Algorithm for 2d Hubbard model analysis on square lattice

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The model

$$\begin{aligned}\hat{H} &= \sum_{\mathbf{k}\sigma}(\epsilon_{\mathbf{k}\sigma}-\mu)\hat{n}_{\mathbf{k}\sigma}+U_0\sum_{\mathbf{i}}\hat{n}_{\mathbf{i}\sigma}\hat{n}_{\mathbf{i}-\sigma}\\ &= \sum_{\mathbf{k}\sigma}(\epsilon_{\mathbf{k}\sigma}-\mu_{eff})\hat{n}_{\mathbf{k}\sigma}+U_0\sum_{\mathbf{i}}\left(\hat{n}_{\mathbf{i}\sigma}-\frac{1}{2}\right)\left(\hat{n}_{\mathbf{i}-\sigma}-\frac{1}{2}\right)+\frac{U}{4}\text{Vol}\end{aligned} \quad (1)$$

The half filled Hubbard model ($\mu=\frac{U_0}{2}\equiv\mu_{eff}=0$) There are $4N^2$ electrons and $4N^2$ sites (i.e. $8N^2$ states) therefore filling is $\nu=\frac{4N^2}{8N^2}=\frac{1}{2}$,

Step-1 Focussing on the Fermi surface Geometry

Capture the square Fermi surface (F) defined as a collection of wave-vectors $\mathbf{k}_F(\hat{s})$ (where $\hat{s}$ parametrizes the Fermi surface) such that $\epsilon_{\mathbf{k}_F(\hat{s})}=E_F=\mu_{eff}$ where $\mu_{eff}=-\frac{U_0}{2}$ and define all the wave-vectors as ,

$$\mathbf{k}_{\Lambda\hat{s}} = \mathbf{k}_{F\hat{s}}+\Lambda\hat{s}\ ,\ \hat{s}\in\left\{\hat{s}_i=\frac{\nabla\epsilon_{\mathbf{k}}}{|\nabla\epsilon_{\mathbf{k}}|}|_{\mathbf{k}\to\mathbf{k}_{Fi}},\epsilon_{\mathbf{k}_{Fi}}=0\ ,\ i=[1,N_F]\right\}\ , \quad (2)$$

with N_F being the number of points in F. This way we use the Fermi surface as a reference to characterize all wave-vector directions on the Fermi surface, where $\hat{s}$ provides the orientation of wave-vectors and Λ provides the distance from the Fermi surface. The creation/annihilation operator in terms of this indexes is given by $c^\dagger_{\mathbf{k}_{\Lambda\hat{s}}\sigma}=c^\dagger_{\Lambda\hat{s}\sigma}$.

Step-2 Forming most relevant(*problem dependent*) pseudospin subspaces

We now define (1/2) doublon-holon or two spinon pseudospin vectors using e-e ($f^{c\dagger}_{\Lambda\hat{s}}$) or e-h ($f^{s\dagger}_{\Lambda\hat{s}}$) pseudospinors as,

$$\begin{aligned}f^{c\dagger}_{\Lambda,\hat{s}} &= (c^\dagger_{\Lambda\hat{s}\uparrow}\ \ c_{-\Lambda T\hat{s}\downarrow})\ ,\ f^{s\dagger}_{\Lambda,\hat{s}}=(c^\dagger_{\Lambda\hat{s}\uparrow}\ \ c^\dagger_{-\Lambda T\hat{s}\downarrow})\\ \mathbf{C}_{\Lambda,\hat{s}} &= f^{c\dagger}_{\Lambda\hat{s}}\frac{\sigma}{2}f^{c\dagger}_{\Lambda\hat{s}}\ ,\ \mathbf{S}_{\Lambda,\hat{s}}=f^{s\dagger}_{\Lambda\hat{s}}\frac{\sigma}{2}f^{s\dagger}_{\Lambda\hat{s}}\ ,\quad\text{where } T(s_x,s_y)=(s_y,s_x)\end{aligned} \quad (3)$$

The total momentum of the doublon-holon pseudospin states are given by,

$$\begin{aligned}\mathbf{k}_{\Lambda\hat{s}} + \mathbf{k}_{-\Lambda T\hat{s}} &= (k_{F\hat{s},x} + k_{F\hat{s},y})\hat{x} + (k_{F\hat{s},x} + k_{F\hat{s},y})\hat{y} \\ &+ \Lambda(s_x - s_y)\hat{x} + \Lambda(s_y - s_x)\hat{y}\end{aligned} \tag{4}$$

therefore in the $\mathbf{Q}_1 = (\pi,\pi)$ direction the total momentum is ,

$$(\mathbf{k}_{\Lambda\hat{s}} + \mathbf{k}_{-\Lambda T\hat{s}}) \cdot \hat{\mathbf{Q}}_1 = \mathbf{Q}_1 \ . \tag{5}$$

Using the C_4 symmetry of the square lattice all the other pairs about the reciprocal lattice vectors $-\mathbf{Q}_1$ and $\pm\mathbf{Q}_2$ can be also generated.

Justification behind defining such pairs

The $f^{c\dagger}_{\Lambda,\hat{s}}$ pairs with momenta $\mathbf{k}_{\Lambda_0}(\hat{s}), \mathbf{k}_{-\Lambda_0}(T\hat{s})$ are maximally prone to nesting via the **Umklapp scattering event**. To observe that we sum over the 2nd order transition matrix element connecting the nested surfaces $\hat{s} \to -\hat{s}$ via all possible pairs with total momenta along nodal direction given by $(\mathbf{k}_{\Lambda+\delta\Lambda,\hat{s}} + \mathbf{k}_{-\Lambda,T\hat{s}}) \cdot \hat{\mathbf{Q}}_1 = 2\pi + \delta\Lambda$,

$$\begin{aligned}\lim_{\Omega\to 0} T^{(2),\delta\Lambda_0}_{\hat{s}\to-\hat{s}}(\Omega) &= \lim_{\Omega\to 0} \sum_{\Delta\epsilon^{pair}_{\Lambda,\delta\Lambda}(\hat{s}) = \Delta\epsilon^{pair}_{\Lambda,\delta\Lambda 0}(\hat{s})}^{W} \frac{U^2}{\Omega - \Delta\epsilon^{pair}_{\Lambda,\delta\Lambda}(\hat{s})} \ , \ \text{bandwidth } W \\ &= \frac{U^2}{W} \ln \frac{W}{\Delta\epsilon^{pair}_{\Lambda,\delta\Lambda}(\hat{s})} \ , \\ \Delta\epsilon^{pair}_{\Lambda,\delta\Lambda}(\hat{s}) &= (\epsilon_{\Lambda\hat{s}} + \epsilon_{-\Lambda+\delta\Lambda T\hat{s}}) - (\epsilon_{-\Lambda-\hat{s}} + \epsilon_{\Lambda-\delta\Lambda T\hat{s}}) \ .\end{aligned} \tag{6}$$

The transition matrix has a leading order logarithmic divergence with the branch cut located along the line $\delta\Lambda = 0$ indicating the **resonant pairs**$(\delta\Lambda = 0)$ as against the off-resonant pairs$(\delta\Lambda \neq 0)$ most susceptible to the umklapp instability. A similar instability can be shown due to **spin backscattering** across the Fermi surface for the pairs $f^{s\dagger}_{\Lambda,\hat{s}}$. This completes our justification in choosing the resonant pairs for the basis formation.

resonant pairs = doublon-holon or two spinon pseudospins

Completeness relation in the pseudospin basis

The pair of single electronic Hilbert spaces $|n_{\Lambda,\hat{s};\sigma}\rangle$ belongs to $(2\times 2 = 4)$ possible configurations i.e. $\{n_{\Lambda,\hat{s};\sigma}, n_{-\Lambda,\hat{s};-\sigma}\} = [(0,0),(1,0),(0,1),(1,1)]$. These can be recasted as eigenstates of a pair of $(S = \frac{1}{2})$ pseudospin operators $\mathbf{S}_{\Lambda,\hat{s}}, \mathbf{C}_{\Lambda,\hat{s}}$ in the following way,

$$\{n_{\Lambda,\hat{s};\sigma}, n_{-\Lambda,\hat{s};-\sigma}\} = \{\{|S^z_{\Lambda,\hat{s}} = \pm\frac{1}{2}\rangle\}, \{|C^z_{\Lambda,\hat{s}} = \pm\frac{1}{2}\rangle\}\} \ . \tag{7}$$

The commutation relations satisfied by this pseudospins are as follows,

$$[S^i_{\Lambda,\hat{s}}, S^j_{\Lambda',\hat{s}'}] = i\delta_{\Lambda\Lambda'}\delta_{oo'}\epsilon^{ijk}S^k_{\Lambda,\hat{s}} \ , \ [C^i_{\Lambda,\hat{s}}, C^j_{\Lambda',\hat{s}'}] = i\delta_{\Lambda\Lambda'}\delta_{\hat{s}\hat{s}'}\epsilon^{ijk}C^k_{\Lambda,\hat{s}} \ , \ [S^i_{\Lambda,\hat{s}}, C^j_{\Lambda,\hat{s}}] = 0 \tag{8}$$

For this pair of states the completeness relation can be recasted in terms of the spin pseudospin operators,

$$\begin{aligned} I_{\Lambda,\hat{s}} &= \sum_{n_{\Lambda,\hat{s};\sigma}, n_{-\Lambda,\hat{s};-\sigma}} |n_{\Lambda,\hat{s};\sigma}, n_{-\Lambda,\hat{s};-\sigma}\rangle\langle n_{\Lambda,\hat{s};\sigma}, n_{-\Lambda,\hat{s};-\sigma}| \\ &= (\hat{n}_{\Lambda,\hat{s};\sigma} + \hat{n}_{-\Lambda,\hat{s};-\sigma} - 1)^2 + (\hat{n}_{\Lambda,\hat{s};\sigma} - \hat{n}_{-\Lambda,\hat{s};-\sigma})^2 \\ &= \frac{4}{3}(\mathbf{S}^2_{\Lambda,\hat{s}} + \mathbf{C}^2_{\Lambda,\hat{s}}) \end{aligned} \tag{9}$$

Therefore the complete set of states can be recomposed in terms of a direct product of the two electronic state subspaces in the following fashion,

$$I_{tot} = \prod_{\substack{\mathbf{k}_{\Lambda\hat{s}} \in BZ \\ \hat{s} \in F}} I_{\Lambda,\hat{s}} = \left(\frac{4}{3}\right)^{4N^2} \prod_{\substack{\mathbf{k}_{\Lambda\hat{s}} \in BZ \\ \hat{s} \in F}} (\mathbf{S}^2_{\Lambda\hat{s}} + \mathbf{C}^2_{\Lambda,\hat{s}}) \ . \tag{10}$$

Total number operator is connected to the net pseudospin angular momentum operator in the following way

$$\hat{N}_{tot} = \sum_k \hat{n}_{k\sigma} = \frac{1}{2} \sum_{\substack{\mathbf{k}_{\Lambda\hat{s}} \in BZ, \\ \hat{s}}} (C^z_{\Lambda,\hat{s}} + S^z_{\Lambda,\hat{s}} + 1), \tag{11}$$

from here one can confirm that the eigenvalue of the total number operator $\hat{N}$ is indeed $\hat{N}_{tot}|\mathbf{P}_{cm} = 0, N_e, \mathrm{NFS}\rangle = 4N^2|\mathbf{P}_{cm} = 0, N_e, \mathrm{NFS}\rangle$ such that it reproduces the value $4N^2$ and hence the half filling condition $\nu = \frac{4N^2}{8N^2} = \frac{1}{2}$.

All statements below are problem independent.

Step-3 Recasting the Hamiltonian in the projected subspace of resonant pairs

Recasting the Kinetic energy term in the pseudospin basis

The kinetic energy Hamiltonian in terms of the pseudospin operators is rewritten as ,

$$\sum_{\Lambda\hat{s}\sigma} \epsilon_{\Lambda\hat{s}\sigma}\hat{n}_{\Lambda,\hat{s},\sigma} = \sum_{\Lambda\hat{s}} \epsilon^c_{\Lambda\hat{s}} C^z_{\Lambda\hat{s}} + \epsilon^s_{\Lambda\hat{s}} S^z_{\Lambda\hat{s}} \tag{12}$$

here ,$\epsilon^{c,s}_{\Lambda,\hat{s}} = \epsilon_{\Lambda\hat{s}} \pm \epsilon_{-\Lambda T\hat{s}}$.

Manybody eigenbasis constituting $4N$ electrons in the pseudospin language

The complete basis set of all possible manybody wavefunctions constituting $N_e = 4N$ occupied electronic states among $8N$ total single fermion states with total spin angular momentum $\mathbf{S} = \sum_{\mathbf{r}} \mathbf{S}_{\mathbf{r}} = 0$, $\mathbf{S}_{\mathbf{r}} = (c^{\dagger}_{\mathbf{r}\sigma}\ c^{\dagger}_{\mathbf{r}-\sigma})\boldsymbol{\sigma}(c_{\mathbf{r}\sigma}\ c_{\mathbf{r}-\sigma})^T$ in the pseudospin language is given by,

$$\mathcal{B}_{4N,\mathbf{S}=0} = \{\prod_{\Lambda,o} \delta_{(\hat{N}_{tot}-4N)|C_{\Lambda,\hat{s}},C^z_{\Lambda,\hat{s}};S_{\Lambda,\hat{s}},S^z_{\Lambda,\hat{s}}\rangle=0}|C_{\Lambda,\hat{s}},C^z_{\Lambda,\hat{s}};S_{\Lambda,\hat{s}},S^z_{\Lambda,\hat{s}}\rangle\}\ ,\ \mathbf{C}^2_{\Lambda,\hat{s}} + \mathbf{S}^2_{\Lambda,\hat{s}} = \frac{3}{4} \tag{13}$$

Projecting Hamiltonian onto resonant pairs scattering subspace

We will now project onto a reduced set of basis states in which the charge and spin pseudospin are only globally entangled leading to dynamics of the pairs $C_{\Lambda,\hat{s}}$,$S_{\Lambda,\hat{s}}$ that are connected to there partner pairs around the Fermi surface $C_{\Lambda,\hat{s}}$,$S_{\Lambda,\hat{s}}$,

$$\begin{aligned}\hat{P}^{(2)} &= \sum_{\{C^z_{\Lambda,\hat{s}}\}}\prod_{\Lambda,\hat{s}}|C_{\Lambda,\hat{s}}=\frac{1}{2},C^z_{\Lambda,\hat{s}};S_{\Lambda,\hat{s}}=0\rangle\prod_{\Lambda,\hat{s}}\langle C_{\Lambda,\hat{s}}=\frac{1}{2},C^z_{\Lambda,\hat{s}};S_{\Lambda,\hat{s}}=0| \\ &+ \sum_{\{S^z_{\Lambda,\hat{s}}\}}\prod_{\Lambda,\hat{s}}|C_{\Lambda,\hat{s}}=0;S_{\Lambda,\hat{s}}=\frac{1}{2},S^z_{\Lambda,\hat{s}}\rangle\prod_{\Lambda,\hat{s}}\langle C_{\Lambda,o}=0;S_{\Lambda,\hat{s}}=\frac{1}{2},S^z_{\Lambda,\hat{s}}|\ ,\end{aligned} \tag{14}$$

obeying momentum conservation.

Hubbard interaction in the pseudospin basis $\hat{P}^{(2)}$

The Hubbard interaction in the two particle projected pseudospin basis is given as,

$$\begin{aligned}\hat{P}^{(2)}_{C,S}\left[U_0\sum_{i=1}^{2N}\left(n_{i\uparrow}-\frac{1}{2}\right)\left(n_{i\downarrow}-\frac{1}{2}\right)\right]\hat{P}^{(2)} &= \frac{U_0}{4N^2}\left(\sum_{\Lambda\Lambda',\hat{s}\hat{s}'}\mathbf{C}_{\Lambda,\hat{s}}\cdot\mathbf{C}_{\Lambda',\hat{s}'}+\mathbf{S}_{\Lambda,\hat{s}}\cdot\mathbf{S}_{\Lambda',\hat{s}'}\right)\ , \\ &= V_0(\mathbf{C}^2+\mathbf{S}^2)\ ,\ V_0=\frac{U_0}{4N^2}\end{aligned} \tag{15}$$

where $\mathbf{C} = \sum_{\Lambda,\hat{s}} \mathbf{C}_{\Lambda,\hat{s}}, \mathbf{S} = \sum_{\Lambda,o} \mathbf{S}_{\Lambda,\hat{s}'}$ are the total (charge/spin) pseudospin angular momentum operators.

Reduced Hamiltonian in the resonant pairs basis is therefore given by

The complete Hamiltonian in the two particle projected subspace can be written in the following way,

$$\begin{aligned}\hat{H}^{(2)}_{C,S} &= \sum_{\Lambda\hat{s}\neq\hat{T}s}\epsilon^c_{\Lambda,\hat{s}}(C^z_{\Lambda,\hat{s}}+C^z_{\Lambda,T\hat{s}}+C^z_{\Lambda,-\hat{s}}+C^z_{\Lambda,-T\hat{s}})+\epsilon^s_{\Lambda,\hat{s}}(S^z_{\Lambda,\hat{s}}+S^z_{\Lambda,T\hat{s}}+S^z_{\Lambda,-\hat{s}}+S^z_{\Lambda,-T\hat{s}}) \\ &+ \frac{V_0}{4}\left[\sum_{\Lambda\hat{s}\neq T\hat{s}}(\mathbf{C}_{\Lambda\hat{s}}+\mathbf{C}_{\Lambda T\hat{s}})\right]^2+\frac{V_0}{4}\left[\sum_{\Lambda\hat{s}\neq T\hat{s}}(\mathbf{S}_{\Lambda\hat{s}}+\mathbf{S}_{\Lambda T\hat{s}})\right]^2\end{aligned} \tag{16}$$

Step-4 Exact '0' energy wavefunctions for the resonant pair reduced Hamiltonian The reduced Hamiltonian $\hat{H}^{(2)}_{C,S}$ has a family of eigenstates in order to tabulate them we define the following momentum space singlets formed with doublon-holon or two spinon pseudospins ,

$$\begin{aligned}|\pm,\Lambda_{\hat{s},T\hat{s}}\rangle &= \frac{1}{\sqrt{2}}\left[|\mathbf{C}_{\Lambda\hat{s}}+\mathbf{C}_{\Lambda T\hat{s}}=0\rangle \pm |\mathbf{S}_{\Lambda\hat{s}}+\mathbf{S}_{\Lambda T\hat{s}}=0\rangle\right] \\ |\pm,\Lambda_{\hat{s},-T\hat{s}}\rangle &= \frac{1}{\sqrt{2}}\left[|\mathbf{C}_{\Lambda\hat{s}}+\mathbf{C}_{\Lambda -T\hat{s}}=0\rangle \pm |\mathbf{S}_{\Lambda\hat{s}}+\mathbf{S}_{\Lambda -T\hat{s}}=0\rangle\right] \end{aligned} \tag{17}$$

The many body eigenstates can be written down in terms of this singlets as,

$$|\{\{\Lambda_{\hat{s},T\hat{s},o}\}_{p_{\hat{s},o}}\}_{N_F}\ ;\ \{\{\Lambda_{\hat{s},-T\hat{s},o}\}_{q_{\hat{s},o}}\}_{N_F}\rangle = \prod_{\substack{j=1 \\ \hat{s}\in\{\hat{s}_i;i=[1,N_F]\}}}^{p_{\hat{s},o}} |o,\Lambda_j,\hat{s},T\hat{s}\rangle \prod_{\substack{j=1 \\ \hat{s}\in\{\hat{s}_i;i=[1,N_F]\}}}^{q_{\hat{s},o}} |o,\Lambda_j,\hat{s},-T\hat{s}\rangle\ , \tag{18}$$

Step-5 Renormalization Group procedure

Choosing the form for the many-body wave functions

The many body wave-function is formed in such a way that the longitudinal (i.e. forward and backward), tangential scattering can be independently handled.

step-1

To focus on forward and backward scattering events along a given direction along FS i.e. $\hat{s}$, freeze all tangential scattering dynamics in the other directions i.e. $\hat{s}\rightarrow\hat{s}'$ this can be done by writing the part of the many body wave-function susceptible towards longitudinal scattering in the following way,

Forward Scattering

$$\begin{aligned}|\Psi^{fwd}_{long}(E),\{m\}_{N_F}\rangle &= \frac{1}{\sqrt{N_F}}\sum_{\hat{s}}\Bigg[\underbrace{\prod_{\substack{j=0, \\ \hat{s}'\neq\hat{s}}}^{N}|\mathbf{C}_{\Lambda_j\hat{s}'}+\mathbf{C}_{\Lambda_j T\hat{s}'}=0\rangle + \prod_{\substack{j=0, \\ \hat{s}'\neq\hat{s}}}^{N}|\mathbf{S}_{\Lambda_j\hat{s}'}+\mathbf{S}_{\Lambda_j T\hat{s}'}=0\rangle}_{\text{Freeze backward/tangential dynamics from } \hat{s}\to\hat{s}' \text{ in doublon-holon or two spinon channel}} \Bigg] \\ &\quad \otimes\Big(a_{m_{\hat{s}}+1}|\Psi_{N-1,\hat{s}},m_{\hat{s}}+1\rangle\,|p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle + a_{m_{\hat{s}}}|\Psi_{N-1,\hat{s}},m_{\hat{s}}\rangle\,|p,\Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle\Big)\ , \\ |p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle &= \sqrt{p}|\downarrow^c_{\Lambda_N\hat{s}}\downarrow^c_{\Lambda_N T\hat{s}}\rangle + \sqrt{1-p}|\downarrow^s_{\Lambda_N\hat{s}}\downarrow^s_{\Lambda_N T\hat{s}}\rangle \\ |p,\Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle &= \sqrt{p}|\uparrow^c_{\Lambda_N\hat{s}}\downarrow^c_{\Lambda_N T\hat{s}}\rangle + \sqrt{1-p}|\uparrow^s_{\Lambda_N\hat{s}}\downarrow^s_{\Lambda_N T\hat{s}}\rangle \end{aligned} \tag{19}$$

The $H^{(2)}_{C,S}$ in this basis simplifies to a Hamiltonian $H^{(2)}_{C,S,fwd}$ for forward scattering in every direction,

$$\begin{aligned}H^{(2)}_{C,S,fwd} &= \sum_{\hat{s}} H^{(2)}_{C,S,fwd,\hat{s}}\ ,\ H^{(2)}_{C,S,\hat{s},fwd} = \sum_{\Lambda}\epsilon^c_{\Lambda\hat{s}}(C^z_{\Lambda\hat{s}}+C^z_{\Lambda T\hat{s}}) + \epsilon^s_{\Lambda\hat{s}}(S^z_{\Lambda\hat{s}}+S^z_{\Lambda T\hat{s}}) \\ &\quad +\frac{V_0}{4}\left[\sum_{\Lambda}\mathbf{C}_{\Lambda\hat{s}}+\mathbf{C}_{\Lambda T\hat{s}}\right]^2 + \frac{V_0}{4}\left[\sum_{\Lambda}\mathbf{S}_{\Lambda\hat{s}}+\mathbf{S}_{\Lambda T\hat{s}}\right]^2\ . \end{aligned} \tag{20}$$

The Hamiltonian for the forward scattering along direction $\hat{s}$ i.e. $H^{(2)}_{C,S,\hat{s},fwd}$ can be block diagonalized recursively in the following way ($H^{(2)}_{C,S,\hat{s},fwd} = H^{(2),\leq N}_{C,S,\hat{s},fwd}$) firstly by setting up the blocks ,

$$H^{(2),\leq N}_{C,S,\hat{s},fwd}|\Psi_{\leq N}, m_{\hat{s}}, \{\lambda\}\rangle = E_{m_{\hat{s}},\leq N}|\Psi_{\leq N}, m_{\hat{s}}, \{\lambda\}\rangle \text{ eigenvalue eqn for N pseudospins}$$
$$|\Psi_{\leq N}, m_{\hat{s}}, \{\lambda\}\rangle = a_{m_{\hat{s}}+1}\,|\Psi_{\leq N-1,\hat{s}}, m_{\hat{s}}+1, \{\lambda\}\rangle\,|p, \Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle + a_{m_{\hat{s}}}\,|\Psi_{\leq N-1,\hat{s}}, m_{\hat{s}}, \{\lambda\}\rangle\,|p, \Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle \quad (21)$$

The Hamiltonian for 0 to N-1 coupled blocks (i.e. the low energy sector) is given by,

$$H^{(2),\leq N-1}_{C,S,\hat{s},fwd}|\Psi_{\leq N-1}, m_{\hat{s}}, \{\lambda\}\rangle = E_{m_{\hat{s}},\leq N-1}|\Psi_{\leq N-1}, m_{\hat{s}}, \{\lambda\}\rangle \text{ eigenvalue eqn for N-1 pseudospins}$$
$$H^{(2),\leq N-1}_{C,S,\hat{s},fwd} = \sum_{j=1}^{N-1}\epsilon^c_{\Lambda_j\hat{s}}(C^z_{\Lambda_j\hat{s}} + C^z_{\Lambda_jT\hat{s}}) + \epsilon^s_{\Lambda\hat{s}}(S^z_{\Lambda_j\hat{s}} + S^z_{\Lambda_jT\hat{s}}) + \frac{V_0}{4}\left[\sum_{j=1}^{N-1}(\mathbf{C}_{\Lambda_j\hat{s}} + \mathbf{C}_{\Lambda_jT\hat{s}})\right]^2 + \frac{V_0}{4}\left[\sum_{j=1}^{N-1}(\mathbf{S}_{\Lambda_j\hat{s}} + \mathbf{S}_{\Lambda_jT\hat{s}})\right]^2 \quad (22)$$

The Hamiltonian for the Nth block (i.e. the high energy pivot) is given by,

$$H^{(2),N}_{C,S,\hat{s},fwd} = \epsilon^c_{\Lambda_N\hat{s}}(C^z_{\Lambda_N\hat{s}} + C^z_{\Lambda_NT\hat{s}}) + \epsilon^s_{\Lambda\hat{s}}(S^z_{\Lambda_N\hat{s}} + S^z_{\Lambda_NT\hat{s}}) + \frac{V_0}{4}\left[(\mathbf{C}_{\Lambda_N\hat{s}} + \mathbf{C}_{\Lambda_NT\hat{s}})\right]^2 + \frac{V_0}{4}\left[(\mathbf{S}_{\Lambda_N\hat{s}} + \mathbf{S}_{\Lambda_NT\hat{s}})\right]^2 \ . \quad (23)$$

The Hamiltonian coupling the N-1 blocks with the Nth block is given by ,

$$\begin{aligned}
H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd} &= \frac{V_0}{4}\sum_{j=1}^{N-1}(\mathbf{C}_{\Lambda_j\hat{s}} + \mathbf{C}_{\Lambda_jT\hat{s}})\cdot(\mathbf{C}_{\Lambda_N\hat{s}} + \mathbf{C}_{\Lambda_NT\hat{s}}) + \frac{V_0}{4}\sum_{j=1}^{N-1}(\mathbf{S}_{\Lambda_j\hat{s}} + \mathbf{S}_{\Lambda_jT\hat{s}})\cdot(\mathbf{S}_{\Lambda_N\hat{s}} + \mathbf{S}_{\Lambda_NT\hat{s}}) \ , \\
&= \sum_{m_{\hat{s}}}\Bigg(\left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}}|\Psi_{N-1}, m_{\hat{s}}\rangle\langle\Psi_{N-1}, m_{\hat{s}}| \otimes (|p, \Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle\langle p, \Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\,|_N + |p, \Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle\langle p, \Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\,|_N) \\
&\quad + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}-1}|\Psi_{N-1}, m_{\hat{s}}-1\rangle\langle\Psi_{N-1}, m_{\hat{s}}-1| \otimes |p, \Uparrow_{\hat{s}}\Uparrow_{T\hat{s}}\rangle\langle p, \Uparrow_{\hat{s}}\Uparrow_{T\hat{s}}\,|_N \\
&\quad + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1}|\Psi_{N-1}, m_{\hat{s}}+1\rangle\langle\Psi_{N-1}, m_{\hat{s}}+1| \otimes |p, \Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle\langle p, \Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\,|_N \\
&\quad + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1\leftarrow m_{\hat{s}}}|\Psi_{N-1}, m_{\hat{s}}+1\rangle\langle\Psi_{N-1}, m_{\hat{s}}| \otimes |p, \Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle\langle p, \Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\,|_N + h.c. \\
&\quad + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}\leftarrow m_{\hat{s}}-1}|\Psi_{N-1}, m_{\hat{s}}\rangle\langle\Psi_{N-1}, m_{\hat{s}}-1| \otimes |p, \Downarrow_{\hat{s}}\Uparrow_{T\hat{s}}\rangle\langle p, \Uparrow_{\hat{s}}\Uparrow_{T\hat{s}}\,|_N + h.c.\Bigg) \quad (24)
\end{aligned}$$

The Hamiltonian in this basis of $N-1$ blocks and the Nth block is given by ($p_c = p = 1-p_s$) ,

$$\begin{aligned}
H^{(2),N}_{C,S,\hat{s},fwd} = \sum_{m_{\hat{s}}}\Bigg[\Bigg(&\left[H^{(2),\leq N-1}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1} + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}} \\
&+ \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1}\Bigg)|\Psi_{N-1}, m_{\hat{s}}+1\rangle\langle\Psi_{N-1}, m_{\hat{s}}+1,| \otimes |p, \Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle\langle p, \Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\,|_N \\
+\Bigg(&\left[H^{(2),\leq N-1}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}} + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}} \\
&+ \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}}\Bigg)|\Psi_{N-1}, m_{\hat{s}}\rangle\langle\Psi_{N-1}, m_{\hat{s}},| \otimes |p, \Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\rangle\langle p, \Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\,|_N \\
+\sqrt{p_c}&\left[H^{(2),\leq N-1\leftrightarrow N}_{C,\hat{s},fwd}\right]_{m_{\hat{s}}+1\rightarrow m_{\hat{s}}}|\Psi_{N-1}, m_{\hat{s}}\rangle\langle\Psi_{N-1}, m_{\hat{s}}+1| \otimes |\uparrow^c_{\Lambda_N\hat{s}}\downarrow^c_{\Lambda_NT\hat{s}}\rangle\langle p, \Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\,|_N \\
+\sqrt{p_s}&\left[H^{(2),\leq N-1\leftrightarrow N}_{S,\hat{s},fwd}\right]_{m_{\hat{s}}+1\rightarrow m_{\hat{s}}}|\Psi_{N-1}, m_{\hat{s}}\rangle\langle\Psi_{N-1}, m_{\hat{s}}+1| \otimes |\uparrow^s_{\Lambda_N\hat{s}}\downarrow^s_{\Lambda_NT\hat{s}}\rangle\langle p, \Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\,|_N + h.c.\Bigg] \ . \quad (25)
\end{aligned}$$

here,

$$\left[H^{(2),\leq N-1}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1} + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1} = E_{m_{\hat{s}}+1,\leq N-1}\ ,\ \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}} = \frac{1}{4}(p_c V^c_{N\hat{s}} + p_s V^s_{N\hat{s}}) - p_c\epsilon^c_{\Lambda_N\hat{s}} - p_s\epsilon^s_{\Lambda_N\hat{s}}$$
$$\left[H^{(2),\leq N-1}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}} + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}} = E_{m_{\hat{s}},\leq N-1}\ ,\ \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}} = -\frac{1}{4}(p_c V^c_{N\hat{s}} + p_s V^s_{N\hat{s}})\ ,$$
$$\left[H^{(2),\leq N-1\leftrightarrow N}_{C,\hat{s},fwd}\right]_{m_{\hat{s}}+1\to m_{\hat{s}}} = V^c_{N\hat{s}}\langle\Psi_{N-1}, m_{\hat{s}}|C^-_{<\Lambda_N,\hat{s}}|\Psi_{N-1}, m_{\hat{s}}+1\rangle\ ,$$
$$\left[H^{(2),\leq N-1\leftrightarrow N}_{S,\hat{s},fwd}\right]_{m_{\hat{s}}+1\to m_{\hat{s}}} = V^s_{N\hat{s}}\langle\Psi_{N-1}, m_{\hat{s}}|S^-_{<\Lambda_N,\hat{s}}|\Psi_{N-1}, m_{\hat{s}}+1\rangle \tag{26}$$

Using the eigenvalue equation eq(21) and eq(25) we have the following matrix equation ,

$$\begin{pmatrix} \left[H^{(2),\leq N-1}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1} + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}} + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1} & \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1\leftarrow m_{\hat{s}}} \\ \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1\to m_{\hat{s}}} & \left[H^{(2),\leq N-1}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}} + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}} + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}} \end{pmatrix} \begin{pmatrix} a_{m_{\hat{s}}+1} \\ a_{m_{\hat{s}}} \end{pmatrix} = E_{m_{\hat{s}},\leq N} \begin{pmatrix} a_{m_{\hat{s}}+1} \\ a_{m_{\hat{s}}} \end{pmatrix} \tag{27}$$

where the column vector is represented in the ket basis ,

$$\begin{pmatrix} a_{m_{\hat{s}}+1} \\ a_{m_{\hat{s}}} \end{pmatrix} = a_{m_{\hat{s}}+1}\left|\Psi_{\leq N-1,\hat{s}}, m_{\hat{s}}+1\right\rangle \left|p, \Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}\right\rangle + a_{m_{\hat{s}}}\left|\Psi_{\leq N-1,\hat{s}}, m_{\hat{s}}\right\rangle\left|p, \Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}\right\rangle\ . \tag{28}$$

The level spacing between a eigenvalue of 2N pseudospin system and a 2N-2 pseudospin system is given by,

$$\begin{aligned} E_{m_{\hat{s}},\leq N} - E_{m_{\hat{s}},\leq N-1} &= \frac{V_0}{4} + \frac{W}{2} + \omega\ ,\ E_{m_{\hat{s}},\leq N} - E_{m_{\hat{s}}+1,\leq N-1} = \frac{V_0}{4} - \omega \\ E_{m_{\hat{s}},\leq N} &= \frac{V_0}{4} + \frac{W}{4} + \frac{1}{2}(E_{m_{\hat{s}},\leq N-1} + E_{m_{\hat{s}}+1,\leq N-1})\ , \\ E_{m_{\hat{s}}+1,\leq N-1} - E_{m_{\hat{s}},\leq N-1} &= 2\omega - \frac{W}{2} \end{aligned} \tag{29}$$

where ω is a quantum fluctuation scale and V_0 is the bare coupling strength. The characteristic polynomial from the above eq(37) ,

$$\left(\left[H^{(2),\leq N-1}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1} + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}} + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1} - E_{m_{\hat{s}},\leq N}\right)$$
$$\times\left(\left[H^{(2),\leq N-1}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}} + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}} + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}} - E_{m_{\hat{s}},\leq N}\right) = \left|\left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1\leftarrow m_{\hat{s}}}\right|^2 \tag{30}$$

Using the energy level differences in eq(29) the characteristic polynomial can be written as ,

$$\left(\omega - \frac{V_0}{4} + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}}\right)\left(\left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}} - \frac{V_0}{4} - \frac{W}{2} - \omega\right) = \left|\left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1\leftarrow m_{\hat{s}}}\right|^2 . \tag{31}$$

The characteristic polynomial leads to the following constraint ,

$$\left(\omega - \frac{V_0}{4} + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}}\right)\left(\left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}} - \frac{V_0}{4} - \frac{W}{2} - \omega\right) > 0\ . \tag{32}$$

Using eq(37) and eq(29) we have the following relation between the coefficients,

$$\frac{a_{m_{\hat{s}}+1}}{a_{m_{\hat{s}}}} = \frac{\left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1\leftarrow m_{\hat{s}}}}{\frac{V_0}{4} - \omega - \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}}}\ ,\ \frac{a_{m_{\hat{s}}}}{a_{m_{\hat{s}}+1}} = \frac{\left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}\rightarrow m_{\hat{s}}+1}}{\omega + \frac{V_0}{4} + \frac{W}{2} - \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}}} \tag{33}$$

The way the energy differences have been defined allows the condition eq(32) to be fulfilled for $-\frac{W}{2} < \omega < \frac{W}{2}$, that is the variation of kinetic energy for a single particle in the tight binding spectrum. From the above relation the normalized coefficients are determined to be,

$$a_{m_{\hat{s}}} = \sqrt{\frac{\frac{V_0}{4} - \omega - \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}}}{\frac{V_0}{2} + \frac{W}{2} - Tr_{p,\Downarrow_{T\hat{s}}}\left(H^{(2),N}_{C,S,\hat{s},fwd}\right)}}\ ,\ a_{m_{\hat{s}}+1} = \sqrt{\frac{\omega + \frac{V_0}{4} + \frac{W}{2} - Tr_{p,\Downarrow_{T\hat{s}}}\left(H^{(2),N}_{C,S,\hat{s},fwd}\right) + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}}}{\frac{V_0}{2} + \frac{W}{2} - Tr_{p,\Downarrow_{T\hat{s}}}\left(H^{(2),N}_{C,S,\hat{s},fwd}\right)}}\ . \tag{34}$$

The trace of the 2×2 equals the sum of its eigenvalues therefore using eq(29) we can determine the other eigenvalue.

$$\begin{aligned} E_{m_{\hat{s}},\leq N} &= \frac{V_0}{4} + \frac{W}{4} + \frac{1}{2}(E_{m_{\hat{s}},\leq N-1} + E_{m_{\hat{s}}+1,\leq N-1})\ , \\ E'_{m_{\hat{s}},\leq N} &= \text{sum of diagonal elements in eq(37)} - E'_{m_{\hat{s}},\leq N} \\ &= \frac{1}{2}(E_{m_{\hat{s}},\leq N-1} + E_{m_{\hat{s}}+1,\leq N-1}) - p_c\epsilon^c_{\Lambda_N\hat{s}} - p_s\epsilon^s_{\Lambda_N\hat{s}} - \frac{V_0}{4} - \frac{W}{2}\ . \end{aligned} \tag{35}$$

The coefficients for the other eigenstate is ,

$$a'_{m_{\hat{s}}} = -a^*_{m_{\hat{s}}+1}\ ,\ a'_{m_{\hat{s}}+1} = a^*_{m_{\hat{s}}} \tag{36}$$

Using this coefficients and the energy eigenvalues the 2×2 matrix can be written in a diagonal form through the unitary transformation,

$$U_{N\hat{s}}\begin{pmatrix} \left[H^{(2),\leq N-1}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1} + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}} + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1} & 0 \\ + \frac{\left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1\leftarrow m_{\hat{s}}}\left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}\leftarrow m_{\hat{s}}+1}}{\omega + \frac{V_0}{4} + \frac{W}{2} - Tr_{p,\Downarrow_{T\hat{s}}}\left(H^{(2),N}_{C,S,\hat{s},fwd}\right) + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}}} & \\ 0 & \left[H^{(2),\leq N-1}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}} + \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Uparrow_{\hat{s}}\Downarrow_{T\hat{s}}} + \left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}} \\ & + \frac{\left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}\leftarrow m_{\hat{s}}+1}\left[H^{(2),\leq N-1\leftrightarrow N}_{C,S,\hat{s},fwd}\right]_{m_{\hat{s}}+1\leftarrow m_{\hat{s}}}}{\frac{V_0}{4} - \omega - \left[H^{(2),N}_{C,S,\hat{s},fwd}\right]_{p,\Downarrow_{\hat{s}}\Downarrow_{T\hat{s}}}} \end{pmatrix} U^\dagger_{N\hat{s}}U_{N\hat{s}}\begin{pmatrix} a_{m_{\hat{s}}+1} \\ \\ a_{m_{\hat{s}}} \end{pmatrix} = E_{m_{\hat{s}},\leq N}U_{N\hat{s}}\begin{pmatrix} a_{m_{\hat{s}}+1} \\ \\ a_{m_{\hat{s}}} \end{pmatrix} \tag{37}$$

where $U_{N\hat{s}}$ is defined as ,

$$U_{N\hat{s}} = \begin{pmatrix} a_{m_{\hat{s}}} & -a^*_{m_{\hat{s}}+1} \\ a_{m_{\hat{s}}+1} & a^*_{m_{\hat{s}}} \end{pmatrix} \tag{38}$$