Ex1002+Ex1003: Fock formalism for a single site with electrons

Submitted by: Yuri Khodorkovsky and Avishai Sadeh

The problem:
Use the procedure from the lecture notes and express the following operators by 2nd quantization formalism: $\hat{N}$, $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$, $\hat{S}^2$ for one site electronic system. Verify that the commutation relation $[\hat{S}_x, \hat{S}_y] = i\hat{S}_z$ is satisfied. Generalize the expression for many site system.

The solution:

`The answer to 1003 is wrong.`

In order to express the operators in second quantization formalism we shall use the following formula for a one body operator:

$$\hat{V} = \sum_{k,k'} \hat{a}^\dagger_{k'} V_{k',k} \hat{a}_k.$$

We will write the operators in the spin state basis $(|\uparrow\rangle, |\downarrow\rangle)$. Knowing the matrix elements $(\hat{S}_x)_{k',k}$, $(\hat{S}_y)_{k',k}$, $(\hat{S}_z)_{k',k}$, and summing over $k, k' = \uparrow, \downarrow$ we get:

$$\hat{S}_x = \frac{1}{2}(\hat{a}^\dagger_\downarrow \hat{a}_\uparrow + \hat{a}^\dagger_\uparrow \hat{a}_\downarrow)$$

$$\hat{S}_y = \frac{1}{2} i(\hat{a}^\dagger_\downarrow \hat{a}_\uparrow - \hat{a}^\dagger_\uparrow \hat{a}_\downarrow)$$

$$\hat{S}_z = \frac{1}{2}(\hat{a}^\dagger_\uparrow \hat{a}_\uparrow - \hat{a}^\dagger_\downarrow \hat{a}_\downarrow).$$

Doing the algebra and using the anti-commutation relations

$$[\hat{a}_r, \hat{a}_s]_+ = 0$$

$$[\hat{a}^\dagger_r, \hat{a}^\dagger_s]_+ = 0$$

$$[\hat{a}_r, \hat{a}^\dagger_s]_+ = \delta_{r,s}$$

give us:

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = \frac{1}{4}\left\{\hat{n}_\uparrow(\hat{n}_\uparrow + 2) + \hat{n}_\downarrow(\hat{n}_\downarrow + 2)\right\} - \frac{3}{2}\hat{n}_\uparrow \hat{n}_\downarrow.$$

We see that $\hat{S}^2$ is zero when there are no particles, or two particles of opposite spin in the site, and is $\frac{3}{4}$ when there is one particle, as it should be. Obviously, we have:

$$\hat{N} = \hat{n}_\uparrow + \hat{n}_\downarrow = \hat{a}^\dagger_\uparrow \hat{a}_\uparrow + \hat{a}^\dagger_\downarrow \hat{a}_\downarrow.$$

Now we shall check the commutation relation:

$$[\hat{S}_x, \hat{S}_y] = \frac{1}{4} i \left(-[\hat{a}^\dagger_\downarrow \hat{a}_\uparrow, \hat{a}^\dagger_\uparrow \hat{a}_\downarrow] + [\hat{a}^\dagger_\uparrow \hat{a}_\downarrow, \hat{a}^\dagger_\downarrow \hat{a}_\uparrow] \right) =$$

$$= \frac{1}{2} i [\hat{a}^\dagger_\uparrow \hat{a}_\downarrow, \hat{a}^\dagger_\downarrow \hat{a}_\uparrow] =$$

$$= \frac{1}{2} i \left(\hat{a}_\uparrow^\dagger [\hat{a}_\downarrow, \hat{a}_\downarrow^\dagger \hat{a}_\uparrow] + [\hat{a}_\uparrow^\dagger, \hat{a}_\downarrow^\dagger \hat{a}_\uparrow] \hat{a}_\downarrow \right) =$$

$$= \frac{1}{2} i \left\{ \hat{a}_\uparrow^\dagger \left(\hat{a}_\downarrow^\dagger [\hat{a}_\downarrow, \hat{a}_\uparrow] + [\hat{a}_\downarrow, \hat{a}_\downarrow^\dagger] \hat{a}_\uparrow \right) + \left(\hat{a}_\downarrow^\dagger [\hat{a}_\uparrow^\dagger, \hat{a}_\uparrow] + [\hat{a}_\uparrow^\dagger, \hat{a}_\downarrow^\dagger] \hat{a}_\uparrow \right) \hat{a}_\downarrow \right\} =$$

$$= \frac{1}{2} i \left\{ 2\hat{a}_\uparrow^\dagger \hat{a}_\downarrow^\dagger \hat{a}_\downarrow \hat{a}_\uparrow + \hat{a}_\uparrow^\dagger \left(1 - 2\hat{a}_\downarrow^\dagger \hat{a}_\downarrow \right) \hat{a}_\uparrow - \hat{a}_\downarrow^\dagger \left(1 - 2\hat{a}_\uparrow^\dagger \hat{a}_\uparrow \right) \hat{a}_\downarrow - 2\hat{a}_\downarrow^\dagger \hat{a}_\uparrow^\dagger \hat{a}_\uparrow \hat{a}_\downarrow \right\} = i\hat{S}_z.$$

To get the last line we have used the anti-commutation relations stated above and:

$$[\hat{a}_r, \hat{a}_r^\dagger] = 1 - 2\hat{a}_r^\dagger \hat{a}_r.$$

Now, for many site system, we just add the spin operators of all the N sites:

$$\hat{S}_x^{tot} = \sum_{i=1}^{N} \hat{S}_{x,i} = \frac{1}{2} \sum_{i=1}^{N} (\hat{a}_{\downarrow,i}^\dagger \hat{a}_{\uparrow,i} + \hat{a}_{\uparrow,i}^\dagger \hat{a}_{\downarrow,i})$$

and similar expressions for $\hat{S}_y^{tot}$ and $\hat{S}_z^{tot}$.

Note about ex. 1003: We are asked to prove Hubbard-Sternovich identity

$$\mathrm{e}^{-\alpha\left(\hat{n}_\uparrow - \frac{1}{2}\right)\left(\hat{n}_\downarrow - \frac{1}{2}\right)} = \frac{1}{2} \mathrm{e}^{-\alpha/4} \sum_{\sigma=\pm 1} \mathrm{e}^{\lambda\sigma(\hat{n}_\uparrow - \hat{n}_\downarrow)}.$$

We can just trivially check it for all the 4 combinations of $\hat{n}_\uparrow$ and $\hat{n}_\downarrow$. This way we find that λ should be equal to $i \arccos(e^{\alpha/2})$. We see that $\alpha \leq 0$ shoul be satisfied.