Aufgabe 35

a) $$\hat{H} = \underbrace{-\mu B \sum_{i=1}^{N} \hat{\sigma}_z^{(i)}}_{\text{Energie der } N \text{ magn. Momente im B-Feld}} - \underbrace{I \sum_{i=1}^{N} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(i+1)}}_{\text{Wechselwirkung zwischen nächsten Nachbarn: } i \leftrightarrow i+1}$$

mögliche Energiewerte ohne WW : $\pm \mu B$

b) $$Z = Sp\left(e^{-\frac{1}{k_BT}\hat{H}} \right)$$

$$= Sp\left(\exp\left\{ \frac{\mu B}{k_BT} \sum_{i=1}^{N} \hat{\sigma}_z^{(i)} + \frac{I}{k_BT} \sum_{i=1}^{N} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(i+1)} \right\} \right)$$

Basis: $\left\{ |+\rangle^{(1)}, |-\rangle^{(1)} \right\} \otimes \left\{ |+\rangle^{(2)}, |-\rangle^{(2)} \right\} \otimes \dots \otimes \left\{ |+\rangle^{(N)}, |-\rangle^{(N)} \right\}$

mit $\hat{\sigma}_z^{(i)} |\sigma_i\rangle^{(i)} = \sigma_i |\sigma_i\rangle^{(i)}$, $\sigma_i = \pm 1$

$\Rightarrow$ Jetzt explizite Spurbildung mit dieser Basis:

$$Z = \sum_{\sigma_1=\pm1} \sum_{\sigma_2=\pm1} \dots \sum_{\sigma_N=\pm1} {}^{(1)}\langle\sigma_1| {}^{(2)}\langle\sigma_2| \dots {}^{(N)}\langle\sigma_N| \exp\left\{ \frac{\mu B}{k_BT} \sum_{j=1}^{N} \hat{\sigma}_z^{(j)} + \frac{I}{k_BT} \sum_{j=1}^{N} \hat{\sigma}_z^{(j)} \hat{\sigma}_z^{(j+1)} \right\} |\sigma_1\rangle^{(1)} \dots |\sigma_N\rangle^{(N)}$$

$$= \sum_{\substack{\sigma_1=\pm1 \\ \vdots \\ \sigma_N=\pm1}} \exp\left\{ \frac{\mu B}{k_BT} \sum_{i=1}^{N} \sigma_i + \frac{I}{k_BT} \sum_{i=1}^{N} \sigma_i \sigma_{i+1} \right\}$$

Jetzt: $$\sum_{i=1}^{N} \sigma_i = \frac{1}{2} \left(\sum_{i=1}^{N} \sigma_i + \sum_{i=1}^{N} \sigma_i \right)$$

$$= \frac{1}{2} \sum_{i=1}^{N} \sigma_i + \frac{1}{2} \left(\sum_{i=1}^{N-1} \sigma_{i+1} + \sigma_1 \right)$$

$$= \frac{1}{2} \sum_{i=1}^{N} \sigma_i + \frac{1}{2} \left(\sum_{i=1}^{N-1} \sigma_{i+1} + \sigma_{N+1} \right) \quad \text{, da } \mu_{N+1} = \mu_1$$

$$= \frac{1}{2} \sum_{i=1}^{N} \sigma_i + \frac{1}{2} \sum_{i=1}^{N} \sigma_{i+1} = \frac{1}{2} \sum_{i=1}^{N} (\sigma_i + \sigma_{i+1})$$

$$\Rightarrow Z = \sum_{\substack{\sigma_1=\pm1 \\ \sigma_N=\pm1}} \exp\left\{ \frac{1}{2} \frac{\mu B}{k_BT} \sum_{i=1}^{N} (\sigma_i + \sigma_{i+1}) + \frac{I}{k_BT} \sum_{i=1}^{N} \sigma_i \sigma_{i+1} \right\}$$

$$= \sum_{\substack{\sigma_1=\pm1 \\ \vdots \\ \sigma_N=\pm1}}' e^{\frac{1}{2}\frac{\mu B}{k_B T}(\sigma_1+\sigma_2)+\frac{I}{k_B T}\sigma_1\sigma_2} \cdots e^{\frac{1}{2}\frac{\mu B}{k_B T}(\sigma_{N-1}+\sigma_N)+\frac{I}{k_B T}\sigma_{N-1}\sigma_N} \, e^{\frac{1}{2}\frac{\mu B}{k_B T}(\sigma_N+\sigma_1)+\frac{I}{k_B T}\sigma_N\sigma_1}$$

$$= \underbrace{\sum_{\substack{\sigma_1=\pm1 \\ \vdots \\ \sigma_N=\pm1}}' P_{\sigma_1,\sigma_2} \cdot P_{\sigma_2,\sigma_3} \cdot \ldots \cdot P_{\sigma_{N-1},\sigma_N} \cdot P_{\sigma_N,\sigma_1}}_{\text{Matrixmultiplikation mit anschließender Spurbildung}} \quad , \quad P_{\sigma,\sigma'} = e^{\frac{1}{2}\frac{\mu B}{k_B T}(\sigma+\sigma')+\frac{I}{k_B T}\sigma\sigma'}$$

$$Sp(A \cdot B) = \sum_i' (A \cdot B)_{ii} = \sum_i' \sum_j' A_{ij} B_{ji}$$

$$\Rightarrow \quad Z = Sp(P^N) \quad \text{mit}$$

$$P = \begin{pmatrix} P_{++} & P_{+-} \\ P_{-+} & P_{--} \end{pmatrix} = \begin{pmatrix} e^{\frac{I+\mu B}{k_B T}} & e^{\frac{-I}{k_B T}} \\ e^{-\frac{I}{k_B T}} & e^{\frac{I-\mu B}{k_B T}} \end{pmatrix}$$

c) <u>Diagonalisieren:</u>

$$P = U \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} U^T \quad , \text{mit} \quad UU^T = \mathbb{1} = U^T U$$

$$P^N = U \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} U^T U \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} U^T \ldots U \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} U^T = U \begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix} U^T$$

$$Z = Sp(P^N) = Sp\left(U \begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix} U^T\right) = Sp\left(U^T U \begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix}\right)$$

$$= Sp \begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix} = \lambda_1^N + \lambda_2^N$$

d) <u>explizit:</u> $x = \frac{\mu B}{k_B T}$, $y = \frac{I}{k_B T}$

$$P = \begin{pmatrix} e^{y+x} & e^{-y} \\ e^{-y} & e^{y-x} \end{pmatrix}$$

$$\det \begin{pmatrix} e^{y+x} - \lambda & e^{-y} \\ e^{-y} & e^{y-x} - \lambda \end{pmatrix} = \left(e^{y+x} - \lambda\right)\left(e^{y-x} - \lambda\right) - e^{-2y}$$

$$= e^{2y} - \lambda\left(e^{y+x} + e^{y-x}\right) + \lambda^2 - e^{-2y}$$

$$= \lambda^2 - \lambda e^y \, 2\cosh x + 2\sinh 2y$$

$$\lambda_{1,2} = e^{y}\cosh x \pm \sqrt{e^{2y}\cosh^2 x - 2\sinh 2y}$$

$$= e^{y}\cosh x \pm \sqrt{e^{2y}\cosh^2 x - e^{2y} + e^{-2y}}$$

$$= e^{y}\cosh x \pm \sqrt{e^{2y}(\cosh^2 x - 1) + e^{-2y}}$$

$$= e^{y}\cosh x \pm \sqrt{e^{2y}\sinh^2 x + e^{-2y}}$$

$$= e^{y}\left(\cosh x \pm \sqrt{e^{-4y} + \sinh^2 x}\right) \Rightarrow \lambda_1 \text{ immer} > 0$$

i) $y > 0$: $\lambda_1 \cdot \lambda_2 = 2\sinh 2y > 0$

zusammen mit $\lambda_1 > 0 \Rightarrow \lambda_2 > 0$

Also ist $\lambda_1 > \lambda_2$!

ii) $y < 0$: $\lambda_1 \cdot \lambda_2 = 2\sinh 2y < 0$

zusammen mit $\lambda_1 > 0 \Rightarrow \lambda_2 < 0$

aber $\lambda_1 + \lambda_2 = 2e^{y}\cosh x$

$$|\lambda_1| - |\lambda_2| = 2e^{y}\cosh x$$

Also $|\lambda_2| = |\lambda_1| - \underbrace{2e^{y}\cosh x}_{>0} < |\lambda_1|$

Es gilt also immer $|\lambda_2| < |\lambda_1|$

bzw. $\dfrac{|\lambda_2|}{|\lambda_1|} < 1$

e) $\langle M \rangle = \mu \left\langle \sum_{i=1}^{N} \hat{\sigma}_z^{(i)} \right\rangle \quad , \hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}}$

$$= \mu \, Sp\left(\sum_{i=1}^{N} \hat{\sigma}_z^{(i)} \frac{1}{Z} e^{-\frac{\hat{H}}{k_B T}} \right)$$

$$= \mu \frac{1}{Z} \sum_{\substack{\sigma_1 = \pm 1 \\ \vdots \\ \sigma_N = \pm 1}} \sum_{i=1}^{N} \sigma_i \exp\left(\frac{\mu B}{k_B T} \sum_{j=1}^{N} \sigma_j + \frac{I}{k_B T} \sum_{j=1}^{N} \sigma_j \sigma_{j+1} \right)$$

$$= \mu \frac{\sum\limits_{\substack{\sigma_1 = \pm 1 \\ \vdots \\ \sigma_N = \pm 1}} \sum\limits_{i=1}^{N} \sigma_i \exp\left\{ \frac{\mu B}{k_B T} \sum\limits_{j=1}^{N} \sigma_j + \frac{I}{k_B T} \sum\limits_{j=1}^{N} \sigma_j \sigma_{j+1} \right\}}{\sum\limits_{\substack{\sigma_1 = \pm 1 \\ \vdots \\ \sigma_N = \pm 1}} \exp\left\{ \frac{\mu B}{k_B T} \sum\limits_{j=1}^{N} \sigma_j + \frac{I}{k_B T} \sum\limits_{j=1}^{N} \sigma_j \sigma_{j+1} \right\}}$$

$$= \mu \frac{kT}{\mu} \frac{\partial}{\partial B} \ln \left\{ \sum_{\substack{\sigma_1 = \pm 1 \\ \vdots \\ \sigma_N = \pm 1}} \exp\left\{ \frac{\mu B}{k_B T} \sum_{j=1}^{N} \sigma_j + \frac{I}{k_B T} \sum_{j=1}^{N} \sigma_j \sigma_{j+1} \right\} \right\}$$

$$= k_B T \frac{\partial}{\partial B} \ln Z = -\left(\frac{\partial F}{\partial B} \right)_{T,N} \quad ; F = -k_B T \ln Z$$

f) $Z = \lambda_1^N + \lambda_2^N \quad , \quad F = -k_B T \ln Z = -k_B T \ln(\lambda_1^N + \lambda_2^N) \quad , x = \frac{\mu B}{k_B T}$

$$M = -\frac{\partial F}{\partial B} = k_B T \frac{\partial \ln Z}{\partial B} = k_B T \frac{N \lambda_1^{N-1} \frac{\partial \lambda_1}{\partial B} + N \lambda_2^{N-1} \frac{\partial \lambda_2}{\partial B}}{\lambda_1^N + \lambda_2^N}$$

$$\frac{\partial \lambda_\pm}{\partial B} = \frac{\partial x}{\partial B} \frac{\partial \lambda_\pm}{\partial x} = \frac{\mu}{k_B T} e^{y} \left(\sinh x \pm \frac{2 \sinh x \cosh x}{2\sqrt{e^{-4y} + \sinh^2 x}} \right)$$

$$= \pm \frac{\mu}{k_B T} \frac{\sinh x}{\sqrt{e^{-4y} + \sinh^2 x}} \lambda_\pm$$

$$M = N \mu \frac{\sinh x}{\sqrt{e^{-4y} + \sinh^2 x}} \frac{\lambda_1^N - \lambda_2^N}{\lambda_1^N + \lambda_2^N}$$

$$\boxed{\left(\frac{\lambda_2}{\lambda_1} \right)^N \xrightarrow{N \to \infty} 0}$$

$$= N \mu \frac{\sinh x}{\sqrt{e^{-4y} + \sinh^2 x}} \frac{1 - \left(\frac{\lambda_2}{\lambda_1} \right)^N}{1 + \left(\frac{\lambda_2}{\lambda_1} \right)^N}$$

$$\Rightarrow \lim_{N \to \infty} m = \lim_{N \to \infty} \frac{M}{N} = \lim_{N \to \infty} \mu \frac{\sinh x}{\sqrt{e^{-4y} + \sinh^2 x}}$$