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1 Exact diagonalization of the two-site Hubbard model

The Hamiltonian

$$\mathcal{H} = -t \sum_{\sigma} \left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \hat{N} \tag{1}$$

I have two lattice sites, indexed by 1 and 2, occupied by electrons. μ is the chemical potential, $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are the fermionic creation and annihilation operators at the i^{th} site, with spin-index σ. σ can take values $\uparrow$ and $\downarrow$, denoting spin-up and spin-down states respectively. $\hat{n}_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the number operator for the i^{th} site and at spin-index σ; it counts the number of fermions with the designated quantum numbers. $\hat{N} = \sum_{i\sigma} \hat{n}_{i\sigma}$ is the total number operator; it counts the total number of fermions at all sites and spin-indices. t is the hopping strength; the more the t, the more are the electrons likely to hop between sites. U is the on-site repulsion cost; it represents the increase in energy when two electrons occupy the same site.

1.1 Symmetries of the problem

The following operators commute with the Hamiltonian.

1. **Total number operator**: $\left[\mathcal{H}, \hat{N}\right] = 0$.

   Proof. The last term in the Hamiltonian is the number operator itself. Ignoring that, there are three terms that I need to individually consider.

   - $c^{\dagger}_{1\sigma} c_{2\sigma}$

$$\begin{aligned} \left[c^{\dagger}_{1\sigma} c_{2\sigma}, \hat{n}_{i\sigma'}\right] &= \left[c^{\dagger}_{1\sigma} c_{2\sigma}, c^{\dagger}_{i\sigma'} c_{i\sigma'}\right] \\ &= c^{\dagger}_{1\sigma} \left[c_{2\sigma}, c^{\dagger}_{i\sigma'} c_{i\sigma'}\right] + \left[c^{\dagger}_{1\sigma}, c^{\dagger}_{i\sigma'} c_{i\sigma'}\right] c_{2\sigma} \\ &= \delta_{i,2}\, c^{\dagger}_{1\sigma} \left[c_{2\sigma}, c^{\dagger}_{2\sigma'} c_{2\sigma'}\right] + \delta_{i,1} \left[c^{\dagger}_{1\sigma}, c^{\dagger}_{1\sigma'} c_{1\sigma'}\right] c_{2\sigma} \\ &= \delta_{i,2}\, c^{\dagger}_{1\sigma} \left\{c_{2\sigma}, c^{\dagger}_{2\sigma'}\right\} c_{2\sigma'} - \delta_{i,1} c^{\dagger}_{1\sigma'} \left\{c_{1\sigma'}, c^{\dagger}_{1\sigma}\right\} c_{2\sigma} \\ &= \delta_{\sigma,\sigma'} c^{\dagger}_{1\sigma} c_{1\sigma} \left(\delta_{i,2} - \delta_{i,1}\right) \end{aligned} \tag{2}$$

     The third line follows because the electrons on different sites are distinguishable and hence, the *creation and anhillation operators of different sites will commute among themselves.* Therefore,

$$\left[c^{\dagger}_{1\sigma} c_{2\sigma}, \hat{N}\right] = \sum_{i\sigma'} \left[c^{\dagger}_{1\sigma} c_{2\sigma}, \hat{n}_{i\sigma'}\right] = c^{\dagger}_{1\sigma} c_{1\sigma} \sum_{i=\{1,2\}} \left(\delta_{i,2} - \delta_{i,1}\right) = 0 \tag{3}$$

   - $c^{\dagger}_{2\sigma} c_{1\sigma}$: Since the operator $\hat{N}$ is symmetric with respect to the site indices 1 and 2, I can go through the last proof again with the site indices 1 and 2 exchanged and since the proof does not depend on the site indices, this commutator will also be zero.
   - $\hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$:

$$\begin{aligned} \left[\hat{n}_{i\uparrow} \hat{n}_{j\downarrow}, \hat{n}_{j\sigma}\right] &= \hat{n}_{i\uparrow} \left[\hat{n}_{i\downarrow}, \hat{n}_{j\sigma}\right] - \left[\hat{n}_{i\uparrow}, \hat{n}_{j\sigma}\right] \hat{n}_{i\downarrow} \\ &= \delta_{ij} \left(\hat{n}_{i\uparrow} \left[\hat{n}_{i\downarrow}, \hat{n}_{i\sigma}\right] - \left[\hat{n}_{i\uparrow}, \hat{n}_{i\sigma}\right] \hat{n}_{i\downarrow}\right) \\ &= \delta_{ij} \left(\delta_{\sigma\uparrow} \hat{n}_{i\uparrow} \left[\hat{n}_{i\downarrow}, \hat{n}_{i\uparrow}\right] - \delta_{\sigma\downarrow} \left[\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}\right] \hat{n}_{i\downarrow}\right) \\ &= \delta_{ij} \left(\delta_{\sigma\downarrow} \hat{n}_{i\downarrow} - \delta_{\sigma\uparrow} \hat{n}_{i\uparrow}\right) \left[\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}\right] \\ &= \delta_{ij} \left(\delta_{\sigma\downarrow} \hat{n}_{i\downarrow} - \delta_{\sigma\uparrow} \hat{n}_{i\uparrow}\right) \left(c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} - c^{\dagger}_{i\downarrow} c_{i\downarrow} c^{\dagger}_{i\uparrow} c_{i\uparrow}\right) \\ &= \delta_{ij} \left(\delta_{\sigma\downarrow} \hat{n}_{i\downarrow} - \delta_{\sigma\uparrow} \hat{n}_{i\uparrow}\right) \left(c^{\dagger}_{i\downarrow} c_{i\downarrow} c^{\dagger}_{i\uparrow} c_{i\uparrow} - c^{\dagger}_{i\downarrow} c_{i\downarrow} c^{\dagger}_{i\uparrow} c_{i\uparrow}\right) = 0 \end{aligned} \tag{4}$$

     Therefore, $\left[\hat{n}_{i\uparrow} \hat{n}_{j\downarrow}, \hat{N}\right] = \sum_{j,\sigma} \left[\hat{n}_{i\uparrow} \hat{n}_{j\downarrow}, \hat{n}_{j\sigma}\right] = 0$

The total Hamiltonian is just a sum of the three terms; since the number operator commutes individually with these terms, it obviously commutes with the total Hamiltonian. □

2. **Magnetization operator**: $\hat{S}^z_{tot} \equiv \frac{1}{2}\sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$, $\left[\mathcal{H}, \hat{S}^z_{tot}\right] = 0$.

   Proof. The magnetization operator can be rewritten as $\hat{S}^z_{tot} = \frac{1}{2}\sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} - 2\hat{n}_{i\downarrow}) = \hat{N} - 2\sum_i \hat{n}_{i\downarrow}$. Since $\hat{N}$ commutes with $\mathcal{H}$, I just need to prove that $[\mathcal{H}, \sum_i \hat{n}_{i\downarrow}]$. From eq. 2,

   $$\left[c^\dagger_{1\sigma}c_{2\sigma}, \sum_i \hat{n}_{i\downarrow}\right] = c^\dagger_{1\downarrow}c_{1\downarrow}\sum_{i=\{1,2\}}(\delta_{i,2} - \delta_{i,1}) = 0 \tag{5}$$

   Again using the symmetry of the magnetization operator with the exchange of indices, its obvious that $\left[c^\dagger_{2\sigma}c_{1\sigma}, \sum_i \hat{n}_{i\downarrow}\right] = 0$

   Using eq. 4, $[\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \hat{n}_{i\downarrow}] = 0$.

   Finally, $[N, \hat{n}_{i\downarrow}] = \sum_{j\sigma}[\hat{n}_{j\sigma}, \hat{n}_{i\downarrow}] = [\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}] = c^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow} - c^\dagger_{i\downarrow}c_{i\downarrow}c^\dagger_{i\uparrow}c_{i\uparrow} = 0$. Since $\hat{S}^z_{tot}$ commutes with each part individually, it commutes with the total Hamiltonian. □

3. **Two-site parity operator** $\hat{P}$: The action of $\hat{P}$ is defined as follows. If $|\Psi_{\alpha\beta}\rangle$ is a wavefunction with site indices α and β,

   $$\hat{P}\,|\Psi(\alpha,\beta)\rangle = |\Psi(\beta,\alpha)\rangle \tag{6}$$

   That is, it operates on each electron and reverses it's site indices.

   Proof. I now rewrite the Hamiltonian by explcitly showing the two site indices:

   $$\mathcal{H}(\alpha,\beta) = -t\sum_\sigma(c^\dagger_{\alpha\sigma}c_{\beta\sigma} + c^\dagger_{\beta\sigma}c_{\alpha\sigma}) + U(n_{\alpha\uparrow}n_{\alpha\downarrow} + n_{\beta\uparrow}n_{\beta\downarrow}) - \mu\sum_\sigma(n_{\alpha\sigma} + n_{\beta\sigma}) \tag{7}$$

   Its obvious that $\mathcal{H}$ is symmetric in the site indices: $\mathcal{H}(\alpha,\beta) = \mathcal{H}(\beta,\alpha)$. This means that the eigenvalues also have this symmetry. Let $|\Phi(\alpha,\beta)\rangle$ be an eigenstate of $\mathcal{H}(\alpha,\beta)$ with eigenvalue $E(\alpha,\beta)$. Then,

   $$\begin{aligned}\hat{P}\mathcal{H}\,|\Phi(\alpha,\beta)\rangle &= E(\alpha,\beta)\hat{P}\,|\Phi(\alpha,\beta)\rangle = E(\beta,\alpha)\,|\Phi(\beta,\alpha)\rangle\\ &= \mathcal{H}\,|\Phi(\beta,\alpha)\rangle = \mathcal{H}\hat{P}\,|\Phi(\alpha,\beta)\rangle\\ \implies \mathcal{H}\hat{P}\,|\Phi(\alpha,\beta)\rangle &= \hat{P}\mathcal{H}\,|\Phi(\alpha,\beta)\rangle\end{aligned} \tag{8}$$

   Since any general wavefunction can be expanded in terms of these wavefunctions and since both the operator are linear, the above result will also hold for a general wavefunction $|\Psi(\alpha,\beta)\rangle$:

   $$\mathcal{H}\hat{P}\,|\Psi(\alpha,\beta)\rangle = \hat{P}\mathcal{H}\,|\Psi(\alpha,\beta)\rangle \implies [\mathcal{H}, \hat{P}] = 0 \tag{9}$$

   □

1.2 Partitioning the Hilbert space

THe Hamiltonian commutes with the three operators. This means that is possible to simultaneously diagonalize these four operators: $\mathcal{H}, \hat{N}, S^{tot}_z, \hat{P}$. I will be able to label the eigenstates of the total Hamiltonian using the eigenvalues of these operatos. First take the total number operator. $\hat{N}$ can take four values for a two-site system, 1 through 4. The eigenstates labelled by a particular number, say N=2 will be orthogonal to the eigenstates labelled by another number, say N=4. This means each eigenvalue of $\hat{N}$ will have a distinct subspace orthogonal to the other values of $\hat{N}$. I will be able to diagonalize each such subspace independently of each other, because they will not have any overlap. This feature enables us to block-diagonalize the total Hamiltonian into four blocks, each block belonging to each value $\hat{N}$.

Inside each block, I will be able to repeat the procedure by next using the eigenvalues of S_z^{tot}. Each block of the Hamiltonian will again break up to smaller blocks for each value of the total magnetization. The eigenvalues of parity operator provide a further partitioning of the blocks of magnetization.

From this point, all the states I will work with will necessarily be eigenfunctions of $\hat{N}$, so it doesn't make sense to keep the last term in the Hamiltonian, $\mu\hat{N}$. I redefine the Hamiltonian by absorbing this term: $\mathcal{H} \to \mathcal{H} + \mu\hat{N} = -t\sum_\sigma \left(c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}\right) + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$. This will keep the eigenvectors unaltered, but will increase the eigenvalues by μN, where N is the number of particles in the eigenstate I are considering.

1.3 N = 1

For writing the state kets, I use the following notation: $|\uparrow,\downarrow\rangle$ means electron on site 1 has spin up and that on site 2 has spin-down. $|\downarrow,0\rangle$ means electron on site 1 has spin-down and there is no electron on site 2.

For one electron on two lattice sites, I start by writing down the eigenstates of S_z^{tot}. For odd number of electrons, zero magnetization is not possible. So,

- $S_z^{tot} = -1$: $|\downarrow,0\rangle, |0,\downarrow\rangle$
- $S_z^{tot} = +1$: $|\uparrow,0\rangle, |0,\uparrow\rangle$

Each eigenvalue will have a separate subspace and can be separately diagonalized. I need to find the matrix elements of $\mathcal{H}$ in these eigenkets. Since there is no possibility of two electrons occupying same site, I ignore the U-term for the time being.

1.3.1 $S_z^{tot} = -1$

Let us first see the action of the Hamiltonian on the eigenfunctions with $S_z^{tot} = -1$.

$$\begin{aligned} \mathcal{H}|\downarrow,0\rangle &= -tc_{2\downarrow}^\dagger c_{1\downarrow}|\downarrow,0\rangle = -t|0,\downarrow\rangle \\ \mathcal{H}|0,\downarrow\rangle &= -tc_{1\downarrow}^\dagger c_{2\downarrow}|0,\downarrow\rangle = -t|\downarrow,0\rangle \end{aligned} \tag{10}$$

We get the following matrix for this tiny subspace of the Hamiltonian:

$$\begin{array}{c} \\ |\downarrow,0\rangle \\ \\ |0,\downarrow\rangle \end{array} \begin{array}{c} \begin{array}{cc} |\downarrow,0\rangle & |0,\downarrow\rangle \end{array} \\ \begin{pmatrix} 0 & -t \\ & \\ -t & 0 \end{pmatrix} \end{array} \tag{11}$$

The eigenvalues and eigenvectors of this matrix are $\frac{|\downarrow,0\rangle \pm |0,\downarrow\rangle}{\sqrt{2}}$, with eigenvalues $\mp t$. These are also the eigenvalues of the parity operator, as expected.

$$\begin{aligned} \hat{P}\left(|\downarrow,0\rangle + |0,\downarrow\rangle\right) &= |0,\downarrow\rangle + |\downarrow,0\rangle \implies \hat{P} = 1 \\ \hat{P}\left(|\downarrow,0\rangle - |0,\downarrow\rangle\right) &= |0,\downarrow\rangle - |\downarrow,0\rangle \implies \hat{P} = -1 \end{aligned} \tag{12}$$

1.3.2 $S_z^{tot} = +1$

Now I look at the spin-up states.

$$\begin{aligned} \mathcal{H}|\uparrow,0\rangle &= -tc_{2\uparrow}^\dagger c_{1\uparrow}|\uparrow,0\rangle = -t|0,\uparrow\rangle \\ \mathcal{H}|0,\uparrow\rangle &= -tc_{1\uparrow}^\dagger c_{2\uparrow}|0,\uparrow\rangle = -t|\uparrow,0\rangle \end{aligned} \tag{13}$$

Clearly, this gives the same matrix as the spin-down states:

$$\begin{array}{c} \\ |\uparrow,0\rangle \\ \\ |0,\uparrow\rangle \end{array} \begin{array}{c} \begin{array}{cc} |\uparrow,0\rangle & |0,\uparrow\rangle \end{array} \\ \begin{pmatrix} 0 & -t \\ & \\ -t & 0 \end{pmatrix} \end{array} \tag{14}$$

and hence similar eigenfunctions: $\frac{|\uparrow,0\rangle \pm |0,\uparrow\rangle}{\sqrt{2}}$, with eigenvalues $\mp t$.

1.4 N=3

I once again write down the eigenstates of S_z^{tot}, this time with three electrons.

- $S_z^{tot} = -1$: $|\uparrow\downarrow,\downarrow\rangle, |\downarrow,\uparrow\downarrow\rangle$
- $S_z^{tot} = +1$: $|\uparrow\downarrow,\uparrow\rangle, |\uparrow,\uparrow\downarrow\rangle$

1.4.1 $S_z^{tot} = -1$

$$\begin{aligned} \mathcal{H}|\uparrow\downarrow,\downarrow\rangle &= -tc^\dagger_{2\uparrow}c_{1\uparrow}|\uparrow\downarrow,\downarrow\rangle + U|\uparrow\downarrow,\downarrow\rangle = -t|\downarrow,\uparrow\downarrow\rangle + U|\uparrow\downarrow,\downarrow\rangle \\ \mathcal{H}|\downarrow,\uparrow\downarrow\rangle &= -tc^\dagger_{1\uparrow}c_{2\uparrow}|\downarrow,\uparrow\downarrow\rangle + U|\downarrow,\uparrow\downarrow\rangle = -t|\uparrow\downarrow,\downarrow\rangle + U|\downarrow,\uparrow\downarrow\rangle \end{aligned} \tag{15}$$

$$\begin{array}{c|cc} & |\uparrow\downarrow,\downarrow\rangle & |\downarrow,\uparrow\downarrow\rangle \\ \hline |\uparrow\downarrow,\downarrow\rangle & U & -t \\ |\downarrow,\uparrow\downarrow\rangle & -t & U \end{array} \tag{16}$$

This matrix has eigenvalues $U \mp t$, and corresponding eigenvectors $\frac{|\uparrow\downarrow,\downarrow\rangle \pm |\downarrow,\uparrow\downarrow\rangle}{\sqrt{2}}$

1.4.2 $S_z^{tot} = +1$

$$\begin{aligned} \mathcal{H}|\uparrow\downarrow,\uparrow\rangle &= -tc^\dagger_{2\downarrow}c_{1\downarrow}|\uparrow\downarrow,\uparrow\rangle + U|\uparrow\downarrow,\uparrow\rangle = tc^\dagger_{2\downarrow}c_{1\downarrow}|\downarrow\uparrow,\uparrow\rangle + U|\uparrow\downarrow,\uparrow\rangle \\ &= t|\uparrow,\downarrow\uparrow\rangle + U|\uparrow\downarrow,\uparrow\rangle = -t|\uparrow,\uparrow\downarrow\rangle + U|\uparrow\downarrow,\uparrow\rangle \\ \mathcal{H}|\uparrow,\uparrow\downarrow\rangle &= -tc^\dagger_{1\downarrow}c_{2\downarrow}|\uparrow,\uparrow\downarrow\rangle + U|\uparrow,\uparrow\downarrow\rangle = tc^\dagger_{1\downarrow}c_{2\downarrow}|\uparrow,\downarrow\uparrow\rangle + U|\uparrow,\uparrow\downarrow\rangle \\ &= t|\downarrow\uparrow,\uparrow\rangle + U|\uparrow,\uparrow\downarrow\rangle = -t|\uparrow\downarrow,\uparrow\rangle + U|\uparrow,\uparrow\downarrow\rangle \end{aligned} \tag{17}$$

$$\begin{array}{c|cc} & |\uparrow\downarrow,\uparrow\rangle & |\uparrow,\uparrow\downarrow\rangle \\ \hline |\uparrow\downarrow,\uparrow\rangle & U & -t \\ |\uparrow,\uparrow\downarrow\rangle & -t & U \end{array} \tag{18}$$

This matrix has eigenvalues $U \mp t$, and corresponding eigenvectors $\frac{|\uparrow\downarrow,\uparrow\rangle \pm |\uparrow,\uparrow\downarrow\rangle}{\sqrt{2}}$

1.5 N=4

With four electrons, the only possible state is $|\uparrow\downarrow,\uparrow\downarrow\rangle$. Its easy to find the eigenvalue. Since all states are filled, no hopping can take place, so the hopping term is zero. Therefore,

$$\mathcal{H}|\uparrow\downarrow,\uparrow\downarrow\rangle = 2U|\uparrow\downarrow,\uparrow\downarrow\rangle \tag{19}$$

So, $|\uparrow\downarrow,\uparrow\downarrow\rangle$ is an eigenvector with eigenvalue $2U$.

1.6 N=2

This is the eigenvalue that has the largest subspace.

- $S_z^{tot} = -1$: $|\downarrow,\downarrow\rangle$
- $S_z^{tot} = +1$: $|\uparrow,\uparrow\rangle$
- $S_z^{tot} = 0$: $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |0,\uparrow\downarrow\rangle, |\uparrow\downarrow,0\rangle$

1.6.1 $S_z^{tot} = \pm 1$

These two subspaces have a single state each, so theya are obviously eigenstates. Since they both have identical spins on both sites, the hopping term is 0, and the U-term is also zero because of single occupation. As a result, they both have zero eigenvalue

$$\mathcal{H}\left|\downarrow,\downarrow\right\rangle = \mathcal{H}\left|\uparrow,\uparrow\right\rangle = 0 \tag{20}$$

1.6.2 $S_z^{tot} = 0$

This subspace has four eigenvectors,

$$\left|\uparrow,\downarrow\right\rangle, \quad \left|\downarrow,\uparrow\right\rangle, \quad \left|0,\uparrow\downarrow\right\rangle, \quad \left|\uparrow\downarrow,0\right\rangle \tag{21}$$

so it is not possible to directly diagonalize this subspace. First we organize these states into eigenstates of parity. It is easy by inspection.

$$\begin{aligned} \hat{P}\left(\left|\uparrow,\downarrow\right\rangle \pm \left|\downarrow,\uparrow\right\rangle\right) &= \pm\left(\left|\uparrow,\downarrow\right\rangle \pm \left|\downarrow,\uparrow\right\rangle\right) \\ \hat{P}\left(\left|\uparrow\downarrow,0\right\rangle \pm \left|0,\uparrow\downarrow\right\rangle\right) &= \pm\left(\left|\uparrow\downarrow,0\right\rangle \pm \left|0,\uparrow\downarrow\right\rangle\right) \end{aligned} \tag{22}$$

I have the parity eigenstates for this subspace, so its most convenient to work in the basis of these eigenstates

- $\hat{P} = 1 : \frac{\left|\uparrow,\downarrow\right\rangle + \left|\downarrow,\uparrow\right\rangle}{\sqrt{2}}, \quad \frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}}$
- $\hat{P} = -1 : \frac{\left|\uparrow,\downarrow\right\rangle - \left|\downarrow,\uparrow\right\rangle}{\sqrt{2}}, \quad \frac{\left|\uparrow\downarrow,0\right\rangle - \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}}$

Each eigenvalue subspace can now be diagonalized separately. First I look at the eigenstates of $\hat{P} = 1$. I find the matrix of $\mathcal{H}$ in the subspace spanned by these two vectors and then diagonalize that subspace.

$$\begin{aligned} \mathcal{H}\,\frac{\left|\uparrow,\downarrow\right\rangle + \left|\downarrow,\uparrow\right\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}}\left\{\left(c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\uparrow}c_{1\uparrow}\right)\left|\uparrow,\downarrow\right\rangle + \left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right)\left|\downarrow,\uparrow\right\rangle\right\} \\ &= -\frac{t}{\sqrt{2}}\left\{\left|\downarrow\uparrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle + \left|\uparrow\downarrow,0\right\rangle + \left|0,\downarrow\uparrow\right\rangle\right\} = 0 \\ \mathcal{H}\,\frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}}\left\{\left(c^\dagger_{2\uparrow}c_{1\uparrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right)\left|\uparrow\downarrow,0\right\rangle + \left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{1\downarrow}c_{2\downarrow}\right)\left|0,\uparrow\downarrow\right\rangle\right\} + U\frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}} \\ &= -\frac{t}{\sqrt{2}}\left\{\left|\downarrow,\uparrow\right\rangle - \left|\uparrow,\downarrow\right\rangle + \left|\uparrow,\downarrow\right\rangle - \left|\downarrow,\uparrow\right\rangle\right\} + U\frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}} = U\frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}} \end{aligned} \tag{23}$$

We get the following matrix

$$\begin{array}{c|cc} & \frac{\left|\uparrow,\downarrow\right\rangle + \left|\downarrow,\uparrow\right\rangle}{\sqrt{2}} & \frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}} \\ \hline \frac{\left|\uparrow,\downarrow\right\rangle + \left|\downarrow,\uparrow\right\rangle}{\sqrt{2}} & 0 & 0 \\ \frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}} & 0 & U \end{array} \tag{24}$$

As it appears, the subspace is already diagonal in the eigenbasis of $\hat{P}$. The $\hat{P} = 1$ eigenstates are eigenstates of $\mathcal{H}$, with eigenvalues 0 and U. Next I look at the eigenstates of $\hat{P} = -1$.

$$
\begin{aligned}
\mathcal{H}\,\frac{|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}}\left\{\left(c^\dagger_{1\downarrow}c_{2\downarrow}c^\dagger_{2\uparrow}c_{1\uparrow}\right)|\uparrow,\downarrow\rangle-\left(c^\dagger_{1\uparrow}c_{2\uparrow}+c^\dagger_{2\downarrow}c_{1\downarrow}\right)|\downarrow,\uparrow\rangle\right\} \\
&= -\frac{t}{\sqrt{2}}\left\{|\downarrow\uparrow,0\rangle+|0,\uparrow\downarrow\rangle-|\uparrow\downarrow,0\rangle-|0,\downarrow\uparrow\rangle\right\} \\
&= 2t\frac{|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle}{\sqrt{2}} \\
\mathcal{H}\,\frac{|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}}\left\{\left(c^\dagger_{2\uparrow}c_{1\uparrow}+c^\dagger_{2\downarrow}c_{1\downarrow}\right)|\uparrow\downarrow,0\rangle-\left(c^\dagger_{1\uparrow}c_{2\uparrow}+c^\dagger_{1\downarrow}c_{2\downarrow}\right)|0,\uparrow\downarrow\rangle\right\}+U\,\frac{|\uparrow\downarrow,0\rangle+|0,\uparrow\downarrow\rangle}{\sqrt{2}} \\
&= -\frac{t}{\sqrt{2}}\left\{|\downarrow,\uparrow\rangle-|\uparrow,\downarrow\rangle-|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle\right\}+U\,\frac{|\uparrow\downarrow,0\rangle+|0,\uparrow\downarrow\rangle}{\sqrt{2}} \\
&= 2t\frac{|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle}{2}+U\,\frac{|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle}{\sqrt{2}}
\end{aligned}
\tag{25}
$$

$$
\begin{array}{c|cc}
 & \frac{|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle}{\sqrt{2}} & \frac{|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle}{\sqrt{2}} \\
\hline
\frac{|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle}{\sqrt{2}} & 0 & 2t \\
\frac{|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle}{\sqrt{2}} & 2t & U
\end{array}
\tag{26}
$$

This subspace is not automatically diagonal, but is easily diagonalized. The eigenvectors are

$$
\begin{aligned}
&\frac{1}{N_\pm}\left\{2t\frac{(|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle)}{\sqrt{2}}+\frac{U\pm\sqrt{U^2+16t^2}}{2}\,\frac{(|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\} \\
&N_\pm=\left\{\frac{U}{2}\left[U\pm\sqrt{U^2+16t^2}\right]+16t^2\right\}^{\frac{1}{2}}
\end{aligned}
\tag{27}
$$

with eigenvalues $\frac{U\pm\sqrt{U^2+16t^2}}{2}$ respectively.

1.7 The total spectrum

The final spectrum is already obtained. One final thing to do is to just add the respective values of $-\mu N$ to the eigenvalues.

$\hat{N}$	S_z^{tot}	$\hat{P}$	E	$\lvert\Phi\rangle$
0	-	-	0	$\lvert 0,0\rangle$
1	-1	1	-t-μ	$\frac{\lvert\downarrow,0\rangle+\lvert 0,\downarrow\rangle}{\sqrt{2}}$
		-1	t-μ	$\frac{\lvert\downarrow,0\rangle-\lvert 0,\downarrow\rangle}{\sqrt{2}}$
	1	1	-t-μ	$\frac{\lvert\uparrow,0\rangle+\lvert 0,\uparrow\rangle}{\sqrt{2}}$
		-1	t-μ	$\frac{\lvert\uparrow,0\rangle-\lvert 0,\uparrow\rangle}{\sqrt{2}}$
2	-1	1	0-2μ	$\lvert\downarrow,\downarrow\rangle$
	0	1	0-2μ	$\frac{\lvert\uparrow,\downarrow\rangle+\lvert\downarrow,\uparrow\rangle}{\sqrt{2}}$
		1	U-2μ	$\frac{\lvert\uparrow\downarrow,0\rangle+\lvert 0,\uparrow\downarrow\rangle}{\sqrt{2}}$
		-1	$\frac{U+\sqrt{U^2+16t^2}}{2}-2\mu$	$\frac{1}{N_\pm}\left\{2t\frac{(\lvert\uparrow,\downarrow\rangle-\lvert\downarrow,\uparrow\rangle)}{\sqrt{2}}+\frac{U\pm\sqrt{U^2+16t^2}}{2}\frac{(\lvert\uparrow\downarrow,0\rangle-\lvert 0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\}$
		-1	$\frac{U-\sqrt{U^2+16t^2}}{2}-2\mu$	$\frac{1}{N_-}\left\{2t\frac{(\lvert\uparrow,\downarrow\rangle-\lvert\downarrow,\uparrow\rangle)}{\sqrt{2}}+\frac{U-\sqrt{U^2+16t^2}}{2}\frac{(\lvert\uparrow\downarrow,0\rangle-\lvert 0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\}$
	1	1	0-2μ	$\lvert\uparrow,\uparrow\rangle$
3	-1	1	U-t-3μ	$\frac{\lvert\uparrow\downarrow,\downarrow\rangle+\lvert\downarrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
		-1	U+t-3μ	$\frac{\lvert\uparrow\downarrow,\downarrow\rangle-\lvert\downarrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
	1	1	U-t-3μ	$\frac{\lvert\uparrow\downarrow,\uparrow\rangle+\lvert\uparrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
		-1	U+t-3μ	$\frac{\lvert\uparrow\downarrow,\uparrow\rangle-\lvert\uparrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
4	0	1	2U-4μ	$\lvert\uparrow\downarrow,\uparrow\downarrow\rangle$