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, 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,

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

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

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

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 $N\sigma$,

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

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

$$\eta_1^\dagger\eta_1 = \hat{n}_1, \tag{38}$$

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,

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

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

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

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

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

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

$$\hat{\omega}\hat{n}_1 + \hat{\omega}'(1-\hat{n}_1) = (V-2\mu)\hat{n}_1\hat{n}_2 + (t-\mu)\hat{n}_1(1-\hat{n}_2) + (-t-\mu)\hat{n}_2(1-\hat{n}_1)$$

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,

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

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.