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# 1 Exact diagonalization of the two-site Hubbard model

**The Hamiltonian**

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

I have two lattice sites, indexed by 1 and 2, occupied by electrons. $\mu$ is the chemical potential, $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are the fermionic creation and annihilation operators at the $\mathrm{i}^{\mathrm{th}}$ site, with spin-index $\sigma$. $\sigma$ 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 $\sigma$; 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**:

$$\left[\mathcal{H}, \hat{N}\right] = 0$$

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

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

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

Because the electrons on different sites are distinguishable, creation and anhillation operators of different sites will commute among themselves.

$$\begin{aligned}\left[c^{\dagger}_{1\sigma}c_{2\sigma}, \hat{N}\right] &= \sum_{i\sigma'}\left(c^{\dagger}_{1\sigma}\delta_{i,2}\left[c_{2\sigma}, c^{\dagger}_{2\sigma'}c_{2\sigma'}\right] + \delta_{i,1}\left[c^{\dagger}_{1\sigma}, c^{\dagger}_{1\sigma'}c_{1\sigma'}\right]c_{2\sigma}\right) \\ &= \sum_{\sigma'}\left(c^{\dagger}_{1\sigma}\left\{c_{2\sigma}, c^{\dagger}_{2\sigma'}\right\}c_{2\sigma'} - c^{\dagger}_{1\sigma'}\left\{c_{1\sigma'}, c^{\dagger}_{1\sigma}\right\}c_{2\sigma}\right) \\ &= \sum_{\sigma'}\left(c^{\dagger}_{1\sigma}\delta_{\sigma,\sigma'}c_{2\sigma'} - c^{\dagger}_{1\sigma'}\delta_{\sigma,\sigma'}c_{2\sigma}\right) = 0\end{aligned}$$

- $c^\dagger_{2\sigma}c_{1\sigma}$: Since the operator $\hat{N}$ is symmetric with respect to the site indices 1 and 2, we 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.
- $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$:

$$\begin{aligned}
\left[\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \hat{N}\right] &= \sum_{j\sigma}\left[\hat{n}_{i\uparrow}\hat{n}_{j\downarrow}, \hat{n}_{j\sigma}\right] \\
&= \sum_{\sigma}\left[\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \hat{n}_{i\sigma}\right] \\
&= \hat{n}_{i\uparrow}\left[\hat{n}_{i\downarrow}, \hat{n}_{i\uparrow}\right] + \left[\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}\right]\hat{n}_{i\downarrow} = 0
\end{aligned}$$

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