# Statistical Physics & Condensed Matter Theory I: Exercise

## Superexchange and antiferromagnetism: Solutions

**a)** Action of $\hat{H}_t$ on $S^z_{\text{tot}} = 0$ states:

$$\hat{H}_t|s_1\rangle = -t\sum_\sigma (a^\dagger_{1\sigma}a_{2\sigma} + a^\dagger_{2\sigma}a_{1\sigma})a^\dagger_{1\uparrow}a^\dagger_{2\downarrow}|0\rangle = -t(a^\dagger_{1\uparrow}a^\dagger_{1\downarrow}|0\rangle + a^\dagger_{2\uparrow}a^\dagger_{2\downarrow}|0\rangle)$$
$$= -t(|d_1\rangle + |d_2\rangle) = \hat{H}_t|s_2\rangle$$
$$\hat{H}_t|d_1\rangle = ... = -t(|s_1\rangle + |s_2\rangle) = \hat{H}_t|d_2\rangle.$$

The action of $\hat{H}_u$ is very simple:

$$\hat{H}_U|s_i\rangle = 0, \qquad \hat{H}_U|d_i\rangle = U|d_i\rangle.$$

**b)** The first part simply requires expanding the exponentials to order $t^2$ on both sides:

$$\hat{H}' = (1 + it\hat{O} - \frac{t^2}{2}\hat{O}^2 + ...)\hat{H}(1 - it\hat{O} - \frac{t^2}{2}\hat{O}^2 + ...)$$
$$= \hat{H} + it[\hat{O},\hat{H}] + t^2(\hat{O}\hat{H}\hat{O} - \frac{1}{2}(\hat{O}^2\hat{H} + \hat{H}\hat{O}^2)) + ... = \hat{H} + it[\hat{O},\hat{H}] - \frac{t^2}{2}[\hat{O},[\hat{O},\hat{H}]] + ...$$

The second part is obtained by straight substitution:

$$\text{Linear in t of}(\hat{H} + it[\hat{O},\hat{H}] - \frac{t^2}{2}[\hat{O},[\hat{O},\hat{H}]] + ...) = \hat{H}_t + it[\hat{O},\hat{H}_U].$$

The third part becomes:

$$\hat{H}' = \hat{H}_t + \hat{H}_U + it[\hat{O},\hat{H}_t] + it[\hat{O},\hat{H}_U] - \frac{t^2}{2}[\hat{O},[\hat{O},\hat{H}_t]] - \frac{t^2}{2}[\hat{O},[\hat{O},\hat{H}_U]] + O(t^3)$$
$$= \hat{H}_U - it[\hat{H}_t,\hat{O}] + (O(t^3)) - \frac{it}{2}[\hat{O},\hat{H}_t] + O(t^3)$$

so we get

$$\hat{H}' = \hat{H}_U + \frac{it}{2}[\hat{O},\hat{H}_t] + O(t^3)$$

**c)** We have

$$[\hat{0},\hat{H}_U] = i\alpha U[\begin{pmatrix} \mathbf{0} & -\mathbf{f} \\ \mathbf{f} & \mathbf{0} \end{pmatrix}, \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix}] = -i\alpha U \begin{pmatrix} \mathbf{0} & \mathbf{f} \\ \mathbf{f} & \mathbf{0} \end{pmatrix} = i\alpha\frac{U}{t}H_t$$

so $\alpha = i/U$. Proving the relation using the second way:

$$[\hat{H}_U,\hat{O}] = \hat{H}_U\hat{O} - \hat{O}\hat{H}_U = \frac{i}{Ut}\left(\hat{H}_U\hat{P}_s\hat{H}_t\hat{P}_d - \hat{H}_U\hat{P}_d\hat{H}_t\hat{P}_s - \hat{P}_s\hat{H}_t\hat{P}_d\hat{H}_U + \hat{P}_d\hat{H}_t\hat{P}_s\hat{H}_U\right)$$

Using the fact that $\hat{H}_U\hat{P}_s = 0 = \hat{P}_s\hat{H}_U$, $\hat{H}_U\hat{P}_d = U\hat{P}_d = \hat{P}_d\hat{H}_U$, we get

$$[\hat{H}_U, \hat{O}] = \frac{i}{Ut}\left(0 - U\hat{P}_d\hat{H}_t\hat{P}_s - U\hat{P}_s\hat{H}_t\hat{P}_d + 0\right) = \frac{-i}{t}\hat{H}_t$$

since $\hat{P}_s\hat{H}_t\hat{P}_s = 0 = \hat{P}_d\hat{H}_t\hat{P}_d$ and $\hat{P}_s + \hat{P}_d = \mathbf{1}$.

**d)** Substituting and projecting onto singly-occupied subspace,

$$\hat{P}_s\hat{H}'\hat{P}_s = \frac{it}{2}\hat{P}_s[\hat{O}, \hat{H}_t]\hat{P}_s = \frac{-1}{2U}\hat{P}_s\left(\hat{H}_t\hat{P}_s\hat{H}_t\hat{P}_d - \hat{P}_s\hat{H}_t\hat{P}_d\hat{H}_t - \hat{H}_t\hat{P}_d\hat{H}_t\hat{P}_s + \hat{P}_d\hat{H}_t\hat{P}_s\hat{H}_t\right)\hat{P}_s$$
$$= \frac{-1}{U}\hat{P}_s\hat{H}_t\hat{P}_d\hat{H}_t\hat{P}_s$$

We have

$$\hat{H}_t\hat{P}_d\hat{H}_t = \hat{H}_t\sum_i |d_i\rangle\langle d_i|\hat{H}_t = 2t^2(|s_1\rangle + |s_2\rangle)(\langle s_1| + \langle s_2|)$$
$$= 2t^2(\sum_i |s_i\rangle\langle s_i| + |s_1\rangle\langle s_2| + |s_2\rangle\langle s_1|)$$

**e)** But the earlier $\mathbb{P}$ permutation operator switches the spins on 1 and 2, *i.e.* $\mathbb{P}|s_1\rangle = \mathbb{P}a^\dagger_{1\uparrow}a^\dagger_{2\downarrow}|0\rangle = a^\dagger_{1\downarrow}a^\dagger_{2\uparrow}|0\rangle = -a^\dagger_{2\uparrow}a^\dagger_{1\downarrow}|0\rangle = -|s_2\rangle$ so this operator is represented in this subspace as $\mathbb{P} = -(|s_1\rangle\langle s_2| + |s_2\rangle\langle s_1|)$. We therefore get

$$\hat{P}_s\hat{H}_t\hat{P}_d\hat{H}_t\hat{P}_s = 2t^2(\mathbf{1} - \mathbb{P})$$

With our earlier result that

$$\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 = -\frac{1}{4}\mathbf{1} + \frac{1}{2}\mathbb{P} \qquad \rightarrow \mathbf{1} - \mathbb{P} = -2(\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 - \frac{1}{4})$$

we get

$$P_s\hat{H}'P_s = J\left(\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 - \frac{1}{4}\right)$$

with $J = 4\frac{t^2}{U}$ is the **antiferromagnetic exchange** strength.