相互作用のない系での静的一様磁場に対する帯磁率　(T. Matsumura, 2011.3.17)

(2011. 3. 17)

〈静磁場 $\vec{H}$ に対する帯磁率〉

$$\mathcal{H} = \mathcal{H}_0 + g\mu_B \vec{J}\cdot\vec{H} = \mathcal{H}_0 + g\mu_B \sum_\alpha J_\alpha H_\alpha \qquad (\alpha = x, y, z)$$

$$\mathcal{H}_0 \varphi_n = \mathcal{E}_n^0 \varphi_n$$

$$\mathcal{E}_n = \mathcal{E}_n + g\mu_B \sum_\alpha H_\alpha \langle n|J_\alpha|n\rangle + g^2\mu_B^2 \sum_m \frac{\langle n|\sum_\alpha J_\alpha H_\alpha|m\rangle\langle m|\sum_\beta J_\beta H_\beta|n\rangle}{\mathcal{E}_n^0 - \mathcal{E}_m^0} \qquad ①$$

$$Z = \sum_n e^{-\mathcal{E}_n/\tau}, \qquad F = -\tau \log Z \qquad ②$$

ここは第0近似で $\mathcal{E}_n^0$ を使う.

$$\frac{\partial F}{\partial H_\alpha} = -\frac{\tau}{Z}\frac{\partial Z}{\partial H_\alpha} = -\frac{\tau}{Z}\sum_n\left(-\frac{1}{\tau}\right)e^{-\mathcal{E}_n^0/\tau}\frac{\partial \mathcal{E}_n}{\partial H_\alpha} = \frac{1}{Z}\sum_n e^{-\mathcal{E}_n^0/\tau}\frac{\partial \mathcal{E}_n}{\partial H_\alpha} = \left\langle\frac{\partial E}{\partial H_\alpha}\right\rangle = -M_\alpha \qquad ③$$

$$\frac{\partial^2 F}{\partial H_\beta \partial H_\alpha} = -\frac{1}{Z^2}\frac{\partial Z}{\partial H_\beta}\cdot\sum_n e^{-\mathcal{E}_n^0/\tau}\frac{\partial \mathcal{E}_n}{\partial H_\alpha} + \frac{1}{Z}\sum_n\left(-\frac{1}{\tau}\right)e^{-\mathcal{E}_n^0/\tau}\left(\frac{\partial \mathcal{E}_n}{\partial H_\beta}\right)\cdot\left(\frac{\partial \mathcal{E}_n}{\partial H_\alpha}\right)$$
$$+ \frac{1}{Z}\sum_n e^{-\mathcal{E}_n^0/\tau}\frac{\partial^2 \mathcal{E}_n}{\partial H_\beta \partial H_\alpha}$$
$$= -\frac{1}{Z^2}\left\{\sum_n\left(-\frac{1}{\tau}\right)e^{-\mathcal{E}_n^0/\tau}\frac{\partial \mathcal{E}_n}{\partial H_\beta}\right\}\cdot\left\{\sum_n e^{-\mathcal{E}_n^0/\tau}\frac{\partial \mathcal{E}_n}{\partial H_\alpha}\right\} - \frac{1}{\tau}\cdot\frac{1}{Z}\sum_n e^{-\mathcal{E}_n^0/\tau}\left(\frac{\partial \mathcal{E}_n}{\partial H_\beta}\right)\cdot\left(\frac{\partial \mathcal{E}_n}{\partial H_\alpha}\right)$$
$$+ \frac{1}{Z}\sum_n e^{-\mathcal{E}_n^0/\tau}\frac{\partial^2 \mathcal{E}_n}{\partial H_\beta \partial H_\alpha}$$

帯磁率はFの2回微分

$$= \left\langle\frac{\partial^2 E}{\partial H_\beta \partial H_\alpha}\right\rangle - \frac{1}{\tau}\underbrace{\left\{\left\langle\left(\frac{\partial E}{\partial H_\beta}\right)\cdot\left(\frac{\partial E}{\partial H_\alpha}\right)\right\rangle - \left\langle\frac{\partial E}{\partial H_\beta}\right\rangle\left\langle\frac{\partial E}{\partial H_\alpha}\right\rangle\right\}} = -\chi_{\alpha\beta} \qquad ④$$

↳ $\alpha = \beta$ のとき. $\langle M_\alpha^2\rangle - \langle M_\alpha\rangle^2 = \langle(M_\alpha - \langle M_\alpha\rangle)^2\rangle = \langle\Delta M_\alpha^2\rangle$

であり、これは "磁化のゆらぎ" のこと.

①より、

$$\left\langle\frac{\partial^2 E}{\partial H_\beta \partial H_\alpha}\right\rangle = \frac{g^2\mu_B^2}{Z}\sum_n e^{-\mathcal{E}_n^0/\tau}\sum_m\left(\frac{\langle n|J_\alpha|m\rangle\langle m|J_\beta|n\rangle}{\mathcal{E}_n^0 - \mathcal{E}_m^0} + \frac{\langle n|J_\beta|m\rangle\langle m|J_\alpha|n\rangle}{\mathcal{E}_n^0 - \mathcal{E}_m^0}\right) \qquad ⑤$$

$$\left\langle\left(\frac{\partial E}{\partial H_\beta}\right)\left(\frac{\partial E}{\partial H_\alpha}\right)\right\rangle = \frac{g^2\mu_B^2}{Z}\sum_n e^{-\mathcal{E}_n^0/\tau}\langle n|J_\alpha|n\rangle\langle n|J_\beta|n\rangle \qquad ⑥$$

$$\left\langle\frac{\partial E}{\partial H_\beta}\right\rangle\left\langle\frac{\partial E}{\partial H_\alpha}\right\rangle = g^2\mu_B^2\left(\sum_n \frac{e^{-\mathcal{E}_n^0/\tau}}{Z}\langle n|J_\alpha|n\rangle\right)\left(\sum_n \frac{e^{-\mathcal{E}_n^0/\tau}}{Z}\langle n|J_\beta|n\rangle\right) \qquad ⑦$$

従って、

$$\chi_{\alpha\beta} = \frac{g^2\mu_B^2}{Z}\sum_n e^{-\mathcal{E}_n^0/\tau}\left\{\frac{\langle n|J_\alpha|n\rangle\langle n|J_\beta|n\rangle}{\tau} - \sum_m \frac{\langle n|J_\alpha|m\rangle\langle m|J_\beta|n\rangle + \langle n|J_\beta|m\rangle\langle m|J_\alpha|n\rangle}{\mathcal{E}_n^0 - \mathcal{E}_m^0}\right\}$$
$$- \frac{g^2\mu_B^2}{\tau}\left(\sum_n \frac{e^{-\mathcal{E}_n^0/\tau}}{Z}\langle n|J_\alpha|n\rangle\right)\left(\sum_n \frac{e^{-\mathcal{E}_n^0/\tau}}{Z}\langle n|J_\beta|n\rangle\right) \qquad ⑧$$

← 有限の期待値をもつ部分を差し引くことに相当

$$= \chi_{\alpha\beta}(\text{curie}) + \chi_{\alpha\beta}(\text{VV}) - \chi_{\alpha\beta}(\text{ave})$$

$$\chi_{\alpha\beta}(\text{VV}) = -\frac{g^2\mu_B^2}{Z}\cdot\sum_{n,m}\frac{1}{2}\frac{\langle n|J_\alpha|m\rangle\langle m|J_\beta|n\rangle + \langle n|J_\beta|m\rangle\langle m|J_\alpha|n\rangle}{\mathcal{E}_n^0 - \mathcal{E}_m^0}\cdot\underbrace{\left(e^{-\mathcal{E}_n^0/\tau} - e^{-\mathcal{E}_m^0/\tau}\right)}$$

$$= e^{-\mathcal{E}_n^0/\tau}\underbrace{\left\{1 - e^{(\mathcal{E}_n^0 - \mathcal{E}_m^0)/\tau}\right\}}$$

↓ $|\mathcal{E}_n - \mathcal{E}_m| \ll \tau$ のとき

$$\approx -\frac{\mathcal{E}_n^0 - \mathcal{E}_m^0}{\tau}$$

$|\mathcal{E}_n - \mathcal{E}_m| \ll \tau$ のとき

$$\approx \frac{g^2\mu_B^2}{Z}\sum_{n,m} e^{-\mathcal{E}_n^0/\tau}\frac{\langle n|J_\alpha|m\rangle\langle m|J_\beta|n\rangle + \langle n|J_\beta|m\rangle\langle m|J_\alpha|n\rangle}{2\tau}$$

↳ $\chi_{\alpha\beta}(\text{curie})$ と. 計算上. 同一にできる.