \delta_{l^i_{e,j},l}\right)\left(1 - \sum_{k=1}^{q_i} \delta_{l^i_{e,k},l}\right)\hat{O}_i$$
$$+ \sum_{\substack{j'=1,\\k'=1}}^{p_i,q_i} \delta_{l^i_{e,j'},l}\delta_{l^i_{h,k'},l} \times e^{i\pi[(j'-1)+(q_i-k')]} \prod_{\substack{j=1,\\j\neq j'}}^{p_i} c^\dagger_{l^i_{e,j}} \prod_{\substack{k=1,\\k\neq k'}}^{q_i} c_{l^i_{h,j}} . \quad (3)$$

Using the above definition eq(3) the following three identities can be derived,

$$Tr_l(\hat{B}_i\hat{n}_l)\hat{n}_l = e^{i\pi(p_i+q_i)}\left[\left(1 - \sum_{j=1}^{p_i} \delta_{l^i_{e,j},l}\right)\left(1 - \sum_{k=1}^{q_i} \delta_{l^i_{e,k},l}\right)\hat{n}_l + \sum_{\substack{j'=1,\\k'=1}}^{p_i,q_i} \delta_{l^i_{e,j'},l}\delta_{l^i_{h,k'},l}\right]\hat{O}_i \ ,$$

$$Tr_l(c^\dagger_l\hat{B}_i)c_l = \left(1 - \sum_{j'=1}^{p_i} \delta_{l^i_{e,j'},l}\right)\sum_{k'=1}^{q_i} \delta_{l^i_{h,k'},l}\hat{O}_i \ ,$$

$$c^\dagger_l Tr_l(\hat{B}_i c_l) = \left(1 - \sum_{k'=1}^{q_i} \delta_{l^i_{h,k'},l}\right)\sum_{j'=1}^{p_i} \delta_{l^i_{e,j'},l}\hat{O}_i \ . \quad (4)$$

The above three identities lead to the fourth relation as a corollary,

$$Tr_l(\hat{B}_i(1 - \hat{n}_l))(1 - \hat{n}_l) = \left(2 - e^{i\pi(p_i+q_i)}\right)\left(1 - \sum_{j=1}^{p_i} \delta_{l^i_{e,j},l}\right) \times \left(1 - \sum_{k=1}^{q_i} \delta_{l^i_{e,k},l}\right)\hat{B}_i(1 - \hat{n}_l) \ . \quad (5)$$

The operator $\hat{O}_i$ can now be reconstructed using the partial traced operators with respect to the state l multiplied by the triad of operators $\hat{n}_l - \frac{1}{2}, c_l^\dagger, c_l$ using eq(4) and eq(5) ,

$$\hat{B}_i = e^{i\pi(p_i+q_i)} Tr_l(\hat{B}_i \hat{n}_l)\hat{n}_l + Tr_l(c_l^\dagger \hat{O}_i)c_l + c_l^\dagger Tr_l(\hat{B}_i c_l) + \left(2 - e^{i\pi(p_i+q_i)}\right)^{-1} Tr_l(\hat{O}_i(1-\hat{n}_l))(1-\hat{n}_l) \ .$$

Hence any arbitrary N.O. fermionic operator can be reconstructed in terms of partial traced operators and the triad $\hat{n}_l - \frac{1}{2}, c_l^\dagger, c_l$ as ,

$$\hat{B} = \sum_i \left[e^{i\pi(p_i+q_i)} Tr_l(\hat{O}_i \hat{n}_l)\hat{n}_l + Tr_l(c_l^\dagger \hat{O}_i)c_l + c_l^\dagger Tr_l(\hat{O}_i c_l) + \left(2 - e^{i\pi(p_i+q_i)}\right)^{-1} Tr_l(\hat{O}_i(1-\hat{n}_l))(1-\hat{n}_l) \right] . \quad (6)$$

The operator decomposition proved above allows for a block matrix representation of the operator $\hat{O}$,

$$\hat{B} = \begin{pmatrix} \sum_i e^{i\pi(p_i+q_i)} Tr_l(\hat{B}_i \hat{n}_l)\hat{n}_l & c_l^\dagger Tr_l(\hat{B}_i c_l) \\ Tr_l(c_l^\dagger \hat{B}_i)c_l & \sum_i \left(2 - e^{i\pi(p_i+q_i)}\right)^{-1} Tr_l(\hat{B}_i(1-\hat{n}_l))(1-\hat{n}_l) \end{pmatrix} . \quad (7)$$

II. BLOCK DIAGONALIZATION OF A FERMIONIC HAMILTONIAN IN SINGLE FERMION NUMBER OCCUPANCY BASIS

Theorem 2 *A fermionic Hamiltonian describing a system of 2N fermionic single particle state defined in the number occupancy (eigenstates of number operator $\hat{n}_{j\sigma}$) basis as $|1_{j\sigma}\rangle, |0_{j\sigma}\rangle$ 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,*

$$\begin{aligned} \hat{H}_{2N} &= (\hat{n}_{N\sigma} + 1 - \hat{n}_{N\sigma})\hat{H}_{2N}(\hat{n}_{N\sigma} + 1 - \hat{n}_{N\sigma}) \\ &= \begin{pmatrix} \hat{n}_{N\sigma}\hat{H}_{2N}\hat{n}_{N\sigma} & \hat{n}_{N\sigma}\hat{H}_{2N}(1-\hat{n}_{N\sigma}) \\ (1-\hat{n}_{N\sigma})\hat{H}_{2N}\hat{n}_{N\sigma} & (1-\hat{n}_{N\sigma})\hat{H}_{2N}(1-\hat{n}_{N\sigma}) \end{pmatrix} \end{aligned} \quad (8)$$

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,*

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

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,

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

Proof:
Case-1 Hamiltonian composed of operators containing even number of $c^\dagger$'s and c's.
A Fermionic Hamiltonian of the size $2^{2N} \times 2^{2N}$ composed of operators containing even number of Fermion operators can be written as a block matrix in terms of diagonal and off-diagonal blocks of size $2^{2N-1} \times 2^{2N-1}$ in the basis of single fermion identity operator($\hat{I}_{N\sigma}$) $\hat{n}_{N\sigma} + \hat{I}_{N\sigma} - \hat{n}_{N\sigma} = \hat{I}_{N\sigma}$ as,

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

where,

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

We ask for such a basis in which this matrix attains a block diagonal form with respect to the state $N\sigma$ i.e.,

$$H|\psi\rangle = H'|\psi\rangle, \text{ where } [H', \hat{n}_{N\sigma}] = 0 \ .$$

A form of $\hat{H}' = \hat{E}_{[N\sigma]} \otimes I_{N\sigma}$ satisfies the block diagonal equation,

$$\begin{pmatrix} H_{N\sigma,e}\hat{n}_{N\sigma} & c_{N\sigma}^\dagger\hat{T}_{N\sigma,e-h} \\ \hat{T}_{N\sigma,e-h}^\dagger c_{N\sigma} & H_{N\sigma,h} \end{pmatrix}|\psi\rangle = \hat{I}_2 \otimes \hat{E}_{[N\sigma]}|\psi\rangle \quad (9)$$

where $\hat{E}_{[N\sigma]}$ is a matrix of size $2^{2N-1} \times 2^{2N-1}$ and $\hat{I}_2$ is the 2×2 identity . For this equation we will now implement the Gauss Jordan Block diagonalization procedure as follows, firstly we write $|\psi\rangle$ as ,

$$\begin{aligned} |\psi\rangle &= \mathcal{N}(1 + \eta_{N\sigma} + \eta_{N\sigma}^\dagger)|\Psi_{N\sigma}^1, 1_{N\sigma}\rangle \\ &= \mathcal{N}'(1 + \eta_{N\sigma} + \eta_{N\sigma}^\dagger)|\Psi_{N\sigma}^0, 0_{N\sigma}\rangle \ , \end{aligned} \quad (10)$$

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

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

where $\eta^2_{N\sigma} = 0$. The properties of $\eta^\dagger_{N\sigma}$ follows from above. Using the definition eq(10) and the block diagonalization equation eq(9) we can write down the following matrix equations,

$$\begin{pmatrix} H_{N\sigma,e}\hat{n}_{N\sigma} & c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h} \\ \hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} & H_{N\sigma,h}(1-\hat{n}_{N\sigma}) \end{pmatrix} \begin{pmatrix} 1 \\ \eta_{N\sigma} \end{pmatrix} = \hat{E}_{[N\sigma]} \begin{pmatrix} 1 \\ \eta_{N\sigma} \end{pmatrix}$$
$$\begin{pmatrix} H_{N\sigma,e}\hat{n}_{N\sigma} & c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h} \\ \hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} & H_{N\sigma,h}(1-\hat{n}_{N\sigma}) \end{pmatrix} \begin{pmatrix} \eta^\dagger_{N\sigma} \\ 1 \end{pmatrix} = \hat{E}_{[N\sigma]} \begin{pmatrix} \eta^\dagger_{N\sigma} \\ 1 \end{pmatrix} \ . \tag{11}$$

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

$$\hat{\eta}_{N\sigma} = \hat{G}_h(\hat{E}_{[N\sigma]})\hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} \ ,$$
$$\hat{\eta}^\dagger_{N\sigma} = \hat{G}_e(\hat{E}_{[N\sigma]})c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h} \ , \tag{12}$$

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 $N\sigma$,

$$\left[H_{N\sigma,e}\hat{n}_{N\sigma} + c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{[N\sigma]})\hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma}\right]|\Psi^1_{N\sigma},1_{N\sigma}\rangle = \hat{E}_{[N\sigma]}\hat{n}_{N\sigma}|\Psi^1_{N\sigma},1_{N\sigma}\rangle \ ,$$
$$\left[H_{N\sigma,h}(1-\hat{n}_{N\sigma}) + \hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma}\hat{G}_e(\hat{E}_{[N\sigma]})c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h}\right]|\Psi^0_{N\sigma},0_{N\sigma}\rangle = \hat{E}_{[N\sigma]}(1-\hat{n}_{N\sigma})|\Psi^0_{N\sigma},0_{N\sigma}\rangle. \tag{13}$$

From the two equations of the transition operators eq(12) we have the following identity,

$$\hat{G}_h(\hat{E}_{[N\sigma]})\hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} = \hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma}\hat{G}_e(\hat{E}_{[N\sigma]}) \ . \tag{14}$$

The above operator ordering relation eq(14) and form of the block diagonal operators eq(13) we have,

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

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

$$[\eta^\dagger_{N\sigma},\eta_{N\sigma}] = 2\hat{n}_{N\sigma} - 1 \ , \ \{\eta^\dagger_{N\sigma},\eta_{N\sigma}\} = 1 \ . \tag{15}$$

For every $|\psi\rangle$ of the form eq(10) there is a $|\psi^\perp\rangle$ of the form,

$$|\psi^\perp\rangle = \mathcal{N}(1-\eta_{N\sigma}-\eta^\dagger_{N\sigma})|\Psi^1_{N\sigma},1_{N\sigma}\rangle$$
$$= \mathcal{N}'(1-\eta_{N\sigma}-\eta^\dagger_{N\sigma})|\Psi^0_{N\sigma},0_{N\sigma}\rangle \ ,$$

from the algebra of the $\eta_{N\sigma}$ operators one can check that $\langle\psi|\psi^\perp\rangle = 0$. To get the other blocks of the final block diagonal form we start with the block diagonal equation satisfied by $|\psi^\perp\rangle$ which is given by,

$$\begin{pmatrix} H_{N\sigma,e}\hat{n}_{N\sigma} & c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h} \\ \hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} & H_{N\sigma,h}(1-\hat{n}_{N\sigma}) \end{pmatrix} \begin{pmatrix} 1 \\ -\eta_{N\sigma} \end{pmatrix} = \hat{E}'_{[N\sigma]} \begin{pmatrix} 1 \\ -\eta_{N\sigma} \end{pmatrix}$$
$$\begin{pmatrix} H_{N\sigma,e}\hat{n}_{N\sigma} & c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h} \\ \hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} & H_{N\sigma,h}(1-\hat{n}_{N\sigma}) \end{pmatrix} \begin{pmatrix} -\eta^\dagger_{N\sigma} \\ 1 \end{pmatrix} = \hat{E}'_{[N\sigma]} \begin{pmatrix} -\eta^\dagger_{N\sigma} \\ 1 \end{pmatrix} \tag{16}$$

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

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

which leads to a further consistency condition using eq(12),

$$-\hat{G}_h(\hat{E}'_{[N\sigma]})\hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} = \hat{G}_h(\hat{E}_{[N\sigma]})\hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} \ ,$$
$$-\hat{G}_e(\hat{E}'_{[N\sigma]})\hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} = \hat{G}_e(\hat{E}_{[N\sigma]})\hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} \ . \tag{17}$$

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 $N\sigma$,

$$c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{[N\sigma]})\hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma}|\Psi^1_{N\sigma},1_{N\sigma}\rangle$$
$$= (H_{N\sigma,e} - \hat{E}'_{[N\sigma]})\hat{n}_{N\sigma}|\Psi^1_{N\sigma},1_{N\sigma}\rangle \ ,$$
$$\hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma}\hat{G}_e(\hat{E}_{[N\sigma]})c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h}|\Psi^0_{N\sigma},0_{N\sigma}\rangle$$
$$= (H_{N\sigma,h} - \hat{E}'_{[N\sigma]})(1-\hat{n}_{N\sigma})|\Psi^0_{N\sigma},0_{N\sigma}\rangle. \tag{18}$$

The block diagonal equation can be reconstructed now as,

$$\begin{pmatrix} \hat{E}_{N\sigma} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hat{E}_{[N\sigma]} \begin{pmatrix} 1 \\ 0 \end{pmatrix} ,$$
$$\begin{pmatrix} \hat{E}_{N\sigma} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hat{E}'_{[N\sigma]} \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \tag{19}$$

By identifying the two blocks $\hat{E}_{[N\sigma]}$ and $\hat{E}'_{[N\sigma]}$ using eq(13) and eq(18) the block diagonalized Hamiltonian is given by,

$$\begin{aligned} \hat{H}' &= \hat{E}_{[N\sigma]}\hat{n}_{N\sigma} + \hat{E}'_{[N\sigma]}(1-\hat{n}_{N\sigma}) \\ &= \frac{1}{2}Tr_{N\sigma}(\hat{H}_{2N}) + \left(\hat{n}_{N\sigma} - \frac{1}{2}\right)\{c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h}, \eta_{N\sigma}\} \end{aligned} \tag{20}$$

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,

$$\begin{aligned} &\frac{1}{\sqrt{2}} \begin{pmatrix} H_{N\sigma,e}\hat{n}_{N\sigma} & c^\dagger_{N\sigma}\hat{T}_{N\sigma,e-h} \\ \hat{T}^\dagger_{N\sigma,e-h}c_{N\sigma} & H_{N\sigma,h} \end{pmatrix} \begin{pmatrix} 1 & \eta^\dagger_{N\sigma} \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \frac{1}{\sqrt{2}}\hat{E}_{[N\sigma]} \begin{pmatrix} 1 & \eta^\dagger_{N\sigma} \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} . \end{aligned} \tag{21}$$

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 ,

$$\begin{aligned} &\begin{pmatrix} \hat{E}_{[N\sigma]} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} \hat{U}_{N\sigma} \begin{pmatrix} 1 & \eta^\dagger_{N\sigma} \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \hat{U}_{N\sigma}\hat{E}_{[N\sigma]}U^\dagger_{[N\sigma]}U_{[N\sigma]} \begin{pmatrix} 1 & \eta^\dagger_{N\sigma} \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} . \end{aligned} \tag{22}$$

The requirement of the block diagonal equation eq(19) is,

$$\hat{U}_{N\sigma} \begin{pmatrix} 1 & \eta^\dagger_{N\sigma} \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = c \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \tag{23}$$

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

$$\hat{U}_{N\sigma} = \frac{1}{\sqrt{2}}(1 + \eta^\dagger_{N\sigma} - \eta_{N\sigma}) . \tag{24}$$

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(15). Below we show the fulfillment of the requirement eq(23) ,

$$\begin{pmatrix} 1 & \eta^\dagger_{N\sigma} \\ -\eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 & \eta^\dagger_{N\sigma} \\ \eta_{N\sigma} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} . \tag{25}$$

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

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

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,

$$U_{N\sigma}\hat{H}_{2N}U^\dagger_{N\sigma} = \begin{pmatrix} \hat{E}_{[N\sigma]} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} . \tag{26}$$

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

$$\begin{aligned} \eta^\dagger_{N\sigma} &= \hat{n}_{N\sigma}\hat{H}(1-\hat{n}_{N\sigma})\frac{1}{\hat{E}_{[N\sigma]} - (1-\hat{n}_{N\sigma})\hat{H}_{2N}(1-\hat{n}_{N\sigma})} , \\ \hat{U}_{N\sigma} &= \frac{1}{\sqrt{2}}\left[1 + \hat{\eta}_{N\sigma} - \hat{\eta}^\dagger_{N\sigma}\right] , \\ \hat{E}_{[N\sigma]} &= \hat{n}_{N\sigma}\hat{H}_{2N}\hat{n}_{N\sigma} + \eta^\dagger_{N\sigma}(1-\hat{n}_{N\sigma})\hat{H}_{2N}\hat{n}_{N\sigma} \end{aligned} \tag{27}$$

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

1.
$$\begin{aligned} &\begin{pmatrix} \hat{E}_{[N\sigma]} & 0 \\ 0 & \hat{E}'_{[N\sigma]} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hat{U}_{N\sigma}\hat{E}_{[N\sigma]}\hat{U}^\dagger_{N\sigma} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &\implies \hat{U}_{N\sigma}\hat{E}_{[N\sigma]}\hat{U}^\dagger_{N\sigma} = \hat{E}_{[N\sigma]} . \end{aligned} \tag{28}$$

2.
$$\begin{aligned} &\begin{pmatrix} 0 & 1 \end{pmatrix} \hat{E}_{N\sigma} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \implies \begin{pmatrix} 1 & 0 \end{pmatrix} U^\dagger_{N\sigma}\hat{E}_{N\sigma}U_{N\sigma} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hat{E}_{N\sigma} \\ &\implies \begin{pmatrix} \eta_{N\sigma} & 1 \end{pmatrix} \hat{E}_{N\sigma} \begin{pmatrix} 1 \\ -\eta_{N\sigma} \end{pmatrix} = \hat{E}_{N\sigma} \rightarrow [\hat{E}_{[N\sigma]}, \eta_{N\sigma}] = 0 \end{aligned} \tag{29}$$

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,

$$\begin{aligned} \hat{E}_{N\sigma}\eta_{N\sigma} &= \hat{E}_{N\sigma}\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h}c_{N\sigma} \\ &= \Big(1 + Tr_{N\sigma}(H(1-\hat{n}_{N\sigma}))\hat{G}_h(\hat{E}_{N\sigma})\Big) T^\dagger_{N\sigma,e-h}c_{N\sigma} . \end{aligned} \tag{30}$$

As eq(14) 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(9) therefore,

$$\begin{aligned} &Tr_{N\sigma}(H(1-\hat{n}_{N\sigma}))\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h}c_{N\sigma} \\ &= T^\dagger_{N\sigma,e-h}c_{N\sigma}Tr_{N\sigma}(H\hat{n}_{N\sigma})\hat{G}_e(\hat{E}_{N\sigma}) \ . \end{aligned} \tag{31}$$

Using eq(31) we have the transition operator rearrangement relation,

$$\begin{aligned} \left(1+Tr_{N\sigma}(H(1-\hat{n}_{N\sigma}))\hat{G}_h(\hat{E}_{N\sigma})\right)T^\dagger_{N\sigma,e-h}c_{N\sigma} &= T^\dagger_{N\sigma,e-h}c_{N\sigma}\left(1+Tr_{N\sigma}(H\hat{n}_{N\sigma})\hat{G}_e(\hat{E}_{N\sigma})\right) \\ \hat{E}_{N\sigma}\eta_{N\sigma} &= T^\dagger_{N\sigma,e-h}c_{N\sigma}\hat{E}_{N\sigma}G_e(\hat{E}_{N\sigma}) \ . \end{aligned} \tag{32}$$

From eq(29) we have $[\hat{E}_{[N\sigma]}, \eta_{N\sigma}] = 0$ therefore,

$$\begin{aligned} T^\dagger_{N\sigma,e-h}c_{N\sigma}\hat{E}_{N\sigma}G_e(\hat{E}_{N\sigma}) &= \eta_{N\sigma}\hat{E}_{N\sigma} \\ T^\dagger_{N\sigma,e-h}c_{N\sigma}[\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] &= [\eta_{N\sigma} - T^\dagger_{N\sigma,e-h}c_{N\sigma}G_e(\hat{E}_{N\sigma})]\hat{E}_{N\sigma}[\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] \ . \end{aligned} \tag{33}$$

Using $\eta_{N\sigma} = T^\dagger_{N\sigma,e-h}c_{N\sigma}G_e(\hat{E}_{N\sigma})$ we can prove our assertion in the following way,

$$\begin{aligned} T^\dagger_{N\sigma,e-h}c_{N\sigma}[\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] &= 0 \\ c^\dagger_{N\sigma}T_{N\sigma,e-h}G_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h}c_{N\sigma}[\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] &= 0 \\ \hat{G}_e^{-1}(\hat{E}_{N\sigma})\eta^\dagger_{N\sigma}\eta_{N\sigma}[\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] &= 0 \\ \implies [\hat{E}_{N\sigma}, G_e(\hat{E}_{N\sigma})] &= 0 \ . \end{aligned} \tag{34}$$

III. INVERTING THE DENOMINATOR IN THE $\eta_{N\sigma}$ AND $\eta^\dagger_{N\sigma}$ OPERATORS

The denominator in the resolvent $\eta_{N\sigma}$ contains two parts,

$\hat{E}_{[N\sigma]}$, :The block diagonalized Hamiltonian ,

$Tr_{N\sigma}(H\hat{n}_{N\sigma})$:Diagonal element of the Hamiltonian $\hat{H}_{2N}$ written as a block matrix .

Theorem 3

$$\begin{aligned} \eta^\dagger_{N\sigma} &= \sum_{i=1}^{2^{2N-1}} \eta_{N\sigma}(\omega_i)\hat{O}(\omega_i) \ , \\ \textit{where } \eta^\dagger_{N\sigma}(\omega_i) &= \frac{1}{\omega_i - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})}c^\dagger_{N\sigma}T_{N\sigma,e-h} \ , \\ \left[\eta_{N\sigma}(\omega_i), \hat{O}(\omega_i)\right] &= 0 \end{aligned} \tag{35}$$

$\{\hat{O}_{\omega_i}, \hat{O}_{\omega_j}\} = 2\delta_{ij}\hat{O}_{\omega_i}$, $\sum_{i=1}^{2^{2N-1}}\hat{O}_{\omega_i} = I$ and ω_i are numbers. The operator $Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})$ has the following commutation relation $[Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma}), \hat{n}_i] = 0$ for all $i \in [1,N]\times[\sigma,-\sigma]$. These corresponds to the diagonal piece of the $Tr_{N\sigma}(H\hat{n}_{N\sigma})$ with respect to all nodes.

Proof: Before we go into the proof we will prove two lemmas.

Lemma 1 *$\hat{E}_{[N\sigma]} - Tr_{N\sigma}(H_{2N}\hat{n}_{N\sigma}) = \hat{\omega}_{N\sigma} - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})$, where $[Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma}), \hat{n}_{i\sigma}] = 0$ for all $i \in [1,N]\times[\sigma,-\sigma]$ and $\hat{\omega}_{N\sigma}$ constitutes the quantum fluctuations associated with the other nodes in $[1,N]\times[\sigma,-\sigma]$.*

The block Hamiltonian $\hat{H}_{2N}$ satisfies the block diagonal equation eq(9),

$$\begin{pmatrix} Tr_{N\sigma}(H_{2N}\hat{n}_{N\sigma}) & c^\dagger_{N\sigma}T_{N\sigma,e-h} \\ T^\dagger_{N\sigma,e-h}c_{N\sigma} & Tr_{N\sigma}(H_{2N}(1-\hat{n}_{N\sigma}))|\psi\rangle \end{pmatrix} = \hat{E}_{[N\sigma]}|\psi\rangle, \tag{36}$$

where the diagonal elements of the block Hamiltonian can be expressed as,

$$\begin{aligned} Tr_{N\sigma}(H_{2N}\hat{n}_{N\sigma}) &= \frac{1}{2}Tr_{N\sigma}(H_{2N}) + Tr_{N\sigma}\left(H_{2N}\left(\hat{n}_{N\sigma} - \frac{1}{2}\right)\right) \ , \\ Tr_{N\sigma}(H_{2N}(1-\hat{n}_{N\sigma})) &= \frac{1}{2}Tr_{N\sigma}(H_{2N}) - Tr_{N\sigma}\left(H_{2N}\left(\hat{n}_{N\sigma} - \frac{1}{2}\right)\right) \ , \\ Tr_{N\sigma}(H_{2N}) &= Tr^D_{N\sigma}(H_{2N}) + Tr_{N\sigma}(H_{2N}) - Tr^D_{N\sigma}(H_{2N}) \ , \\ Tr^D_{N\sigma}(H_{2N}) &= \sum_{l=1,\mathcal{P}_l}^{2N} Tr(\hat{H}_{2N}\hat{B}_{\mathcal{P}_l})\hat{B}_{\mathcal{P}_l} \ , \\ \hat{B}_{\mathcal{P}_l} &= \hat{n}_{N\sigma}\prod_{(j\sigma)=1}^{l}\hat{n}_{\mathcal{P}_l(j\sigma)}\prod_{(j\sigma)=l+1}^{2N}(1-\hat{n}_{\mathcal{P}_l(j\sigma)}) \ , \end{aligned} \tag{37}$$

here $Tr^D_{N\sigma}(H_{2N})$ contains all the diagonal elements with respect to all nodes, therefore $(Tr_{N\sigma}(H_{2N}) -$

$Tr^D_{N\sigma}(H_{2N})$) contains only the off-diagonal elements with respect to all the nodes apart from $N\sigma$. The number diagonal form of $Tr^D_{N\sigma}(H_{2N})$ with respect to all nodes leads to the following commutation relation,

$$[Tr^D_{N\sigma}(H_{2N}), \hat{n}_i] = 0 \ , \ i \in [1, N] \times [\sigma, -\sigma] \ . \quad (38)$$

Using eq(37) the block diagonal equation can be written as,

$$\begin{pmatrix} \frac{1}{2}Tr^D_{N\sigma}(H_{2N}) + Tr_{N\sigma}\Big(H_{2N}\Big(\hat{n}_{N\sigma} - \frac{1}{2}\Big)\Big) & c^\dagger_{N\sigma}T_{N\sigma,e-h} \\ T^\dagger_{N\sigma,e-h}c_{N\sigma} & \frac{1}{2}Tr^D_{N\sigma}(H_{2N}) - Tr_{N\sigma}\Big(H_{2N}\Big(\hat{n}_{N\sigma} - \frac{1}{2}\Big)\Big) \end{pmatrix}|\psi\rangle$$
$$= \left[\hat{E}_{[N\sigma]} - \frac{1}{2}(Tr_{N\sigma}(H_{2N}) - Tr^D_{N\sigma}(H_{2N}))\right]|\psi\rangle \ . \quad (39)$$

We define ,

$$\hat{\omega}_{[N\sigma]} = \hat{E}_{[N\sigma]} - \frac{1}{2}(Tr_{N\sigma}(H_{2N}) - Tr^D_{N\sigma}(H_{2N})) \ ,$$
$$Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma}) = \frac{1}{2}Tr^D_{N\sigma}(H_{2N}) + Tr_{N\sigma}\Big(H_{2N}\Big(\hat{n}_{N\sigma} - \frac{1}{2}\Big)\Big) \ . \quad (40)$$

From eq(38) and the definition eq(40) we arrive at the commutation relation $[Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma}), \hat{n}_i] = 0$, $i \in [1, N] \times [\sigma, -\sigma]$. Using this we prove our assertion ,

$$\hat{E}_{[N\sigma]} - Tr_{N\sigma}(H\hat{n}_{N\sigma}) = \hat{\omega}_{[N\sigma]} - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma}) \ . \quad (41)$$

Lemma 2 *Any Hermitian matrix $\hat{\omega}$ of size $K \times K$ can be written as , $\hat{\omega} = \sum_{i=1}^K \lambda_i \hat{O}_i$, where $\{\hat{O}_i, \hat{O}_j\} = 2\hat{O}_i\delta_{ij}$ and the sum of the operators $\hat{O}_i$ is equal to the identity $\sum_i \hat{O}_i = I$.*

If $\hat{\omega}$ is a Hermitian matrix then there is a Unitary equivalent basis where the matrix is diagonalized ,

$$\hat{\omega} = UDU^\dagger \ , \ D = \sum_{i=1}^K \lambda_i P_i \quad (42)$$

here P_i is the projection operator to the ith eigenstate and λ_i is the ith eigenvalue, where the projection operator fulfills the usual properties $\{P_i, P_j\} = 2\delta_{ij}P_i$. Now by applying the Unitary operator the form of $\hat{\omega}$ becomes,

$$\hat{\omega} = \sum_i \lambda_i \hat{O}_i \ , \ \{\hat{O}_i, \hat{O}_j\} = 2\delta_{ij}\hat{O}_i \ , \quad (43)$$

where $\hat{O}_i = UP_iU^\dagger$. As $\{P_i, P_j\} = 2\delta_{ij}P_i \equiv U\{P_i, P_j\}U^\dagger = 2\delta_{ij}UP_iU^\dagger$, therefore $\{\hat{O}_i, \hat{O}_j\} = 2\delta_{ij}\hat{O}_i$. Furthermore as $\sum_i P_i = I$ so it follows from the unitary mapping between $P_i's$ and $O_i's$ that $\sum_i \hat{O}_i = I$.

The proof of the theorem starts from here where we will use the above lemmas. As $\hat{\omega}_{N\sigma}$ is a $2^{2N-1} \times 2^{2N-1}$ dimensional matrix so we can write this operator as $\hat{\omega}_{N\sigma} = \sum_{i=1}^{2^{2n-1}} \omega_{N\sigma,i}\hat{O}_{\omega_{N\sigma,i}}$ using **Lemma 2** .

The operator $\eta^\dagger_{N\sigma}$ can be rewritten as ,

$$\begin{aligned}\eta^\dagger_{N\sigma} &= \frac{1}{\hat{\omega}_{N\sigma} - Tr^D_{N\sigma}(H_{2N})}c^\dagger_{N\sigma}T_{N\sigma,e-h} \\ &= \frac{1}{\hat{\omega}_{N\sigma} - C + C - Tr^D_{N\sigma}(H_{2N})}c^\dagger_{N\sigma}T_{N\sigma,e-h} \ , \ \text{C is a number} \\ &= \frac{1}{C - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})} \\ &\times \left[1 + \frac{1}{C - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})}(\hat{\omega}_{N\sigma} - C)\right]^{-1} c^\dagger_{N\sigma}T_{N\sigma,e-h} . \end{aligned} \quad (44)$$

From **Lemma 1** the above equation can be expanded into a geometric series in terms of $Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})$ as,

$$\eta^\dagger_{N\sigma} = \frac{1}{C - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})} \times \sum_{n=0}^{\infty}(-1)^n \left[\frac{1}{C - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})}(\hat{\omega}_{N\sigma} - C)\right]^n c^\dagger_{N\sigma}T_{N\sigma,e-h}$$

where by using **Lemma 2** and the commutation relation between the propagator $\hat{G}_e(\hat{\omega}_{N\sigma})$ and probe operator $\hat{\omega}_{N\sigma}$ eq(34) i.e.,$[\hat{G}_e(\hat{\omega}_{N\sigma}), \hat{\omega}_{N\sigma}] = 0$ the series can be resummed to arrive at the expression,

$$\begin{aligned}\eta^\dagger_{N\sigma} &= \frac{1}{C - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})} \\ &\times \sum_{n=0,i=1}^{\infty,2^{2N-1}} \left[\frac{1}{C - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})}(\omega_{N\sigma,i} - C)\right]^n \\ &\times \hat{O}_{\omega_{N\sigma,i}}c^\dagger_{N\sigma}T_{N\sigma,e-h}, \\ &= \sum_{i=1}^{2^{2N-1}} \frac{1}{\omega_{N\sigma,i} - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})}c^\dagger_{N\sigma}T_{N\sigma,e-h}\hat{O}(\omega_{N\sigma,i}) \\ &= \sum_{i=1}^{2^{2N-1}} \eta^\dagger_{N\sigma}(\omega_{N\sigma,i})\hat{O}(\omega_{N\sigma,i}) \ , \end{aligned} \quad (46)$$

where,

$$\eta^{\dagger}_{N\sigma}(\omega_{N\sigma,i}) = \frac{1}{\omega_{N\sigma,i} - Tr^D_{N\sigma}(H_{2N}\hat{n}_{N\sigma})} c^{\dagger}_{N\sigma} T_{N\sigma,e-h} \ . \quad (47)$$

This proves the statement in the theorem.

IV. ALGORITHM FOR THE FINDING THE FORM OF THE $\hat{O}_i's$ OPERATORS

Using the algebra of the $\eta_{N\sigma}$ and $\eta^{\dagger}_{N\sigma}$ operators in sec II and denominator inversion relation in sec III we derive the following relations,

$$\begin{aligned} \eta^{\dagger}_{N\sigma}\eta_{N\sigma} &= \hat{n}_{N\sigma} \\ &= \hat{G}_e(\hat{\omega}_{[N\sigma]}) c^{\dagger}_{N\sigma} T_{N\sigma,e-h} \hat{G}_h(\hat{\omega}_{[N\sigma]}) T^{\dagger}_{N\sigma,e-h} c_{N\sigma} \ , \\ &= \sum_{i=1}^{2^{2N-1}} \hat{O}(\omega_{N\sigma,i}) \eta^{\dagger}_{N\sigma}(\omega_{N\sigma,i}) \eta_{N\sigma}(\omega_{N\sigma,i}) \ , \quad (48) \end{aligned}$$

similarly ,

$$\begin{aligned} \eta_{N\sigma}\eta^{\dagger}_{N\sigma} &= 1 - \hat{n}_{N\sigma} \\ &= \sum_{i=1}^{2^{2N-1}} \hat{O}(\omega_{N\sigma,i}) \eta_{N\sigma}(\omega_{N\sigma,i}) \eta^{\dagger}_{N\sigma}(\omega_{N\sigma,i}) \ . (49) \end{aligned}$$

Using the two constraint relations eq(48) and eq(49) we have the following identity for the $\hat{O}_{\omega_{N\sigma},i}$,

$$\sum_{i=1}^{2^{2N-1}} \hat{O}(\omega_{N\sigma}, i) \{\eta_{N\sigma}(\omega_{N\sigma,i}), \eta^{\dagger}_{N\sigma}(\omega_{N\sigma,i})\} = I \ . \ (50)$$

Using the result $\{\hat{O}(\omega_{N\sigma,i}), \hat{O}(\omega_{N\sigma,j})\} = 2\delta_{ij}\hat{O}(\omega_{N\sigma,i})$ and eq(50) we get a determining equation for $\hat{O}(\omega_{N\sigma,j})$,

$$\hat{O}(\omega_{N\sigma}, i) \{\eta_{N\sigma}(\omega_{N\sigma,i}), \eta^{\dagger}_{N\sigma}(\omega_{N\sigma,i})\} = \hat{O}(\omega_{N\sigma}, i) \ . \quad (51)$$

Let us choose a ansatz for the form of $\{\eta_{N\sigma}(\omega_{N\sigma,i}), \eta^{\dagger}_{N\sigma}(\omega_{N\sigma,i})\}$,

$$\{\eta_{N\sigma}(\omega_{N\sigma,i}), \eta^{\dagger}_{N\sigma}(\omega_{N\sigma,i})\} = \sum_{\substack{j=1 \\ j\neq i}}^{2^{2N-1}} \hat{K}_{\omega_{N\sigma,j}} \hat{O}_{\omega_{N\sigma,j}} + \hat{O}_{\omega_{N\sigma,i}} \ . \ (52)$$

One can check that the ansatz above satisfies eq(51). Again using $\{\hat{O}(\omega_{N\sigma}, i), \hat{O}(\omega_{N\sigma}, j)\} = 2\delta_{ij}\hat{O}(\omega_{N\sigma}, i)$ we get the following relation ,

$$\hat{K}_{\omega_{N\sigma,j}} \hat{O}(\omega_{N\sigma}, i) = \{\eta_{N\sigma}(\omega_{N\sigma,i}), \eta^{\dagger}_{N\sigma}(\omega_{N\sigma,i})\} \hat{O}(\omega_{N\sigma}, i) \ . (53)$$

This leads to the following set of operator equations with $\hat{M}_{\omega_{N\sigma,i}} = \{\eta_{N\sigma}(\omega_{N\sigma,i}), \eta^{\dagger}_{N\sigma}(\omega_{N\sigma,i})\}$,

$$\hat{M}_{\omega_{N\sigma,i}} \sum_{j\neq i, j=1}^{2^{2N-1}} \hat{O}(\omega_{N\sigma}, i) + \hat{O}(\omega_{N\sigma}, i) = \hat{M}_{\omega_{N\sigma,i}} \ (54)$$

These allows us to get the form of the $\hat{O}_{\omega_{N\sigma,j}}$ operators,

$$\begin{pmatrix} \hat{O}_{\omega_{N\sigma,1}} \\ \hat{O}_{\omega_{N\sigma,2}} \\ \vdots \\ \hat{O}_{\omega_{N\sigma,2^{2N-1}}} \end{pmatrix} = \hat{M}^{-1}_{N\sigma} \begin{pmatrix} \hat{M}_{\omega_{N\sigma,1}} \\ \hat{M}_{\omega_{N\sigma,2}} \\ \vdots \\ \hat{M}_{\omega_{N\sigma,2^{2N-1}}} \end{pmatrix} \quad (55)$$

where $\hat{M}_{N\sigma}$ is a superoperator whose elements are given by, $[\hat{M}_{N\sigma}]_{\omega_{N\sigma,i},\omega_{N\sigma,j}} = I\delta_{i,j} + (1-\delta_{i,j})\hat{M}_{\omega_{N\sigma,i}}$. This completes the determination of the Unitary operator.

In the next sections we provide the scheme for block diagonalizing the Hamiltonian H_{2N} using the statements and there proofs given in earlier sections.

V. SCHEMATICS FOR FERMION BLOCK DIAGONALIZATION(FBD)

1. A fermionic Hamiltonian H_{2N} of matrix dimension $dim(H_{2N}) = 2^{2N} \times 2^{2N}$ operating on a 2^{2N} dimensional configuration space made out of 2N single particle states defined in the number occupancy (eigenstates of number operator $\hat{n}_{j\sigma} = c^{\dagger}_{j\sigma}c_{j\sigma}$) basis as $|1_{j\sigma}\rangle, |0_{j\sigma}\rangle$ for all $[j\sigma] \in [1, N] \times [\sigma, -\sigma]$ can be written in the basis of $N\sigma$ as $H_{2N} = H_D + H_X$ i.e. the sum of diagonal H_D and off-diagonal blocks H_{OD} as,

$$H_{2N} = \begin{pmatrix} \hat{n}_{N\sigma}H_{2N}\hat{n}_{N\sigma} & \hat{n}_{N\sigma}\hat{H}_{2N}(1-\hat{n}_{N\sigma}) \\ (1-\hat{n}_{N\sigma})\hat{H}_{2N}\hat{n}_{N\sigma} & (1-\hat{n}_{N\sigma})\hat{H}_{2N}(1-\hat{n}_{N\sigma}) \end{pmatrix} \ (56)$$

where $H_D = \hat{n}_{N\sigma}H_{2N}\hat{n}_{N\sigma} + (1-\hat{n}_{N\sigma})\hat{H}_{2N}(1-\hat{n}_{N\sigma})$ and $H_{OD} = \hat{n}_{N\sigma}\hat{H}_{2N}(1-\hat{n}_{N\sigma}) + (1-\hat{n}_{N\sigma})\hat{H}_{2N}\hat{n}_{N\sigma}$.

2. Using the Hamiltonian block representation eq(56) we outline a procedure in secII to block diagonalize the Hamiltonian i.e. $\tilde{H}_{N\sigma} = U_{N\sigma}H_{N\sigma}U^{\dagger}_{N\sigma}$ where $[\tilde{H}_{N\sigma}, \hat{n}_{N\sigma}] = 0$ and $U_{N\sigma}$ is the unitary operator. The block diagonalized matrix has the form ,

$$\tilde{H}_{2N} = \begin{pmatrix} \begin{matrix} \hat{n}_{N\sigma}\hat{H}_{2N}\hat{n}_{N\sigma} \\ +\frac{1}{2}\{\eta^{\dagger}_{N\sigma}, (1-\hat{n}_{N\sigma})\hat{H}_{2N}\hat{n}_{N\sigma}\} \end{matrix} & 0 \\ 0 & \begin{matrix} (1-\hat{n}_{N\sigma})\hat{H}_{2N}(1-\hat{n}_{N\sigma}) \\ -\frac{1}{2}\{\eta^{\dagger}_{N\sigma}, (1-\hat{n}_{N\sigma})\hat{H}_{2N}\hat{n}_{N\sigma}\} \end{matrix} \end{pmatrix} . (57)$$

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

$$\begin{aligned} \eta_{N\sigma} &= \sum_{j=1}^{2^{2N-1}} \frac{1}{\omega_j - H^D_{h,N\sigma}} (1-\hat{n}_{N\sigma})\hat{H}\hat{n}_{N\sigma}\hat{O}_{N\sigma}(\omega_j) \\ &= \sum_{j=1}^{2^{2N-1}} (1-\hat{n}_{N\sigma})\hat{H}\hat{n}_{N\sigma} \frac{1}{\omega_j - H^D_{e,N\sigma}} \hat{O}_{N\sigma}(\omega_j) (58) \end{aligned}$$

and following the algebra,

$$\{\eta^\dagger_{N\sigma}, \eta_{N\sigma}\} = 1 \ , \ [\eta^\dagger_{N\sigma}, \eta_{N\sigma}] = 2\hat{n}_{N\sigma} - 1 \ . \quad (59)$$

In the above expression ω_j are the probing frequencies for the 2^{2N-1} many body configurations given the state $N\sigma$ is either occupied or unoccupied. The operator $H^D_{(e,h),N\sigma}$ of dimension $dim(H^D_{(e,h),N\sigma}) = 2^{2N-1}\times 2^{2N-1}$ is completely diagonal in the number occupancy basis of the single fermion states $j\sigma'$ i.e. $[H^D_{(e,h),N\sigma}, \hat{n}_{j\sigma'}] = 0$ for all $j\sigma' \in [1, N] \times [\sigma \times -\sigma]$ defined as ,

$$\begin{aligned} H^D_{e,N\sigma} &= \sum_{l=1,\mathcal{P}_l}^{2N} \hat{n}_{N\sigma}\hat{B}_{\mathcal{P}_l}\hat{H}_{2N}\hat{B}_{\mathcal{P}_l}\hat{n}_{N\sigma} \ , \\ \hat{B}_{\mathcal{P}_l} &= \prod_{(j\sigma)=1}^{l} \hat{n}_{\mathcal{P}_l(j\sigma)} \prod_{(j\sigma)=l+1}^{2N} (1 - \hat{n}_{\mathcal{P}_l(j\sigma)}) \ . \end{aligned} \quad (60)$$

Here $\mathcal{P}_l$ represents many body configurations in which l single Fermion labels among $[1, N-1] \times [\sigma, -\sigma] \oplus (N - \sigma)$ are electron occupied and the rest $2N - 1 - l$ labels are electron unoccupied, therefore the number of $P_l's$ is $\binom{2N-1}{l}$. The $\hat{O}_{N\sigma}(\omega_j)$ satisfy the properties $\hat{O}_{N\sigma}(\omega_i)\hat{O}_{N\sigma}(\omega_j) = \delta_{ij}\hat{O}_{N\sigma}(\omega_i)$ and $\sum_i \hat{O}_{N\sigma}(\omega_i) = I$ as can be seen from the spectral decomposition of the block diagonal resolvent in secIII. The operators $\hat{O}_{N\sigma}(\omega_j)$ are determined using there algebraic constraints and the $\eta_{N\sigma}, \eta^\dagger_{N\sigma}$ transition operators algebra eq(59) as shown in secIV and is given by,

$$\begin{aligned} \hat{O}_{N\sigma}(\omega_i) &= \sum_j [\hat{M}^{-1}_{N\sigma}]_{\omega_i,\omega_j} [\hat{G}_{e,N\sigma}(\omega_j)\Delta H_{e,N\sigma}(\omega_j) \\ &\quad + \hat{G}_{h,N\sigma}(\omega_j)\Delta H_{h,N\sigma}(\omega_j)] \\ [\hat{M}_{N\sigma}]_{\omega_i,\omega_j} &= \delta_{ij} + (1 - \delta_{ij})[\hat{G}_{e,N\sigma}(\omega_i)\Delta H_{e,N\sigma}(\omega_i) \\ &\quad + \hat{G}_{h,N\sigma}(\omega_i)\Delta H_{h,N\sigma}(\omega_i)] \end{aligned} \quad (61)$$

where,

$$\begin{aligned} \hat{G}_{(h,e),N\sigma}(\omega_i) &= (\omega_i - H^D_{(h,e),N\sigma})^{-1} \ , \\ \eta_{N\sigma}(\omega_i) &= \hat{G}_{h,N\sigma}(\omega_i)(1 - \hat{n}_{N\sigma})H_{2N}\hat{n}_{N\sigma} \\ \Delta H_{(h,e),N\sigma}(\omega_i) &= \hat{n}_{N\sigma}H_{2N}(1 - \hat{n}_{N\sigma})\eta_{N\sigma}(\omega_i) \ . \end{aligned} \quad (62)$$

In the above $\hat{G}_{(h,e),N\sigma}(\omega_i)$ is the green function associated with the number diagonal part of the Hamiltonian i.e. $H^D_{(h,e),N\sigma}$. The $\eta_{N\sigma}(\omega_i)'s$ operator describes a frequency dependent electron to hole scattering processes which leads to frequency dependent interaction in the block diagonalized Hamiltonian $\tilde{H}$ eq(57) ,

$$\begin{aligned} \tilde{H}_{2N} &= \sum_\omega \tilde{H}_{2N}(\omega)\hat{O}_{N\sigma}(\omega) \\ \tilde{H}_{2N}(\omega) &= \hat{n}_{N\sigma}\hat{H}_{2N}\hat{n}_{N\sigma} + (1 - \hat{n}_{N\sigma})\hat{H}_{2N}(1 - \hat{n}_{N\sigma}) \\ &\quad + \left(\hat{n}_{N\sigma} - \frac{1}{2}\right)[\Delta H_{h,N\sigma}(\omega) + \Delta H_{e,N\sigma}(\omega)] \ . \end{aligned} \quad (63)$$

3. Using the $\hat{O}_{N\sigma}(\omega)$ form eq(61) we can compute the $\hat{\eta}^\dagger_{N\sigma} = \sum_\omega \hat{\eta}^\dagger_{N\sigma}(\omega)\hat{O}_{N\sigma}(\omega)$ exactly this allows to finally construct the unitary operator that block diagonalizes the Hamiltonian,

$$\begin{aligned} U_{N\sigma} &= \frac{1}{\sqrt{2}}[1 + \eta_{N\sigma} - \eta^\dagger_{N\sigma}] \ , \\ \hat{\eta}^\dagger_{N\sigma} &= \sum_\omega \hat{\eta}^\dagger_{N\sigma}(\omega)\hat{O}_{N\sigma}(\omega) \ . \end{aligned} \quad (64)$$

VI. RENORMALIZATION GROUP BASED ON FBD

In the earlier sections sec $(II - VI)$ we have shown how block diagonalization with respect to a state $N\sigma$ can be performed via a Unitary operation. In this section we will show how successive application of block diagonalization procedure forms a Renormalization group. In order to proceed first we describe a useful geometrical representation fig(1) of the configuration space $\mathcal{C}^{2N}$ by writing it down as a antisymmetrized tensor product of $\mathcal{C}^{2N-1}_{N\sigma}$ $(dim(\mathcal{C}^{2N-1}_{N\sigma}) = 2^{2N-1})$ and a single particle Hilbert space $\mathcal{H}_{N\sigma}$ $(dim(H_{N\sigma}) = 2$),

$$\mathcal{C}^{2N} = \mathcal{A}(\mathcal{C}^{2N-1}_{N\sigma} \otimes \mathcal{H}_{N\sigma}) \ , \quad (65)$$

where $0_{N\sigma}$ and $1_{N\sigma}$ represent the unoccupied/occupied

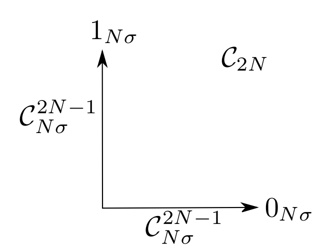

FIG. 1. Geometrical representation of $\mathcal{A}(\mathcal{C}^{2N-1}_{N\sigma} \otimes \mathcal{H}_{N\sigma})$.

configurations of $\mathcal{H}_{N\sigma}$. The parent Hamiltonian $H^{(0)}$ can be written in a block matrix eq(9) form when resolved in the state space of $N\sigma$,

$$H^{(0)} = \begin{pmatrix} H^{(0)}_{1_{N\sigma}} & c^\dagger_{N\sigma}T^{(0)}_{N\sigma,e-h} \\ T^{(0)\dagger}_{N\sigma,e-h}c_{N\sigma} & H^{(0)}_{0_{N\sigma}} \end{pmatrix} \ . \quad (66)$$

The diagonal elements of $H^{(0)}$ operates on $(\mathcal{C}^{2N-1}_{N\sigma}, 1_{N\sigma})$; $(\mathcal{C}^{2N-1}_{N\sigma}, 0_{N\sigma})$ respectively. The off-diagonal elements $c^\dagger_{N\sigma}T^{(0)}_{N\sigma,e-h} = c^\dagger_{N\sigma}Tr_{N\sigma}(H^{(0)}c_{N\sigma})$ and $T^{(0)\dagger}_{N\sigma,e-h}c_{N\sigma} = Tr_{N\sigma}(c^\dagger_{N\sigma}H^{(0)})c_{N\sigma}$ are associated with transitions $(\mathcal{C}^{2N-1}_{N\sigma}, 0_{N\sigma}) \leftrightharpoons (\mathcal{C}^{2N-1}_{N\sigma}, 1_{N\sigma})$. This elements are represented in fig2, The subspaces

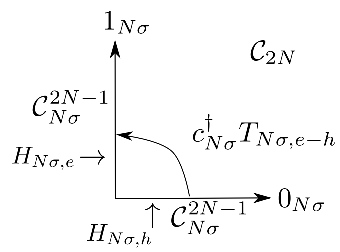

FIG. 2. Geometrical representation of the operations in H.

$(\mathcal{C}^{2N-1}_{N\sigma}, 1_{N\sigma})$ and $(\mathcal{C}^{2N-1}_{N\sigma}, 0_{N\sigma})$ can be represented as,

$$(\mathcal{C}^{2N-1}_{N\sigma}, 1_{N\sigma}) := \begin{pmatrix}1\\0\end{pmatrix} \ , \ (\mathcal{C}^{2N-1}_{N\sigma}, 0_{N\sigma}) := \begin{pmatrix}0\\1\end{pmatrix} \ . \quad (67)$$

Using the subspace representation eq(67) the configuration space $\mathcal{C}^{2N-1}_{N\sigma}$ can be represented as,

$$\mathcal{C}^{2N-1}_{N\sigma} = (1\ 0)\begin{pmatrix}1\\0\end{pmatrix} \oplus (0\ 1)\begin{pmatrix}0\\1\end{pmatrix} \ . \quad (68)$$

We will now geometrically showcase how the successive block diagonalization pursues.

Renormalization step 1, FBD of node $N\sigma$

We then ask for new subspaces $(\tilde{\mathcal{C}}^{2N-1}_{N\sigma}, \tilde{1}_{N\sigma})$ and $(\tilde{\mathcal{C}}^{2N-1}_{N\sigma}, \tilde{0}_{N\sigma})$ attained via rotation,

$$\begin{aligned}(\tilde{\mathcal{C}}^{2N-1}_{N\sigma}, \tilde{1}_{N\sigma}) &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \eta_{N\sigma}\end{pmatrix}\\ (\tilde{\mathcal{C}}^{2N-1}_{N\sigma}, \tilde{0}_{N\sigma}) &= \frac{1}{\sqrt{2}}\begin{pmatrix}-\eta^\dagger_{N\sigma}\\ 1\end{pmatrix} \ ,\end{aligned} \quad (69)$$

in which the block matrix $H^{(0)}$ is rendered a block diagonal form $H^{(1)}$ i.e. $[H^{(1)}, \hat{n}_{N\sigma}] = 0$,

$$H^{(1)} = \begin{pmatrix}H^{(1)}_{1_{N\sigma}} & 0\\ 0 & H^{(1)}_{0_{N\sigma}}\end{pmatrix} \ . \quad (70)$$

The requirement of rotational invariance of configuration space $\mathcal{C}^{2N-1}$ leads to constraint on $\eta_{N\sigma}$ and $\eta^\dagger_{N\sigma}$,

$$\begin{aligned}\frac{1}{2}\left(1\ \eta^\dagger_{N\sigma}\right)\begin{pmatrix}1\\ \eta_{N\sigma}\end{pmatrix} &= (1\ 0)\begin{pmatrix}1\\0\end{pmatrix}\\ \eta^\dagger_{N\sigma}\eta_{N\sigma} &= \hat{n}_{N\sigma} \ ,\\ \frac{1}{2}\left(-\eta_{N\sigma}\ 1\right)\begin{pmatrix}-\eta^\dagger_{N\sigma}\\ 1\end{pmatrix} &= (0\ 1)\begin{pmatrix}0\\1\end{pmatrix}\\ \eta_{N\sigma}\eta^\dagger_{N\sigma} &= 1 - \hat{n}_{N\sigma} \ .\end{aligned} \quad (71)$$

One can also check the orthogonality of this two subspaces given by condition $(-\eta_{N\sigma}\ 1)(1\ \eta_{N\sigma})^T = 0$. Geometrically the rendering of the matrix into a block diagonal form and the associated subspaces is represented in the figure fig(3), In this block diagonal form there is

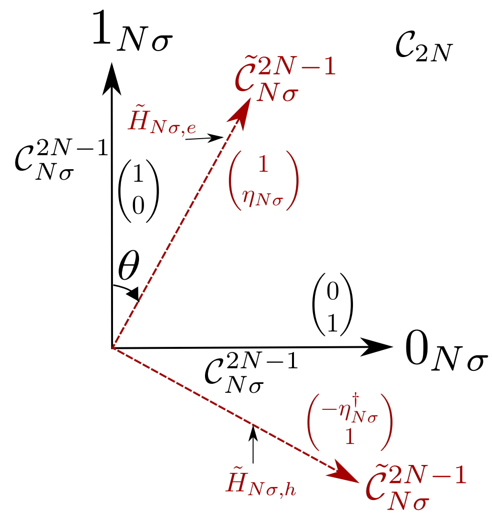

FIG. 3. Block diagonal representation of $H^{(1)}$ in space $(\tilde{C}^{2N-1}_{N\sigma}, \tilde{1}_{N\sigma}) \oplus (\tilde{C}^{2N-1}_{N\sigma}, \tilde{0}_{N\sigma})$.

only the action of diagonal blocks on the new subspaces $(\tilde{\mathcal{C}}^{2N-1}_{N\sigma}, \tilde{1}_{N\sigma})$ and $(\tilde{\mathcal{C}}^{2N-1}_{N\sigma}, \tilde{0}_{N\sigma})$ but absence of any transitions between them as in fig(2. The block diagonal forms of the Hamiltonian $\tilde{H}_{1_{N\sigma}}$ and $\tilde{H}_{0_{N\sigma}}$ is given by eq(57). The unitary operation $U^{(0)}_{N\sigma}$ that renders H block diagonal,

$$\hat{H}^{(1)} = U^{(0)}_{N\sigma}\hat{H}^{(0)}U^{(0)\dagger}_{N\sigma} = \begin{pmatrix}H^{(1)}_{1_{N\sigma}} & 0\\ 0 & H^{(1)}_{0_{N\sigma}}\end{pmatrix} \ , \quad (72)$$

is determined in eq(64). The new Hamiltonian $\hat{H}^{(1)}$ is given by,

$$\begin{aligned}\hat{H}^{(1)} &= \frac{1}{2}Tr_{N\sigma}(H^{(0)})\\ &+ \left(\hat{n}_{N\sigma} - \frac{1}{2}\right)\Big[c^\dagger_{N\sigma}Tr_{N\sigma}(H^{(0)}c_{N\sigma})G^{(0)}_h(\hat{\omega}_{N\sigma})Tr_{N\sigma}(c^\dagger_{N\sigma}H^{(0)})c_{N\sigma}\\ &+ Tr_{N\sigma}(c^\dagger_{N\sigma}H^{(0)})c_{N\sigma}G^{(0)}_e(\hat{\omega}_{N\sigma})c^\dagger_{N\sigma}Tr_{N\sigma}(H^{(0)}c_{N\sigma})\Big].\end{aligned} \quad (73)$$

The angle operator θ is the generator of the subspace rotation whose form can be determined by writing the Unitary matrix $U^{(0)}_{N\sigma}$ eq(26) in a exponential form,

$$\hat{U}^{(0}_{N\sigma} = \exp(i\theta) \ , \ \theta = \arctan(i(\eta_{N\sigma} - \eta^\dagger_{N\sigma})) \ . \quad (74)$$

At the first level of block diagonalization of node $N\sigma$ the effective Hamiltonian obtained have there entries renormalized. To observe the renormalization of the entries in the effective Hamiltonian, we need one mathematical machinery that teases out a general entry in a fermionic matrix. As a first step we define The identity

$I_{2^{2N}\times 2^{2N}}=\sum_{l,\mathcal{P}_l}\prod_{(j\sigma)=1}^{l}\hat{n}_{\mathcal{P}_l(j\sigma)}\prod_{(j\sigma)=l+1}^{2N}(1-\hat{n}_{\mathcal{P}_l(j\sigma)})$ can resolved into a sum of product of pair of state creation operators,

$$I=\sum_{l,\mathcal{P}_l}B^{\dagger}_{\mathcal{P}_l}B_{\mathcal{P}_l}\ ,\ B^{\dagger}_{\mathcal{P}_l}=\prod_{(j\sigma)=1}^{l}c^{\dagger}_{\mathcal{P}_l(j'\sigma')}\prod_{(j\sigma)=l+1}^{2N}c_{\mathcal{P}_l(j\sigma)}\ .\tag{75}$$

Using the state creation operator $B^{\dagger}_{\mathcal{P}_l}$ and the identity eq(75) we can now represent a general entry in a fermionic matrix M as,

$$M=\sum_{\mathcal{P}_l,\mathcal{P}'_{l'}}B^{\dagger}_{\mathcal{P}_l}Tr(B^{\dagger}_{\mathcal{P}'_{l'}}MB_{\mathcal{P}_l})B^{\dagger}_{\mathcal{P}'_{l'}}\ .\tag{76}$$

The identity for the subspace $\mathcal{C}^{2N-1}_{N\sigma}$ is given by $I_{2N-1}=\sum_{l,\mathcal{P}_l}B^{\dagger}_{\mathcal{P}_{N\sigma,l}}B_{\mathcal{P}_{N\sigma,l}}$. The renormalization of the entries in the Hamiltonian matrix in the first step of block diagonlization can be written as using eq(76),

$$\begin{aligned}&Tr_{\bar{N}\sigma}(B^{\dagger}_{\mathcal{P}'_{N\sigma,l'},\mathcal{P}''_{N\sigma,l''},\mathcal{P}_d}\tilde{H}B_{\mathcal{P}_{N\sigma,l},\mathcal{P}'''_{N\sigma,l'''},\mathcal{P}_d})\\&-Tr_{\bar{N}\sigma}(B^{\dagger}_{\mathcal{P}'_{N\sigma,l'},\mathcal{P}''_{N\sigma,l''},\mathcal{P}_d}HB_{\mathcal{P}_{N\sigma,l},\mathcal{P}'''_{N\sigma,l'''},\mathcal{P}_d})\\&=\Big[Tr_{\bar{N}\sigma}(B^{\dagger}_{\mathcal{P}_l}T_{N\sigma,e-h}B_{\mathcal{P}'_{l'}})Tr_{\bar{N}\sigma}(B_{\bar{\mathcal{P}}_d}G_{h,N\sigma}(\omega)B_{\bar{\mathcal{P}}_d})\\&\times Tr_{\bar{N}\sigma}(B^{\dagger}_{\mathcal{P}''_{l''}}T^{\dagger}_{N\sigma,e-h}B_{\mathcal{P}'''_{l'''}})\\&+Tr_{\bar{N}\sigma}(B^{\dagger}_{\mathcal{P}''_{l''}}T^{\dagger}_{N\sigma,e-h}B_{\mathcal{P}'''_{l'''}})Tr_{\bar{N}\sigma}(B_{\bar{\mathcal{P}}_d}G_{e,N\sigma}(\omega)B_{\bar{\mathcal{P}}_d})\\&\times Tr_{\bar{N}\sigma}(B^{\dagger}_{\mathcal{P}_l}T_{N\sigma,e-h}B_{\mathcal{P}'_{l'}})\Big]\left(\hat{n}_{N\sigma}-\frac{1}{2}\right)\ .\end{aligned}\tag{77}$$

Choosing the frequency set for $\hat{\omega}_{N\sigma}$
At the first step of the renormalization procedure the electron and hole transition operators have a frequency channel distribution given by eq(61),

$$\eta^{\dagger}_{N\sigma}=\sum_{j=1}^{2^{2N-1}}\frac{1}{\omega_j-Tr^{D}_{N\sigma}(\hat{H}\hat{n}_{N\sigma})}c^{\dagger}_{N\sigma}Tr_{N\sigma}(Hc_{N\sigma})\ .\tag{78}$$

Operationally we will need to start the block diagonalization scheme with a initial frequency set ω'_is, below we outline a procedure of choosing this frequency set,

1. Define a Hamiltonian H^D containing tree level energies in an appropriately chosen basis. The Hamiltonian H^D is determined uniquely from Hamiltonian $H^{(0)}$ as,

$$\begin{aligned}H^D&=\sum_{l=1,\mathcal{P}_l}^{2N}Tr(H^{(0)}\hat{B}_{\mathcal{P}_l})\hat{B}_{\mathcal{P}_l}\ ,\\\hat{B}_{\mathcal{P}_l}&=\prod_{(j\sigma)=1}^{l}\hat{n}_{\mathcal{P}_l(j\sigma)}\prod_{(j\sigma)=l+1}^{2N}(1-\hat{n}_{\mathcal{P}_l(j\sigma)})\ .\end{aligned}\tag{79}$$

2. Get the minimum and maximum configurational energies of H^D i.e.,

$$E_0=min(Tr(H^{(0)}\hat{B}_{\mathcal{P}_l}))\ ,\ E_1=max(Tr(H^{(0)}\hat{B}_{\mathcal{P}_l}))\ .\tag{80}$$

3. Define the smallest and the highest frequencies with a δ shift ,

$$\omega_0=E_0-\delta\ ,\ \omega_{2^{2N-1}}=E_1+\delta\ ,\tag{81}$$

where the choice of the δ can be made using the maximal strength of the **QF** term that couples the node $N\sigma$ with the rest of the nodes in the graph i.e. $\delta=max(Tr_{N\sigma}(c^{\dagger}_{N\sigma}H^{(0)}))$.

4. The ω set is created as a arithmetic progression on the energy limits ω_0 through $\omega_{2^{2N-1}}$,

$$\omega_j=\omega_0+\frac{j}{2^{2N-1}-1}[\omega_{2^{2N-1}}-\omega_0]\ .\tag{82}$$

Renormalization step 2, FBD of node $N-\sigma$
The 2nd successive step of the block diagonalization

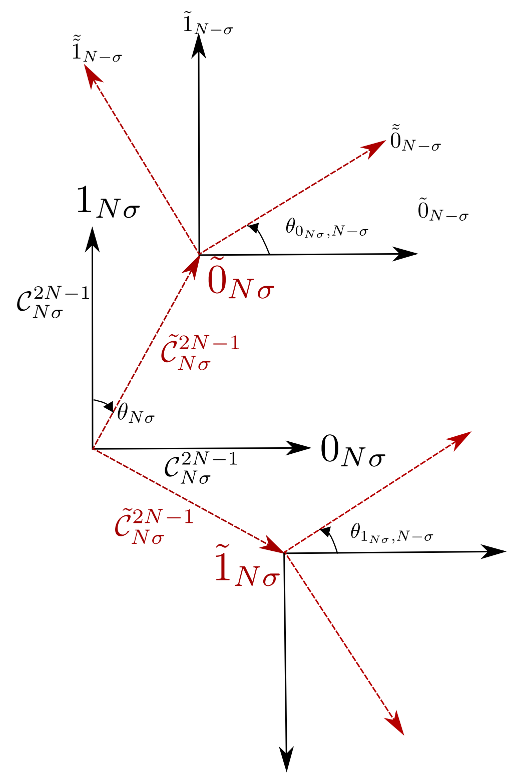

FIG. 4. 2nd succesive step of Block diagonalization RG.

procedure involves writing the configuration subspaces $(\mathcal{C}^{2N-1}_{N\sigma},1_{N\sigma})$ and $(\mathcal{C}^{2N-1}_{N\sigma},0_{N\sigma})$ as,

$$\begin{aligned}\mathcal{C}^{2N}&=\mathcal{A}(\mathcal{C}^{2N-1}_{N\sigma}\otimes\mathcal{H}_{N\sigma})\ ,\\\mathcal{C}^{2N-1}_{N\sigma}&=\mathcal{A}(\mathcal{C}^{2N-1}_{N\sigma,N-\sigma}\otimes\mathcal{H}_{N-\sigma})\ .\end{aligned}\tag{83}$$

At this step we are look for a solution to the block diagonal equation satisfied by $H^{(1)}$ given by eq(70), this is

FBD step-1

$$\begin{pmatrix} H^{(1)}_{1_{N\sigma},1_{N-\sigma}} & c^{\dagger}_{N-\sigma}T^{(1)}_{N-\sigma} & 0 & 0 \\ T^{(1)\dagger}_{N-\sigma}c_{N-\sigma} & H^{(1)}_{1_{N\sigma},0_{N-\sigma}} & 0 & 0 \\ 0 & 0 & H^{(1)}_{0_{N\sigma},1_{N-\sigma}} & c^{\dagger}_{N-\sigma}T^{(1)}_{N-\sigma} \\ 0 & 0 & T^{(1)\dagger}_{N-\sigma}c_{N-\sigma} & H^{(1)}_{1_{N\sigma},0_{N-\sigma}} \end{pmatrix}|\psi\rangle = \hat{E}_{N\sigma,N-\sigma}\otimes I_2\otimes I_2|\psi\rangle\ . \quad (84)$$

By using FBD steps 2-3 we get to a basis where $H^{(1)}$ attains a block diagonal form $H^{(2)}$,

$$H^{(2)} = U^{(1)}_{N-\sigma}H^{(1)}U^{(1)\dagger}_{N-\sigma} = \begin{pmatrix} H^{(2)}_{1_{N\sigma},1_{N-\sigma}} & 0 & 0 & 0 \\ 0 & H^{(2)}_{1_{N\sigma},0_{N-\sigma}} & 0 & 0 \\ 0 & 0 & H^{(2)}_{0_{N\sigma},1_{N-\sigma}} & 0 \\ 0 & 0 & 0 & H^{(2)}_{0_{N\sigma},0_{N-\sigma}} \end{pmatrix}, \quad (85)$$

where $U^{(1)}_{N-\sigma}$ is the unitary map connecting the old basis to the new basis and its form is given by,

$$\begin{aligned} U^{(1)}_{N-\sigma} &= \frac{1}{\sqrt{2}}\left[1+\eta^{(1)\dagger}_{N-\sigma}-\eta^{(1)}_{N-\sigma}\right] \\ &= U^{(1)}_{1_{N\sigma},N-\sigma}\oplus U^{(1)}_{0_{N\sigma},N-\sigma} \\ U^{(1)}_{(1,0)_{N\sigma},N-\sigma} &= \frac{1}{\sqrt{2}}\left[1+\eta^{(1)\dagger}_{(1,0)_{N\sigma},N-\sigma}-\eta^{(1)}_{(1,0)_{N\sigma},N-\sigma}\right] \end{aligned} \quad (86)$$

where,

$$\begin{aligned} \eta^{(1)\dagger}_{N-\sigma} &= \sum_{j=1}^{2^{2N-2}}\eta^{(1)\dagger}_{N-\sigma}(\omega_j)\hat{O}^{(1)}_{N-\sigma}(\omega_j) \\ \eta^{(1)\dagger}_{N-\sigma}(\omega_j) &= \frac{1}{\omega_j - Tr^{D}_{N-\sigma}(H^{(1)}\hat{n}_{N-\sigma})}c^{\dagger}_{N-\sigma}T^{(1)}_{N-\sigma,e-h} \\ T^{(1)}_{N-\sigma,e-h} &= Tr_{N-\sigma}(H^{(1)}c_{N-\sigma}). \end{aligned} \quad (87)$$

This transition operator has a block form given by $\eta^{(1)\dagger}_{N-\sigma} = \eta^{(1)\dagger}_{1_{N\sigma}N-\sigma}\oplus\eta^{(1)\dagger}_{0_{N\sigma}N-\sigma}$ where,

$$\begin{aligned} \eta^{(1)\dagger}_{(1,0)_{N\sigma}N-\sigma} &= \sum_{j=1}^{2^{2N-2}}\eta^{(1)\dagger}_{(1,0)_{N\sigma}N-\sigma}(\omega_j)\hat{O}^{(1)}_{N-\sigma}(\omega_j) \\ \eta^{(1)\dagger}_{(1,0)_{N\sigma},N-\sigma}(\omega_j) &= \frac{1}{\omega_j - Tr^{D}_{N-\sigma}(H^{(1)}_{(1,0)_{N\sigma}}\hat{n}_{N-\sigma})} \\ &\quad\times c^{\dagger}_{N-\sigma}T^{(1)}_{1_{N\sigma},N-\sigma,e-h} \\ T^{(1)}_{(1,0)_{N\sigma},N-\sigma,e-h} &= Tr_{N-\sigma}(H^{(1)}_{(1,0)_{N\sigma}}c_{N-\sigma})\ . \end{aligned} \quad (88)$$

The new blocks in $H^{(2)}$ eq(85) is given by,

$$\begin{aligned} H^{(2)} &= \frac{1}{2}Tr_{N-\sigma}(H^{(1)}) + \left(\hat{n}_{N\sigma}-\frac{1}{2}\right) \\ &\times\Big[c^{\dagger}_{N\sigma}Tr_{N\sigma}(H^{(1)}c_{N\sigma})G^{(1)}_{h}(\hat{\omega}_{N\sigma})Tr_{N\sigma}(c^{\dagger}_{N\sigma}H^{(1)})c_{N\sigma} \\ &+Tr_{N\sigma}(c^{\dagger}_{N\sigma}H^{(1)})c_{N\sigma}G^{(1)}_{e}(\hat{\omega}_{N\sigma})c^{\dagger}_{N\sigma}Tr_{N\sigma}(H^{(1)}c_{N\sigma})\Big]. \end{aligned} \quad (89)$$

Halving the frequency channel count The matrix structure of $\eta^{(0)\dagger}_{N\sigma}$ and $\eta^{(1)\dagger}_{N-\sigma}$ are given as ,

$$\begin{aligned} \eta^{(0)\dagger}_{N\sigma} &= \sum_{j=1}^{2^{2N-1}}\frac{1}{\omega_j - Tr^{D}_{N\sigma}(H^{(0)}\hat{n}_{N\sigma})}T^{(0)\dagger}_{N\sigma,e-h}c_{N\sigma}\hat{O}^{(0)}_{N\sigma}(\omega_j) \\ \eta^{(1)\dagger}_{N-\sigma} &= \sum_{j=1}^{2^{2N-2}}\frac{1}{\omega_j - Tr^{D}_{N-\sigma}(H^{(1)}\hat{n}_{N\sigma})}T^{(1)\dagger}_{N\sigma,e-h}c_{N\sigma}\hat{O}^{(1)}_{N-\sigma}(\omega_j)\ . \end{aligned} \quad (90)$$

Note that $H^{(1)} = \sum_{j=1}^{2^{2N-1}}H^{(1)}(\omega_j)\hat{O}^{(0)}_{N\sigma}(\omega_j)$ where the number of frequency channels were 2^{2N-1} in the 2nd step of block diagonalization of node $N-\sigma$ that reduced to 2^{2N-2}, this is an outcome of the fact that largest dimension of the nontrivial blocks reduced by half from $dim(H^{(1)}_{1_{N\sigma}}) = 2^{2N-1}\to dim(H^{(2)}_{1_{N-\sigma}}) = 2^{2N-2}$. Operationally to perform this iterative block diagonalization based RG procedure we have started from a set of 2^{2N-1} numbers chosen using the scheme given in the earlier paragraph and then next of frequency is completely determined by it,

$$\begin{pmatrix} \omega_1 \\ \omega_2 \\ \vdots \\ \omega_{2^{2N-2}} \\ \omega_{2^{2N-2}+1} \\ \vdots \\ \omega_{2^{2N-1}-1} \\ \omega_{2^{2N-1}} \end{pmatrix} \to \begin{pmatrix} \omega'_1+\delta \\ \omega'_2+\delta \\ \vdots \\ \omega'_{2^{2N-2}}+\delta \\ \omega'_{2^{2N-2}+1}-\delta \\ \vdots \\ \omega'_{2^{2N-1}-1}-\delta \\ \omega'_{2^{2N-1}}-\delta \end{pmatrix} \to \begin{pmatrix} \omega'_1 \\ \omega'_2 \\ \vdots \\ \omega'_{2^{2N-2}} \end{pmatrix} \quad (91)$$

here $\delta = \frac{1}{2}(\omega_{2^{2N-2}+j}-\omega_j)$. With the above scheme effective Hamiltonian blocks in the next steps are given by,

$$H^{(2)} = \sum_{j=1}^{2^{2N-2}}H^{(2)}(\omega'_j)\hat{O}^{(1)}_{N-\sigma}(\omega'_j)\ . \quad (92)$$

In the next paragraph we show the outcome of iteratively doing **FBD** acronymed **IFBD** for k steps.

Renormalization step k (IFBD) of node $2N-k,\sigma$ The kth step Hamiltonian is connected to the k-1th step by the following iterative equation,

$$H^{(k)} = U^{(k-1)}_{n\sigma}H^{(k-1)}U^{(k-1)\dagger}_{n\sigma}\ . \quad (93)$$

The Unitary operator $U^{(k-1)}_{2N-k\sigma} = \exp(i\theta^{(k-1)})$, $\theta^{(k-1)} = \arctan(i(\eta^{(k-1)}_{2N-k\sigma}-\eta^{(k-1)\dagger}_{2N-k\sigma}))$ for the kth step is defined following eq(86) as,

$$U^{(k-1)}_{2N-k\sigma} = U^{(k-1)}_{1_{2N-k+1,-\sigma};2N-k\sigma}\oplus U^{(k-1)}_{0_{2N-k+1,-\sigma};\sigma}\ . \quad (94)$$

Where the electron and hole transition operators composing $U^{(k-1)}_{2N-k\sigma}$ is defined as,

$$\begin{aligned} \eta^{(k-1)}_{2N-k\sigma} &= \sum_{j=1}^{2^k}\frac{1}{\omega_j - Tr^{D}_{2N-k\sigma}(H^{(k-1)}\hat{n}_{2N-k\sigma})} \\ &\quad\times Tr_{2N-k\sigma}(c^{\dagger}_{2N-k\sigma}H^{(k-1)})c_{2N-k\sigma}\hat{O}^{(k-1)}_{2N-k\sigma}\ . \end{aligned} \quad (95)$$

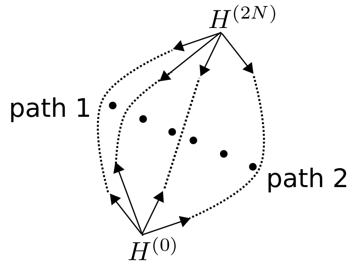

FIG. 5. Paths 1 to $(2N-1)!$ denotes the various ways of arranging the Unitary operations from one node to the next in order to reach the final diagonal Hamiltonian $H^{(2N)}$ from $H^{(0)}$.

The set of $\omega's$ maps to the next set of $\omega's$ using the scheme described in eq(91).

The completely diagonal Hamiltonian

The complete number diagonal Hamiltonian is attained in n-steps given by,

$$\begin{aligned} H^{(2N)} &= U^{(2N-1)}_{1-\sigma} H^{(2N-1)} U^{(2N-1)\dagger}_{1-\sigma} \\ &= [U^{(2N-1)}_{1\sigma} \dots U^{(0)}_{N\sigma}] H^{(0)} [U^{(2N-1)}_{1\sigma} \dots U^{(0)}_{N\sigma}]^{\dagger} \ . \end{aligned} \tag{96}$$

This number diagonal Hamiltonian can be as a collection of 2^{2N} number diagonal strings written using the operators eq(79),

$$H^{(2N)} = \sum_{l,\mathcal{P}_l} Tr(H^{(2N)} \hat{B}_{\mathcal{P}_l}) \hat{B}_{\mathcal{P}_l} \ . \tag{97}$$

This Hamiltonian commutes with $2N$ Hermitian operators $[H^{(2N)}, \hat{n}_{j\sigma}] = 0, \forall j \in [1,N]\times[\sigma,-\sigma]$. This Unitary operation's logarithm can be taken to get the generator of this rotation,

$$\begin{aligned} U^{(2N-1)}_{1\sigma} \dots U^{(0)}_{N\sigma} &= \tilde{U}_{[1,2N]} = \exp\left(i\hat{G}\right) \ , \\ \hat{G}_{[1,2N]} &= -i \log\left(\tilde{U}_{[1,2N]}\right) \ . \end{aligned} \tag{98}$$

The net unitary transformation can be done as a product of infinitesimal rotations $\delta\theta$ on the configuration space as,

$$\begin{aligned} \tilde{U}_{[1,2N]} &= \lim_{L\to\infty} \left[\hat{U}_{[1,2N]}(\delta\theta)\right]^L = \lim_{L\to\infty} \left[1 + \delta\theta \hat{G}_{[1,2N]}\right]^L \ , \\ L\delta\theta &= 1 \\ \hat{U}_{[1,2N]}(\delta\theta) &= \exp\left[i\delta\theta \hat{G}_{[1,2N]}\right] \ . \end{aligned} \tag{99}$$

The generator of the infinitesimal Unitary operation $\hat{G}_{[1,2N]}$ can now be related to the generator of continuous unitary transformations based renormalization group introduced by Wegner, Glazek, Wilson,

$$\begin{aligned} H(\delta\theta) &= \hat{U}_{[1,2N]}(\delta\theta) \hat{H} \hat{U}^{\dagger}_{[1,2N]}(\delta\theta) \\ &= \hat{H} + i\delta\theta \left[\hat{G}_{[1,2N]}, \hat{H}\right] \\ \frac{dH(\theta)}{d\theta} &= i \left[\hat{G}_{[1,2N]}, \hat{H}(\theta)\right] \ . \end{aligned} \tag{100}$$

The completely number diagonal Hamiltonian $H^{(2N)}$ can be reached from $H^{(0)}$ in $(2N-1)!$ different ways depending on how the Unitary operations are arranged. The jth path for example can be association with the jth permutation of the unitary operator set $\prod_{l=1}^{2N} U_{\mathcal{P}_j(l)}$. The figure fig5 shows path-1 and path-2 in the family of journey paths from $H^{(0)}$ to $H^{(2N)}$.