TFY 4210, Quantum theory of many-particle systems

SOLUTION TO TUTORIAL 5

(In this solution we don't write hats (^) on number operators)

(a) Prove $c_{i\sigma}^\dagger c_{i\sigma'} = \frac{1}{2}\delta_{\sigma\sigma'}(n_{i\uparrow} + n_{i\downarrow}) + \vec{S}_i \cdot \vec{\sigma}_{\sigma'\sigma}$ (1)

$\underline{\underline{\sigma = \sigma'}}$

LHS $= c_{i\sigma}^\dagger c_{i\sigma} = n_{i\sigma}$

RHS $= \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) + \vec{S}_i \cdot \vec{\sigma}_{\sigma\sigma}$

$$\vec{S}_i = S_i^x \hat{e}_x + S_i^y \hat{e}_y + S_i^z \hat{e}_z$$

$$\vec{\sigma}_{\sigma\sigma} = \sigma_{\sigma\sigma}^x \hat{e}_x + \sigma_{\sigma\sigma}^y \hat{e}_y + \sigma_{\sigma\sigma}^z \hat{e}_z$$

$$\Rightarrow \vec{S}_i \cdot \vec{\sigma}_{\sigma\sigma} = S_i^x \underbrace{\sigma_{\sigma\sigma}^x}_{=0} + S_i^y \underbrace{\sigma_{\sigma\sigma}^y}_{=0} + S_i^z \underbrace{\sigma_{\sigma\sigma}^z}_{=2\sigma}$$

$$= 2\sigma S_i^z$$

$$= 2\sigma \cdot \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow})$$

$$= \sigma(n_{i\uparrow} - n_{i\downarrow})$$

$$\Rightarrow \quad RHS = \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) + \sigma(n_{i\uparrow} - n_{i\downarrow})$$

$\supset$: if $\sigma = \uparrow = +\frac{1}{2} \Rightarrow RHS = n_{i\uparrow} = n_{i\sigma}$

if $\sigma = \downarrow = -\frac{1}{2} \Rightarrow RHS = n_{i\downarrow} = n_{i\sigma}$

So in either case, $RHS = n_{i\sigma}$, which is the same as LHS. QED.

$\underline{\sigma = -\sigma'}$

$$LHS = c^{\dagger}_{i\sigma} c_{i-\sigma}$$

$$RHS = \vec{S}_i \cdot \vec{\sigma}_{-\sigma,\sigma}$$

$$= S^x_i \underbrace{\sigma^x_{-\sigma,\sigma}}_{=1} + S^y_i \underbrace{\sigma^y_{-\sigma,\sigma}}_{=2\sigma i} \qquad (\sigma^z_{-\sigma\sigma} = 0)$$

$$= S^x_i + 2i\sigma S^y_i$$

$$= \frac{1}{2}(c^{\dagger}_{i\uparrow} c_{i\downarrow} + c^{\dagger}_{i\downarrow} c_{i\uparrow})$$

$$+ 2i\sigma \cdot \frac{1}{2}(-i c^{\dagger}_{i\uparrow} c_{i\downarrow} + i c^{\dagger}_{i\downarrow} c_{i\uparrow})$$

$$= \frac{1}{2}(c^{\dagger}_{i\uparrow} c_{i\downarrow} + c^{\dagger}_{i\downarrow} c_{i\uparrow}$$

$$+ \sigma(c^{\dagger}_{i\uparrow} c_{i\downarrow} - c^{\dagger}_{i\downarrow} c_{i\uparrow})$$

$\supset$: if $\sigma = \uparrow = +\frac{1}{2} \Rightarrow RHS = c^{\dagger}_{i\uparrow} c_{i\downarrow} = c^{\dagger}_{i\sigma} c_{i-\sigma}$

if $\sigma = \downarrow = -\frac{1}{2} \Rightarrow RHS = c^{\dagger}_{i\downarrow} c_{i\uparrow} = c^{\dagger}_{i\sigma} c_{i-\sigma}$

So in either case, RHS $= c^\dagger_{i\sigma} c_{i-\sigma}$, which is the same as LHS. QED.

(b) Prove $c_{i\sigma} c^\dagger_{i\sigma'} = \delta_{\sigma\sigma'}\left(1 - \frac{n_{i\uparrow}+n_{i\downarrow}}{2}\right) - \vec{S}_i \cdot \vec{\sigma}_{\sigma\sigma'}$ (4)

$\sigma = \sigma'$

LHS $= c_{i\sigma} c^\dagger_{i\sigma} = 1 - c^\dagger_{i\sigma} c_{i\sigma}$.

Using (1), this is equal to

$1 - \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) - \vec{S}_i \cdot \vec{\sigma}_{\sigma\sigma}$

which agrees with RHS of (4). QED.

$\sigma = -\sigma'$

LHS $= c_{i\sigma} c^\dagger_{i-\sigma} = - c^\dagger_{i-\sigma} c_{i\sigma}$.

Using (1), this equals $-\vec{S}_i \cdot \vec{\sigma}_{\sigma,-\sigma}$

which agrees with RHS of (4). QED.

(c) Show that $[S^a_j, S^b_j] = i \sum_c \epsilon_{abc} S^c_j$

(drop j subscript in the following)

$$[S^a, S^b] = \left(\frac{1}{2}\right)^2 \sum_{\alpha\beta} \sum_{\gamma\delta} [c_\alpha^\dagger c_\beta, c_\gamma^\dagger c_\delta] \cdot \sigma^a_{\alpha\beta} \sigma^b_{\gamma\delta}$$

Consider the commutator $[c_\alpha^\dagger c_\beta, c_\gamma^\dagger c_\delta]$

$$= c_\alpha^\dagger c_\beta c_\gamma^\dagger c_\delta - c_\gamma^\dagger c_\delta c_\alpha^\dagger c_\beta$$

The second term can be rewritten as

$$c_\gamma^\dagger c_\delta c_\alpha^\dagger c_\beta = c_\gamma^\dagger (\delta_{\alpha\delta} - c_\alpha^\dagger c_\delta) c_\beta$$

$$= c_\gamma^\dagger c_\beta \delta_{\alpha\delta} - c_\gamma^\dagger c_\alpha^\dagger c_\delta c_\beta$$

$$= c_\gamma^\dagger c_\beta \delta_{\alpha\delta} - c_\alpha^\dagger \underbrace{c_\gamma^\dagger c_\beta}_{\delta_{\beta\gamma} - c_\beta c_\gamma^\dagger} c_\delta \cdot (-1)^2$$

$$= c_\gamma^\dagger c_\beta \delta_{\alpha\delta} - c_\alpha^\dagger c_\delta \delta_{\beta\gamma} + c_\alpha^\dagger c_\beta c_\gamma^\dagger c_\delta$$

$$\Rightarrow [c_\alpha^\dagger c_\beta, c_\gamma^\dagger c_\delta]$$
$$= -c_\gamma^\dagger c_\beta \delta_{\alpha\delta} + c_\alpha^\dagger c_\delta \delta_{\beta\gamma}$$

$$\Rightarrow [S^a, S^b] = \left(\frac{1}{2}\right)^2 \sum_{\alpha\beta} \sum_{\gamma\delta}$$

$$[c_\alpha^\dagger c_\delta \delta_{\beta\gamma} - c_\gamma^\dagger c_\beta \delta_{\alpha\delta}] \sigma^a_{\alpha\beta} \sigma^b_{\gamma\delta}$$

$$= \frac{1}{4}\Big[\sum_{\alpha\beta\delta} c_\alpha^\dagger c_\delta \, \sigma^a_{\alpha\beta} \, \sigma^b_{\beta\delta}$$

$$- \sum_{\alpha\beta\gamma} c_\gamma^\dagger c_\beta \, \sigma^a_{\alpha\beta} \, \sigma^b_{\gamma\alpha}\Big]$$

Now rename dummy summation indices to get $c_\alpha^\dagger c_\beta$ in both terms, i.e.

$$[S^a, S^b] = \frac{1}{4} \sum_{\alpha\beta} c_\alpha^\dagger c_\beta$$

$$\cdot \underbrace{\sum_\gamma \left(\sigma^a_{\alpha\gamma}\,\sigma^b_{\gamma\beta} - \sigma^b_{\alpha\gamma}\,\sigma^a_{\gamma\beta}\right)}_{(\sigma^a\sigma^b)_{\alpha\beta} - (\sigma^b\sigma^a)_{\alpha\beta}}$$

$$= \underbrace{[\sigma^a, \sigma^b]}_{2i \sum_c \epsilon_{abc}\,\sigma^c}{}_{\alpha\beta}$$

$$= \frac{1}{4} \sum_{\alpha\beta} c_\alpha^\dagger c_\beta \cdot 2i \sum_c \epsilon_{abc}\, \sigma^c_{\alpha\beta}$$

$$= i \sum_c \epsilon_{abc} \cdot \underbrace{\frac{1}{2} \sum_{\alpha\beta} c_\alpha^\dagger \sigma^c_{\alpha\beta} c_\beta}_{S^c}$$

$$= i \sum_c \epsilon_{abc}\, S^c . \quad \text{QED.}$$

(d) (Again we drop the site subscript.)

Show that $\vec{S}\cdot\vec{S} = \frac{3}{4} n(2-n)$

where $n = \sum_{\alpha=\uparrow,\downarrow} n_\alpha$

$$\vec{S}\cdot\vec{S} = \left(\tfrac{1}{2}\right)^2 \sum_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta c_\gamma^\dagger c_\delta$$

$$\cdot \underbrace{\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta}}_{-\delta_{\alpha\beta}\delta_{\gamma\delta} + 2\delta_{\beta\gamma}\delta_{\alpha\delta}}$$

$$= \frac{1}{4}\sum_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta c_\gamma^\dagger c_\delta \left[-\delta_{\alpha\beta}\delta_{\gamma\delta} + 2\delta_{\beta\gamma}\delta_{\alpha\delta}\right]$$

$$= \frac{1}{4}\Big[-\underbrace{\sum_\alpha n_\alpha}_{n} \underbrace{\sum_\gamma n_\gamma}_{n} + 2\sum_{\alpha\beta} c_\alpha^\dagger c_\beta c_\beta^\dagger c_\alpha$$

We have

$$\sum_{\alpha\beta} c_\alpha^\dagger c_\beta c_\beta^\dagger c_\alpha = \sum_{\alpha\beta} c_\alpha^\dagger c_\beta \left(\delta_{\alpha\beta} - c_\alpha c_\beta^\dagger\right)$$

$$= \sum_\alpha n_\alpha - \sum_{\alpha\beta} c_\alpha^\dagger c_\beta c_\alpha c_\beta^\dagger$$

$$= n + \sum_{\alpha\beta} c_\alpha^\dagger c_\alpha \overbrace{c_\beta c_\beta^\dagger}^{1-n_\beta}$$

$$= n + \sum_\beta \left(\sum_\alpha n_\alpha\right) - \left(\sum_\alpha n_\alpha\right)\left(\sum_\beta n_\beta\right)$$

$$= n + 2n - n^2 = 3n - n^2$$

Therefore

$$\vec{S}\cdot\vec{S} = \frac{1}{4}\left[-n^2 + 2(3n - n^2)\right]$$

$$= \frac{1}{4}(6n - 3n^2) = \underline{\underline{\frac{3}{4}n(2-n)}} \quad \text{QED.}$$

(e) Insert identities (1) and (4) into

$$PH_K^2P = \sum_{ij}\sum_{\sigma\sigma'} |t_{ij}|^2 \, P c_{i\sigma}^\dagger c_{i\sigma'} P \cdot P c_{j\sigma} c_{j\sigma'}^\dagger P$$

Because of the P operators, $n_{i\uparrow} + n_{i\downarrow}$ in the identities can be replaced by 1. Henceforth we drop the P operators as they are superfluous provided that we're only acting on states in LE.

$$\Rightarrow PH_K^2P \rightarrow$$

$$\sum_{ij}\sum_{\sigma\sigma'} |t_{ij}|^2 \left[\frac{1}{2}\delta_{\sigma\sigma'} + \vec{S}_i\cdot\vec{\sigma}_{\sigma'\sigma}\right] \cdot \left[\frac{1}{2}\delta_{\sigma\sigma'} - \vec{S}_j\cdot\vec{\sigma}_{\sigma\sigma'}\right]$$

$$= \sum_{ij} |t_{ij}|^2 \sum_{\sigma\sigma'} \left[\frac{1}{4}\delta_{\sigma\sigma'} + \frac{1}{2}\left(\vec{S}_i\cdot\vec{\sigma}_{\sigma'\sigma} - \vec{S}_j\cdot\vec{\sigma}_{\sigma\sigma'}\right)\delta_{\sigma\sigma'} - \vec{S}_i\cdot\vec{\sigma}_{\sigma'\sigma}\,\vec{S}_j\cdot\vec{\sigma}_{\sigma\sigma'}\right]$$

$$\sum_{\sigma\sigma'} \frac{1}{4} \delta_{\sigma\sigma'} = \frac{1}{4} \sum_{\sigma} = \frac{1}{2}$$

$$\frac{1}{2} \sum_{ij} |t_{ij}|^2 \sum_{\sigma\sigma'} \left(\vec{S}_i \cdot \vec{\sigma}_{\sigma'\sigma} - \vec{S}_j \cdot \vec{\sigma}_{\sigma\sigma'} \right) \delta_{\sigma\sigma'}$$

$$= \frac{1}{2} \sum_{ij} |t_{ij}|^2 \sum_{\sigma} \left(\vec{S}_i - \vec{S}_j \right) \cdot \vec{\sigma}_{\sigma\sigma} = 0$$

since $|t_{ij}|^2 = |t_{ji}|^2$

This leaves

$$P H_K^2 P \rightarrow \sum_{ij} |t_{ij}|^2 \left[\frac{1}{2} - \sum_{\sigma\sigma'} \vec{S}_i \cdot \vec{\sigma}_{\sigma'\sigma} \vec{S}_j \cdot \vec{\sigma}_{\sigma\sigma'} \right]$$

Now

$$\sum_{\sigma\sigma'} \vec{S}_i \cdot \vec{\sigma}_{\sigma'\sigma} \vec{S}_j \cdot \vec{\sigma}_{\sigma\sigma'}$$

$$= \sum_{a,b} \sum_{\sigma\sigma'} S_i^a \sigma^a_{\sigma'\sigma} S_j^b \sigma^b_{\sigma\sigma'}$$

$$= \sum_{ab} S_i^a S_j^b \underbrace{\sum_{\sigma\sigma'} \sigma^a_{\sigma'\sigma} \sigma^b_{\sigma\sigma'}}_{\mathrm{Tr}(\sigma^a \sigma^b) = 2\delta_{ab}}$$

$$= 2 \sum_a S_i^a S_j^a = 2 \vec{S}_i \cdot \vec{S}_j$$

$$\Rightarrow P H_K^2 P = \sum_{ij} |t_{ij}|^2 \left(\frac{1}{2} - 2 \vec{S}_i \cdot \vec{S}_j \right)$$

$$H_{eff} = -\frac{P H_K^2 P}{U}$$

$$= \sum_{ij} \frac{2|t_{ij}|^2}{U} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \right)$$

$$= \sum_{ij} J_{ij} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \right)$$ where

$$J_{ij} = \frac{2|t_{ij}|^2}{U} > 0 .$$ QED.

A comment on the result

$$\vec{S}\cdot\vec{S} = \frac{3}{4}\hat{n}(2-\hat{n})$$

in (e):

The eigenvalues of $\vec{S}\cdot\vec{S}$ should take the form $S(S+1)$ where S is the total spin quantum number. Thus

$$S(S+1) = \frac{3}{4}n(2-n)$$

where n on the RHS is now the eigenvalue of the number operator for the site.

$n=0$): no electrons on the site

$\Rightarrow$ $S(S+1) = \frac{3}{4}\cdot 0(2-0) \Rightarrow S=0$

obvious, since there are no electrons

$n=1$): one electron on the site

$\Rightarrow$ $S(S+1) = \frac{3}{4}\cdot 1\cdot(2-1) = \frac{3}{4} = \frac{1}{2}\left(\frac{1}{2}+1\right) \Rightarrow S=\frac{1}{2}$

so in this case $\vec{S}$ is a spin-1/2 spin operator

$n=2$): two electrons on the site

$\Rightarrow$ $S(S+1) = \frac{3}{4}\cdot 2\cdot(2-2) \Rightarrow S=0$

singlet state ($S=0$) since the two electrons are in the same orbital and so their spin state must be antisymmetric