統計物理学 No.2

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(a)

2 スピン系の XXZ 相互作用ハミルトニアンは

$$\begin{aligned} H &= J(S_1^x S_2^x + S_1^y S_2^y + \Delta S_1^z S_2^z) - h(S_1^z + S_2^z) \\ &= \frac{J}{2}(S_1^+ S_2^- + S_2^+ S_1^-) + J\Delta S_1^z S_2^z - h(S_1^z + S_2^z) \end{aligned} \tag{1}$$

である. このとき

$$\begin{aligned} H\left|\uparrow\uparrow\right\rangle &= \frac{J}{2}\left(0 \otimes S_2^- \left|\uparrow\right\rangle + 0 \otimes S_1^- \left|\uparrow\right\rangle\right) + J\Delta S_1^z \left|\uparrow\right\rangle \otimes S_2^z \left|\uparrow\right\rangle - h\left(S_1^z \left|\uparrow\right\rangle \otimes \left|\uparrow\right\rangle + \left|\uparrow\right\rangle \otimes S_2^z \left|\uparrow\right\rangle\right) \\ &= 0 + J\Delta \frac{1}{2}\left|\uparrow\right\rangle \otimes \frac{1}{2}\left|\uparrow\right\rangle - h\left(\frac{1}{2}\left|\uparrow\right\rangle \otimes \left|\uparrow\right\rangle + \left|\uparrow\right\rangle \otimes \frac{1}{2}\left|\uparrow\right\rangle\right) \\ &= \left(\frac{J\Delta}{4} - h\right)\left|\uparrow\uparrow\right\rangle \end{aligned} \tag{2}$$

$$\begin{aligned} H\left|\downarrow\downarrow\right\rangle &= \frac{J}{2}\left(S_1^+ \left|\downarrow\right\rangle \otimes 0 + S_2^+ \left|\downarrow\right\rangle \otimes 0\right) + J\Delta S_1^z \left|\downarrow\right\rangle \otimes S_2^z \left|\downarrow\right\rangle - h\left(S_1^z \left|\downarrow\right\rangle \otimes \left|\downarrow\right\rangle + \left|\downarrow\right\rangle \otimes S_2^z \left|\downarrow\right\rangle\right) \\ &= 0 + J\Delta \left(-\frac{1}{2}\left|\downarrow\right\rangle\right) \otimes \left(-\frac{1}{2}\left|\downarrow\right\rangle\right) - h\left(\left(-\frac{1}{2}\left|\downarrow\right\rangle\right) \otimes \left|\downarrow\right\rangle + \left|\downarrow\right\rangle \otimes \left(-\frac{1}{2}\left|\downarrow\right\rangle\right)\right) \\ &= \left(\frac{J\Delta}{4} + h\right)\left|\downarrow\downarrow\right\rangle \end{aligned} \tag{3}$$

$$\begin{aligned} H\left|\uparrow\downarrow\right\rangle &= \frac{J}{2}\left(0 \otimes 0 + S_2^+ \left|\downarrow\right\rangle \otimes S_1^- \left|\uparrow\right\rangle\right) + J\Delta S_1^z \left|\uparrow\right\rangle \otimes S_2^z \left|\downarrow\right\rangle - h\left(S_1^z \left|\uparrow\right\rangle \otimes \left|\downarrow\right\rangle + \left|\uparrow\right\rangle \otimes S_2^z \left|\downarrow\right\rangle\right) \\ &= \frac{J}{2}\left|\downarrow\right\rangle \otimes \left|\uparrow\right\rangle + J\Delta \frac{1}{2}\left|\uparrow\right\rangle \otimes \left(-\frac{1}{2}\left|\downarrow\right\rangle\right) - h\left(\frac{1}{2}\left|\uparrow\right\rangle \otimes \left|\downarrow\right\rangle + \left|\uparrow\right\rangle \otimes \left(-\frac{1}{2}\left|\downarrow\right\rangle\right)\right) \\ &= \frac{J}{2}\left|\downarrow\uparrow\right\rangle - \frac{J\Delta}{4}\left|\uparrow\downarrow\right\rangle \end{aligned} \tag{4}$$

$$
\begin{aligned}
H\left|\downarrow\uparrow\right\rangle &= \frac{J}{2}\big(S_1^+\left|\downarrow\right\rangle \otimes S_2^-\left|\uparrow\right\rangle + 0\otimes 0\big) + J\Delta S_1^z\left|\downarrow\right\rangle \otimes S_2^z\left|\uparrow\right\rangle - h\left(S_1^z\left|\downarrow\right\rangle \otimes \left|\uparrow\right\rangle + \left|\downarrow\right\rangle \otimes S_2^z\left|\uparrow\right\rangle\right) \\
&= \frac{J}{2}\left|\uparrow\right\rangle \otimes \left|\downarrow\right\rangle + J\Delta\left(-\frac{1}{2}\left|\downarrow\right\rangle\right) \otimes \frac{1}{2}\left|\uparrow\right\rangle - h\left(\left(-\frac{1}{2}\left|\downarrow\right\rangle\right) \otimes \left|\uparrow\right\rangle + \left|\downarrow\right\rangle \otimes \frac{1}{2}\left|\uparrow\right\rangle\right) \\
&= \frac{J}{2}\left|\uparrow\downarrow\right\rangle - \frac{J\Delta}{4}\left|\downarrow\uparrow\right\rangle
\end{aligned}
\tag{5}
$$

である. ここで

$$
\left|t_{+1}\right\rangle = \left|\uparrow\uparrow\right\rangle,\ \left|t_{-1}\right\rangle = \left|\downarrow\downarrow\right\rangle,\ \left|t_0\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle\right),\ \left|s\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right) \tag{6}
$$

は固有状態であり, それぞれの固有値は

$$
H\left|t_{+1}\right\rangle = \left(\frac{J\Delta}{4} - h\right)\left|t_{+1}\right\rangle \tag{7}
$$

$$
H\left|t_{-1}\right\rangle = \left(\frac{J\Delta}{4} + h\right)\left|t_{-1}\right\rangle \tag{8}
$$

$$
\begin{aligned}
H\left|t_0\right\rangle &= \frac{1}{\sqrt{2}}\left(\frac{J}{2}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right) - \frac{J\Delta}{4}\left(\left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle\right)\right) \\
&= \left(\frac{J}{2} - \frac{J\Delta}{4}\right)\left|t_0\right\rangle
\end{aligned}
\tag{9}
$$

$$
\begin{aligned}
H\left|s\right\rangle &= \frac{1}{\sqrt{2}}\left(-\frac{J}{2}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right) - \frac{J\Delta}{4}\left(\left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle\right)\right) \\
&= -\left(\frac{J}{2} + \frac{J\Delta}{4}\right)\left|s\right\rangle
\end{aligned}
\tag{10}
$$

となる.

(b)(i)

$\left|t_{\pm 1}\right\rangle$ のエネルギーは $h = 0$ において $J\Delta/4$ である. $\Delta \geq 1$ のとき $h \geq 0$ において $E_{t_{+1}}$ は E_{t_0}, E_s とそれぞれ一回ずつ交点をもち, その値は

$$
\begin{aligned}
\frac{J\Delta}{4} - h &= \frac{J}{2} - \frac{J\Delta}{4} \\
\iff \qquad h &= \frac{J}{2}(\Delta - 1)
\end{aligned}
\tag{11}
$$

$$
\begin{aligned}
\frac{J\Delta}{4} - h &= -\frac{J}{2} - \frac{J\Delta}{4} \\
\iff \qquad h &= \frac{J}{2}(\Delta + 1)
\end{aligned}
\tag{12}
$$

である. したがってエネルギースペクトルは図 1 のようになる. 図 1 から $h \leq J/2(\Delta+1)$ での基底状態は $|s\rangle$, $h > J/2(\Delta+1)$ での基底状態は $|t_{+1}\rangle$ である. それぞれの状態での磁化の期待値は

$$\begin{aligned} \langle s \,|\, S_1^z + S_2^z \,|\, s\rangle &= \langle s|\,(S_1^z + S_2^z)\frac{1}{\sqrt{2}}\,(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \\ &= \langle s|\,\frac{1}{\sqrt{2}}\,(S_1^z\,|\uparrow\downarrow\rangle - S_1^z\,|\downarrow\uparrow\rangle + S_2^z\,|\uparrow\downarrow\rangle - S_2^z\,|\downarrow\uparrow\rangle) \\ &= \langle s|\,\frac{1}{\sqrt{2}}\left(\frac{1}{2}\,|\uparrow\downarrow\rangle + \frac{1}{2}\,|\downarrow\uparrow\rangle - \frac{1}{2}\,|\uparrow\downarrow\rangle - \frac{1}{2}\,|\downarrow\uparrow\rangle\right) \\ &= 0 \end{aligned} \tag{13}$$

$$\begin{aligned} \langle t_{+1} \,|\, S_1^z + S_2^z \,|\, t_{+1}\rangle &= \langle\uparrow\uparrow|\,(S_1^z + S_2^z)\,|\uparrow\uparrow\rangle \\ &= \langle\uparrow\uparrow|\left(\frac{1}{2} + \frac{1}{2}\right)|\uparrow\uparrow\rangle = 1 \end{aligned} \tag{14}$$

したがって磁化の期待値は図 2 のように振る舞う.

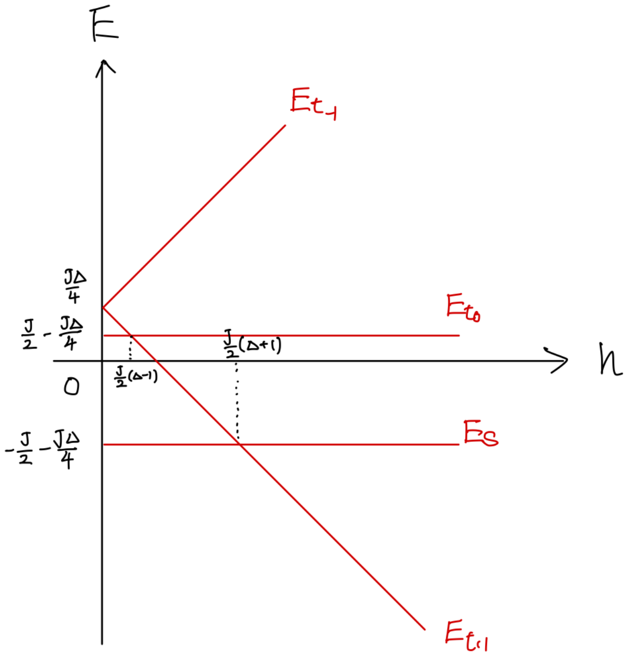

図 1　$\Delta \geq 1$ の場合のエネルギースペクトル

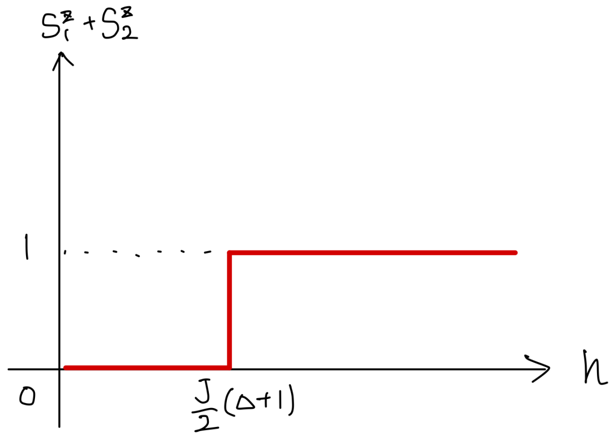

図 2　$\Delta \geq 1$ の場合の磁化の期待値

(b)(ii)