TFY4210, Quantum theory of many-particle systems, 2015: Tutorial 5

Some calculations related to the derivation of the $S = 1/2$ antiferromagnetic Heisenberg model as the strong-interaction limit of the half-filled Hubbard model

Consider the identity

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

where $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$,

$$\boldsymbol{S}_i \equiv \frac{1}{2}\sum_{\sigma,\sigma'} c_{i\sigma}^\dagger \boldsymbol{\sigma}_{\sigma,\sigma'} c_{i\sigma'}, \tag{2}$$

and $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ is the vector of Pauli matrices given by

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \tag{3}$$

here the first row/column corresponds to the index $\sigma = \uparrow = +1/2$ and the second row/column corresponds to $\sigma = \downarrow = -1/2$.

(a) Prove Eq. (1). [For both $\sigma = \sigma'$ and $\sigma = -\sigma'$.]

(b) Show that the identity

$$c_{i\sigma} c_{i\sigma'}^\dagger = \delta_{\sigma\sigma'}\left(1 - \frac{n_{i\uparrow} + n_{i\downarrow}}{2}\right) - \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma\sigma'} \tag{4}$$

follows from Eq. (1).

(c) Show that the spin operator $\boldsymbol{S}_i$ for site i, defined in Eq. (2), satisfies the spin commutation relations

$$[S_j^a, S_j^b] = i\sum_c \epsilon_{abc} S_j^c, \tag{5}$$

where $a, b, c = x, y, z$. You may find the following result helpful: $[\sigma^a, \sigma^b] = 2i\sum_c \epsilon_{abc}\sigma^c$.

(d) Use the identity (you don't need to prove it) $\boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\gamma\delta} = -\delta_{\alpha\beta}\delta_{\gamma\delta} + 2\delta_{\beta\gamma}\delta_{\alpha\delta}$ to show that

$$\boldsymbol{S}_i^2 = \frac{3}{4} n_i(2 - n_i), \tag{6}$$

where $n_i = \sum_{\alpha=\uparrow,\downarrow} n_{i\alpha}$ is the operator for the total number of electrons on site i. From this result one can see that when there is exactly 1 electron per site (as there is in the low-energy subspace (LES) of the half-filled Hubbard model when $U \gg t$), $\boldsymbol{S}_i^2 = S(S+1)$ with $S = 1/2$, which implies that $\boldsymbol{S}_i$ is a spin-1/2 spin operator in this case. Also, when the number of electrons on site i is 0 or 2, the result (6) shows that the spin on the site is 0. These results agree with what one would intuitively expect.

(e) By inserting the identities (1) and (4) into the equation

$$PH_K^2P = \sum_{ij}\sum_{\sigma\sigma'} |t_{ij}|^2 P c_{i\sigma}^\dagger c_{i\sigma'} P \cdot P c_{j\sigma} c_{j\sigma'}^\dagger P. \tag{7}$$

derived in the lectures, show that the effective Hamiltonian $H_{\text{eff}} = -P\frac{H_K^2}{U}P$ for the LES becomes

$$H_{\text{eff}} = \sum_{i,j} J_{ij}(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - 1/4), \tag{8}$$

where

$$J_{ij} = \frac{2|t_{ij}|^2}{U} > 0. \tag{9}$$

You may find the following result helpful: $\mathrm{Tr}(\sigma^a\sigma^b) = 2\delta_{ab}$ where $a, b = x, y, z$.