Hamiltonian commutators, Angular Momentum

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1 Hamiltonian commutators

The Hubbard Hamiltonian is given by $\hat{H} = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} \hat{n}_{i\sigma} + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$. We wish to show that

$$[\hat{S}_\pm, \hat{H}] = [\hat{S}_z, \hat{H}] = [\hat{J}_z, \hat{H}] = 0, \qquad [\hat{H}, \hat{J}_\pm] = \pm(U - 2\mu)\hat{J}_\pm$$

Recall,

$$\hat{S}_+ = \sum_i c^\dagger_{i\uparrow} c_{i\downarrow} \qquad \hat{S}_- = \sum_i c^\dagger_{i\downarrow} c_{i\uparrow} \qquad \hat{S}_z = \frac{1}{2}\sum_i \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}$$
$$\hat{J}_+ = \sum_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} (-1)^{i+1} \quad \hat{J}_z = \sum_i c_{i\downarrow} c_{i\uparrow} (-1)^{i+1} \quad \hat{J}_z = \frac{1}{2}\sum_i (\hat{n}_{i\downarrow} + \hat{n}_{i\uparrow} - 1)$$

First I show $[\hat{S}_+, \hat{H}] = 0$.

$$[\hat{H}, \hat{S}_+] = -\sum_{ijk\sigma} t_{ij} [c^\dagger_{i\sigma} c_{j\sigma}, c^\dagger_{k\uparrow} c_{k\downarrow}] - \mu \sum_{ij\sigma} [c^\dagger_{i\sigma} c_{i\sigma}, c^\dagger_{j\uparrow} c_{j\downarrow}] + U \sum_{ij} [\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, c^\dagger_{j\uparrow} c_{j\downarrow}]$$

To help evaluate the first (hopping) term:

$$\begin{aligned}
[c^\dagger_{i\sigma} c_{j\sigma}, c^\dagger_{k\uparrow} c_{k\downarrow}] &= c^\dagger_{k\uparrow} [c^\dagger_{i\sigma} c_{j\sigma}, c_{k\downarrow}] + [c^\dagger_{i\sigma} c_{j\sigma}, c^\dagger_{k\uparrow}] c_{k\downarrow} \\
&= c^\dagger_{k\uparrow} (c^\dagger_{i\sigma} \{c_{j\sigma}, c_{k\downarrow}\} - \{c^\dagger_{i\sigma}, c_{k\downarrow}\} c_{j\sigma}) + (c^\dagger_{i\sigma} \{c_{j\sigma}, c^\dagger_{k\uparrow}\} - \{c^\dagger_{i\sigma}, c^\dagger_{k\uparrow}\} c_{j\sigma}) c_{k\downarrow} \\
&= -c^\dagger_{k\uparrow} c_{j\sigma} \delta_{ik} \delta_{\sigma\downarrow} + c^\dagger_{i\sigma} c_{k\downarrow} \delta_{jk} \delta_{\sigma\uparrow}
\end{aligned}$$

The first (hopping) term can now be evaluated:

$$-\sum_{ijk\sigma} t_{ij} [c^\dagger_{i\sigma} c_{j\sigma}, c^\dagger_{k\uparrow} c_{k\downarrow}] = \sum_{ij} t_{ij} c^\dagger_{i\uparrow} c_{j\downarrow} - \sum_{ij} t_{ij} c^\dagger_{i\uparrow} c_{j\downarrow} = 0$$

Onto showing that the second term is 0:

$$[\hat{n}_{i\sigma}, c^\dagger_{j\uparrow} c - j \downarrow] = c^\dagger_{j\uparrow} [\hat{n}_{i\sigma}, c_{j\downarrow}] + [\hat{n}_{i\sigma}, c^\dagger_{j\uparrow}] c_{j\downarrow} = \delta_{ij} (c^\dagger_{j\uparrow} c_{j\downarrow} - c^\dagger_{j\uparrow} c - j \downarrow) = 0$$

Which readily implies that the second term is 0. Lastly,

$$\begin{aligned}
[\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, c^\dagger_{j\uparrow} c_{j\downarrow}] &= c^\dagger_{j\uparrow} [\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, c_{j\downarrow}] + [\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, c^\dagger_{j\uparrow}] c_{j\downarrow} \\
&= c^\dagger_{j\uparrow} (\hat{n}_{i\uparrow} [\hat{n}_{i\downarrow}, c_{j\downarrow}] + [\hat{n}_{i\uparrow}, c_{j\downarrow}] \hat{n}_{i\downarrow}) + (\hat{n}_{i\uparrow} [\hat{n}_{i\downarrow}, c^\dagger_{j\uparrow}] + [\hat{n}_{i\uparrow}, c^\dagger_{j\uparrow}] \hat{n}_{i\downarrow}) c_{j\downarrow} \\
&= -c^\dagger_{j\uparrow} \hat{n}_{i\uparrow} c_{j\downarrow} \delta_{ij} + c^\dagger_{j\uparrow} \hat{n}_{i\downarrow} c_{j\downarrow} \delta_{ij} = 0
\end{aligned}$$

The last line follows because if $i = j$ then the left term contains a $(c^\dagger_{i\uparrow})^2$ and the right term contains a $(c_{i\downarrow})^2$ both of which are 0. This shows that the last term in the commutator is 0. Therefore, $[\hat{S}_+, \hat{H}] = 0$, and via a similar calculation, one can verify that $[\hat{S}_-, \hat{H}] = 0$.
Proceeding with the next identity:

$$2[\hat{S}_z, \hat{H}] = -\sum_{ijk\sigma} t_{jk} ([\hat{n}_{i\uparrow}, c^\dagger_{j\sigma} c_{k\sigma}] - [\hat{n}_{i\downarrow}, c^\dagger_{j\sigma} c_{k\sigma}]) - \mu\sigma_{ij\sigma} [\hat{n}_{i\uparrow}, \hat{n}_{j\sigma}] - [\hat{n}_{i\downarrow}, \hat{n}_{i\sigma}] + U \sum_{ij} [\hat{n}_{i\uparrow}, \hat{n}_{j\uparrow}\hat{n}_{i\downarrow}] - [\hat{n}_{i\downarrow}, \hat{n}_{j\uparrow}\hat{n}_{i\downarrow}]$$

It is time to show a useful result for evaluating a commutator with the first term of the Hamiltonian, namely, that the sum of number operators of a given spin σ' over all positions commutes with the first term.

$$\begin{aligned}\sum_{ijk\sigma} t_{jk}[\hat{n}_{i\sigma'}, c^\dagger_{j\sigma}c_{k\sigma}] &= \sum_{ijk\sigma} t_{jk}(c^\dagger_{j\sigma}[\hat{n}_{i\sigma'}, c_{k\sigma}] + [\hat{n}_{i\sigma'}, c^\dagger_{j\sigma}]c_{k\sigma}) \\ &= \sum_{ijk\sigma} t_{jk}(-\delta_{ik}\delta_{\sigma\sigma'}c^\dagger_{j\sigma}c_{k\sigma} + \delta_{ij}\delta_{\sigma\sigma'}c^\dagger_{j\sigma}c_{k\sigma}) \\ &= -\sum_{ij} t_{ij}c^\dagger_{i\sigma'}c_{j\sigma'} + \sum_{ij} t_{ij}c^\dagger_{i\sigma'}c_{j\sigma'} = 0\end{aligned}$$

This now implies that the first term of $[\hat{S}_z, \hat{H}]$ is 0. To show that the other terms are 0, note that number operators commute:

$$[\hat{n}_{i\sigma}, c^\dagger_{j\sigma'}c_{j\sigma'}] = c^\dagger_{j\sigma'}[\hat{n}_{i\sigma}, c_{j\sigma'}] + [\hat{n}_{i\sigma}, c^\dagger_{j\sigma'}]c_{j\sigma'} = \delta_{\sigma\sigma'}\delta_{ij}(-c^\dagger_{j\sigma'}c_{j\sigma'} + c^\dagger_{j\sigma'}c_{j\sigma'}) = 0$$

Therefore, $[\hat{S}_z, \hat{H}] = 0$. Since $\hat{J}_z$ is also the sum of sums of number operators of a given spin over all positions, in fact $[\hat{J}_z, \hat{H}] = 0$ as well. Onto the final identity:

$$[\hat{H}, \hat{J}_+] = -\sum_{ijk\sigma}(-1)^{k+1}t_{ij}[c^\dagger_{i\sigma}c_{j\sigma}, c^\dagger_{k\uparrow}c^\dagger_{k\downarrow}] - \mu\sum_{ij\sigma}(-1)^{j+1}[\hat{n}_{i\sigma}, c^\dagger_{j\uparrow}c^\dagger_{j\downarrow}] + U\sum_{ij}(-1)^{j+1}[\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, c^\dagger_{j\uparrow}c^\dagger_{j\downarrow}]$$

Starting as always with the first term:

$$\begin{aligned}[c^\dagger_{i\sigma}c_{j\sigma}, c^\dagger_{k\uparrow}c^\dagger_{k\downarrow}] &= c^\dagger_{k\uparrow}[c^\dagger_{i\sigma}c_{j\sigma}, c^\dagger_{k\downarrow}] + [c^\dagger_{i\sigma}c_{j\sigma}, c^\dagger_{k\uparrow}]c^\dagger_{k\downarrow} \\ &= c^\dagger_{k\uparrow}(c^\dagger_{i\sigma}\{c_{j\sigma}, c^\dagger_{k\downarrow}\} - \{c^\dagger_{i\sigma}, c^\dagger_{k\downarrow}\}c_{j\sigma}) + (c^\dagger_{i\sigma}\{c_{j\sigma}, c^\dagger_{k\uparrow}\} - \{c^\dagger_{i\sigma}, c^\dagger_{k\uparrow}\}c_{j\sigma})c^\dagger_{k\downarrow} \\ &= c^\dagger_{k\uparrow}c^\dagger_{i\sigma}\delta_{jk}\delta_{\sigma\downarrow} + c^\dagger_{i\sigma}c^\dagger_{k\downarrow}\delta_{jk}\delta_{\sigma\uparrow}\end{aligned}$$

So that

$$\sum_{ijk\sigma}(-1)^{j+1}t_{ij}[c^\dagger_{i\sigma}c_{j\sigma}, c^\dagger_{k\uparrow}c^\dagger_{k\downarrow}] = \sum_{ij} t_{ji}c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}(-1)^{i+1} + \sum_{ij} t_{ij}c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}(-1)^{j+1} = \sum_{ij} t_{ij}c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}((-1)^{i+1} + (-1)^{j+1}) = 0$$

The following facts were used in the above line; that $t_{ij} = t_{ji}$, since t_{ij} is an adjacency matrix, and that adjacent states' numbering differs by an odd number (checkerboard pattern).
Noticing that $\sum_{i\sigma}\hat{n}_{i\sigma}$ differs from $2\hat{J}_z$ by a constant, the middle term can quickly be evaluated:

$$[-\mu\sum_{i\sigma}\hat{n}_{i\sigma}, \hat{J}_\pm] = -2\mu[\hat{J}_z, \hat{J}_\pm] = \mp\mu 2\hat{J}_\pm$$

For the final term:

$$\begin{aligned}[\hat{n}_{i\uparrow}\hat{n}_{j\downarrow}, c^\dagger_{j\uparrow}c^\dagger_{j\downarrow}] &= c^\dagger_{j\uparrow}[\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, c^\dagger_{j\downarrow}] + [\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, c^\dagger_{j\uparrow}]c^\dagger_{j\downarrow} \\ &= c^\dagger_{j\uparrow}(\hat{n}_{i\uparrow}[\hat{n}_{i\downarrow}, c^\dagger_{j\uparrow}] + [\hat{n}_{i\uparrow}, c^\dagger_{j\downarrow}]\hat{n}_{i\downarrow}) + (\hat{n}_{i\uparrow}[\hat{n}_{i\downarrow}, c^\dagger_{j\uparrow}] + [\hat{n}_{i\uparrow}, c^\dagger_{j\uparrow}]\hat{n}_{i\downarrow})c^\dagger_{j\downarrow} \\ &= c^\dagger_{j\uparrow}\hat{n}_{i\uparrow}c^\dagger_{j\downarrow}\delta_{ij} + c^\dagger_{j\uparrow}\hat{n}_{i\downarrow}c^\dagger_{i\downarrow}\delta_{ij}\end{aligned}$$

The first term above goes away because if $i = j$ then the first term contains a $(c^\dagger)^2$. Now, finishing up our calculations:

$$\begin{aligned}U\sum_{ij}(-1)^{j+1}[\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, c^\dagger_{j\uparrow}c^\dagger_{j\downarrow}] &= U\sum_i(-1)^{i+1}c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow}c^\dagger_{i\downarrow} \\ &= U\sum_i(-1)^{i+1}(c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow}c^\dagger_{i\downarrow} + c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}(1 - \{c_{i\downarrow}, c^\dagger_{i\downarrow}\})) \\ &= U\sum_i(-1)^{i+1}c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} = U\hat{J}_+\end{aligned}$$

as desired. The corresponding result for J_- can be verified doing the same calcultaion. Therefore, adding in the contribution from the middle term, $[\hat{H}, \hat{J}_\pm] = \pm(U - 2\mu)\hat{J}_\pm$.

2 Angular momentum

The angular momentum operator has the familiar form $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$. In other words, $L_i = \epsilon_{ijk}\hat{x}_j\hat{p}_k$.
It turns out that $[\hat{L}_i, \hat{L}_j] = \epsilon_{ijk} i\hbar \hat{L}_k$:

$$\begin{aligned}
[\hat{L}_i, \hat{L}_{i'}] &= [\epsilon_{ijk}x_jp_k, \epsilon_{i'j'k'}x_{j'}p_{k'}] \\
&= \epsilon_{ijk}\epsilon_{i'j'k'}[x_jp_k, x_{j'}p_{k'}] \\
&= \epsilon_{ijk}\epsilon_{i'j'k'}(x_{j'}[x_jp_k, p_{k'}] + [x_jp_k, x_{j'}]p_{k'}) \\
&= \epsilon_{ijk}\epsilon_{i'j'k'}(x_{j'}p_k i\hbar\delta_{jk'} - x_jp_{k'} i\hbar\delta_{j'k}) \\
&= i\hbar(\epsilon_{ijk}\epsilon_{i'j'j}x_{j'}p_k - \epsilon_{ijk}\epsilon_{i'kk'}x_jp_{k'}) \\
&= i\hbar\big[(\delta_{ij'}\delta_{ki'} - \delta ii'\delta_{kj'})x_{j'}p_k - (\delta_{ik'}\delta_{ji'} - \delta_{ii'}\delta_{jk'})x_jp_{k'}\big] \\
&= i\hbar(x_ip_{i'} - x_{i'}p_i) = \epsilon_{ii'k} i\hbar\hat{L}_k
\end{aligned}$$

The commutator $[x_i, p_j] = i\hbar\delta_{ij}$ was used. One can see that $\epsilon_{ijk}\epsilon_{i'j'j}$ can be simplified by noting that for it to be nonzero $i' \neq j'$ which implies $i' = i, j' = k$ or $i' = k, j' = i$. Analyzing these cases separately to see if the parity of $i'j'j$ equals or is opposite to that of ijk gives $\delta_{ij'}\delta_{ki'} - \delta_{ii'}\delta_{kj'}$, and the same is done for the other ϵ product.
Now we introduce the $\hat{\mathbf{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ total angular momentum operator. For now it is desirable to show that $\hat{\mathbf{L}}^2$ commutes with $\hat{L}_z$, to justify searching for simultaneous eigenstates of these operators. Making use of Einstein notation:

$$[\hat{\mathbf{L}}^2, \hat{L}_i] = [\hat{L}_j^2, \hat{L}_i] = \hat{L}_j[\hat{L}_j, \hat{L}_i] + [\hat{L}_j, \hat{L}_i]\hat{L}_j = i\hbar\epsilon_{jik}(\hat{L}_j\hat{L}_k + \hat{L}_k\hat{L}_j) = 0$$

The sum is equal to 0 because interchanging j and k switches the sign of ϵ_{jik} while preserving $\hat{L}_j\hat{L}_k + \hat{L}_k\hat{L}_j$. Having shown that $\hat{\mathbf{L}}^2$ commutes with $\hat{L}_z$, take $|lm\rangle$ to be a simultaneous eigenstate of $\hat{\mathbf{L}}^2$ and $\hat{L}_z$, with l and m identifying its eigenvalues:

$$\hat{\mathbf{L}}^2 |lm\rangle = l(l+1)\hbar^2 |lm\rangle \qquad \hat{L}_z |lm\rangle = m\hbar |lm\rangle$$

Now define raising and lowering operators,

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y \qquad \hat{L}_- = \hat{L}_x - i\hat{L}_y$$

with the following commutator identities (which can be obtained easily from the previous identities)

$$[\hat{\mathbf{L}}^2, \hat{L}_\pm] = 0 \qquad [\hat{L}_z, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm \qquad [\hat{L}_+, \hat{L}_-] = 2\hbar\hat{L}_z$$

Some useful identities are:

$$\hat{L}_\pm\hat{L}_\mp = \hat{\mathbf{L}}^2 - \hat{L}_z^2 \pm \hbar\hat{L}_z \qquad \hat{\mathbf{L}}^2 = \frac{1}{2}(\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+) + \hat{L}_z^2$$

As it turns out, these raising and lowering operators when acted upon a state return a state with $\hat{L}_z$ raised or lowered by 1. Because,

$$\hat{L}_z\hat{L}_\pm |lm\rangle = (\pm\hbar\hat{L}_\pm + \hat{L}_\pm\hat{L}_z) |lm\rangle = (m \pm 1)\hbar\hat{L}_\pm |lm\rangle = (m \pm 1)\hbar c_{lm\pm} |l, m \pm 1\rangle$$

The attached constant $c_{lm\pm}$ is unknown. It can be calculated, however, like so (let's take it to be real and positive):

$$\begin{aligned}
c_{lm\pm}^2 = |\hat{L}_\pm |lm\rangle|^2 = \langle lm|\hat{L}_\mp\hat{L}_\pm|lm\rangle = \langle lm|\hat{\mathbf{L}}^2 - \hat{L}_z^2 \mp \hbar\hat{L}_z|lm\rangle = \hbar^2(l(l+1) - m^2 \mp m) \\
\implies c_{lm\pm} = \hbar\sqrt{l(l+1) - m(m \pm 1)} = \hbar\sqrt{(l \mp m)(l \pm m + 1)}
\end{aligned}$$

This also indirectly says that the maximum and minimum values of m are l and $-l$ respectively, that is, $\hat{L}_\pm |l \pm l\rangle = 0$, and that $2l$ is an integer, so then l is a half integer.
Furthermore, by using the formula for $c_{lm+} = \sqrt{(l-m)(l+m+1)}$, an eigenstate can be expressed in terms of $\hat{L}_+$ and $|l - l\rangle$:

$$|lm\rangle = \sqrt{\frac{(2l)!(l+m)!}{(l-m)!}}(\frac{\hat{L}_+}{\hbar})^{l+m} |l - l\rangle$$

Now start looking at $|lm\rangle$ in the θ, ϕ basis, that is $\langle\theta, \phi|lm\rangle = Y_m^l(\theta, \phi)$. By virtue of the fact that $\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$

$$\langle\theta, \phi|\hat{L}_z|lm\rangle = -i\hbar\frac{\partial}{\partial\phi}Y_m^l(\theta, \phi) = \hbar m Y_m^l(\theta, \phi) \implies Y_m^l(\theta, \phi) = f_m^l(\theta)e^{im\phi}$$

To do more with these functions write $\hat{L}_\pm$ in derivatives. Recalling that

$$\hat{L}_x = i\hbar(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}) \quad \hat{L}_y = -i\hbar(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi})$$

$$\hat{L}_\pm = \pm e^{i\phi}\hbar(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}) \qquad \hat{\mathbf{L}}^2 = -\hbar^2(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2})$$

$\hat{L}_- \left| l\, -l \right\rangle = 0$ implies

$$-i\hbar(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi})f^l_{-l}(\theta)e^{-il\phi} = -i\hbar(\frac{\partial}{\partial\theta} - l\cot\theta)f^l_{-l}(\theta)e^{-il\phi} = 0 \implies f^l_{-l} = C\sin^l\theta$$

The rest involves some integration.