Notes for exercise sheet 8

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Exercise 1

As given in a previous exercise, the bcc lattice has 8 nearest neighbours at the positions:

$$\vec{n}_1 = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}, \ \vec{n}_2 = \begin{pmatrix} -1/2 \\ 1/2 \\ 1/2 \end{pmatrix}, \ \vec{n}_3 = \begin{pmatrix} 1/2 \\ -1/2 \\ 1/2 \end{pmatrix}, \ \vec{n}_4 = \begin{pmatrix} 1/2 \\ 1/2 \\ -1/2 \end{pmatrix} \tag{1}$$

$$\vec{n}_5 = \begin{pmatrix} -1/2 \\ -1/2 \\ 1/2 \end{pmatrix}, \ \vec{n}_6 = \begin{pmatrix} -1/2 \\ 1/2 \\ -1/2 \end{pmatrix}, \ \vec{n}_7 = \begin{pmatrix} 1/2 \\ -1/2 \\ -1/2 \end{pmatrix}, \ \vec{n}_8 = \begin{pmatrix} -1/2 \\ -1/2 \\ -1/2 \end{pmatrix}. \tag{2}$$

The antiferromagnetic dispersion relation is given by:

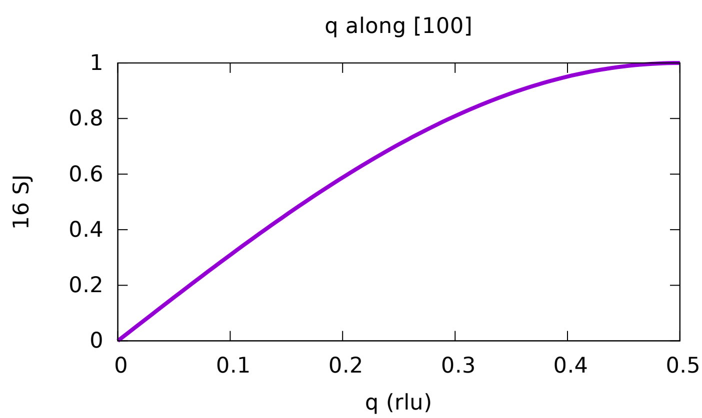
$$E = 2S \cdot \left[\left(\sum_{j \epsilon \{1,..,8\}} J_j \right)^2 - \left(\sum_{j \epsilon \{1,..,8\}} J_j \exp\left(-i2\pi \vec{q} \cdot \vec{n}_j\right) \right)^2 \right]^{1/2} \tag{3}$$

$$E = 2S \cdot \left[64J^2 - \left(\sum_{j \epsilon \{1,..,8\}} J_j \exp\left(-i2\pi \vec{q} \cdot \vec{n}_j\right) \right)^2 \right]^{1/2} \tag{4}$$

- Along an [100] direction:

$$E_{[100]} = 2S \cdot \left[64J^2 - \left(4J \exp\left(-i\pi q_x\right) + 4J \exp\left(i\pi q_x\right)\right)^2 \right]^{1/2} \tag{5}$$

$$E_{[100]} = 2S \cdot \left[64J^2 - 64J^2 \cos^2\left(\pi q_x\right) \right]^{1/2} = 16SJ \cdot \left[1 - \cos^2\left(\pi q_x\right) \right]^{1/2} \tag{6}$$



- Along an [110] direction:

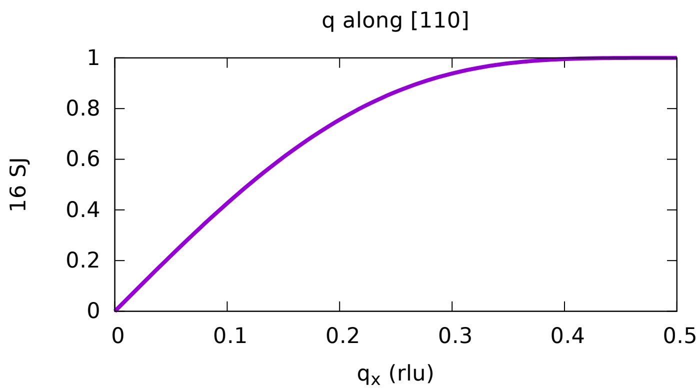
$$E_{[110]} = 2S\cdot\left[64J^2 - \left(2J\exp\left(i\pi q_x + i\pi q_y\right) + 2J\exp\left(-i\pi q_x - i\pi q_y\right) + \overbrace{2J\exp\left(-i\pi q_x + i\pi q_y\right)}^{=2J} + \overbrace{2J\exp\left(i\pi q_x - i\pi q_y\right)}^{=2J}\right)^2\right]^{1/2} \tag{7}$$

Using $q_x = q_y$:

$$E_{[110]} = 2S\cdot\left[64J^2 - \left(4J + 2J\exp\left(i2\pi q_x\right) + 2J\exp\left(-i2\pi q_x\right)\right)^2\right]^{1/2} \tag{8}$$

$$E_{[110]} = 2S\cdot\left[64J^2 - \left(4J\left(1+\cos\left(2\pi q_x\right)\right)\right)^2\right]^{1/2} \tag{9}$$

$$E_{[110]} = 8SJ\cdot\left[4 - \left(1+\cos\left(2\pi q_x\right)\right)^2\right]^{1/2} \tag{10}$$



Exercise 2

$$\mathcal{H} = -J\vec{S}_1\cdot\vec{S}_2 = -J\left(S_{1,x}S_{2,x} + S_{1,y}S_{2,y} + S_{1,z}S_{2,z}\right) \tag{11}$$

Using the ladder operators $S^{\pm} = S_x \pm iS_y$:

$$\mathcal{H} = -\frac{1}{2}J\left(S_1^+S_2^- + S_1^-S_2^+\right) - JS_{1,z}S_{2,z} \tag{12}$$

Applying the Hamilton to the four possible 2-spin states:

$$\mathcal{H}\left|\uparrow\uparrow\right\rangle = -\frac{1}{2}J\left(0+0\right) - J\frac{1}{2}\frac{1}{2}\left|\uparrow\uparrow\right\rangle = -\frac{1}{4}\left|\uparrow\uparrow\right\rangle \tag{13}$$

$$\mathcal{H}\left|\downarrow\downarrow\right\rangle = -\frac{1}{2}J\left(0+0\right) - J\frac{1}{2}\frac{1}{2}\left|\downarrow\downarrow\right\rangle = -\frac{1}{4}\left|\downarrow\downarrow\right\rangle \tag{14}$$

$$\mathcal{H}\left|\uparrow\downarrow\right\rangle = -\frac{1}{2}J\left(\left|\uparrow\downarrow\right\rangle + 0\right) + J\frac{1}{2}\frac{1}{2}\left|\uparrow\downarrow\right\rangle = -\frac{1}{2}J\left|\uparrow\downarrow\right\rangle + \frac{1}{4}J\left|\uparrow\downarrow\right\rangle \tag{15}$$

$$\mathcal{H}\left|\downarrow\uparrow\right\rangle = -\frac{1}{2}J\left(0 + \left|\downarrow\uparrow\right\rangle\right) + J\frac{1}{2}\frac{1}{2}\left|\downarrow\uparrow\right\rangle = -\frac{1}{2}J\left|\downarrow\uparrow\right\rangle + \frac{1}{4}J\left|\downarrow\uparrow\right\rangle \tag{16}$$

The mixed eigenstates are found to be:

- triplet state:

$$|t\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \tag{17}$$

$$\mathcal{H}\,|t\rangle = \frac{1}{\sqrt{2}}\left(-\frac{J}{4}\,|\uparrow\downarrow\rangle - \frac{J}{4}\,|\downarrow\uparrow\rangle\right) \qquad \text{eigenvalue} : -\frac{J}{4} \tag{18}$$

- singlet state:

$$|s\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \tag{19}$$

$$\mathcal{H}\,|s\rangle = \frac{1}{\sqrt{2}}\left(\frac{3}{4}J\,|\uparrow\downarrow\rangle - \frac{3}{4}J\,|\downarrow\uparrow\rangle\right) \qquad \text{eigenvalue} : \frac{3}{4}J \tag{20}$$