

## Übungen zur Theoretischen Physik F SS 09

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## 1. Ising-Modell

(a)

$$Z(N) = \sum_{\{\sigma_i^z\}} \exp \left[ \frac{J}{k_B T} \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z \right] = \sum_{\{\sigma_i^z\}} \prod_{i=1}^{N-1} \exp \left[ \frac{J}{k_B T} \sigma_i^z \sigma_{i+1}^z \right],$$

$$\exp \left[ \frac{J}{k_B T} \sigma_i^z \sigma_{i+1}^z \right] = \cosh \frac{J}{k_B T} + \sigma_i^z \sigma_{i+1}^z \sinh \frac{J}{k_B T},$$

$$Z(N) = 2^N \left[ \cosh \frac{J}{k_B T} \right]^{N-1}.$$

oder

$$\begin{aligned} Z(3) &= \sum_{\{\sigma_i^z\}} \prod_{i=1}^2 \left( \cosh \frac{J}{k_B T} + \sigma_i^z \sigma_{i+1}^z \sinh \frac{J}{k_B T} \right) \\ &= \sum_{\{\sigma_i^z\}} \left( \cosh^2 \frac{J}{k_B T} + (\sigma_1^z \sigma_2^z + \sigma_2^z \sigma_3^z) \cosh \frac{J}{k_B T} \sinh \frac{J}{k_B T} + \sigma_1^z \sigma_2^z \sigma_2^z \sigma_3^z \sinh^2 \frac{J}{k_B T} \right) \\ &= 2^3 \cosh^2 \frac{J}{k_B T}, \end{aligned} \tag{1}$$

weil

$$\sum_{\{\sigma_i^z\}} \sigma_1^z \sigma_2^z = \sum_{\{\sigma_i^z\}} \sigma_2^z \sigma_3^z = 0,$$

und

$$\sum_{\{\sigma_i^z\}} \sigma_1^z \sigma_2^z \sigma_2^z \sigma_3^z = \sum_{\{\sigma_i^z\}} \sigma_1^z \sigma_3^z = 0.$$

(b)

$$F = -k_B T \ln Z(3) = -3k_B T \ln 2 - 2k_B T \ln \cosh \frac{J}{k_B T}.$$

(c)

$$S = -\frac{\partial F}{\partial T} = 3k_B \ln 2 + 2k_B \ln \cosh \frac{J}{k_B T} - 2 \frac{J}{T} \tanh \frac{J}{k_B T},$$

$$c_H = T \left( \frac{\partial S}{\partial T} \right)_H = \frac{J^2}{k_B T^2} \frac{1}{\cosh^2 [J/(k_B T)]}.$$

(d)

$$\langle \sigma_i^z \rangle = \frac{1}{Z(3)} \sum_{\{\sigma_i^z\}} \sigma_i^z \exp \left[ \frac{J}{k_B T} \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z \right] = 0,$$

weil alle Glieder antisymmetrisch sind.

(e)

$$M(H) = \frac{1}{Z(H, N)} \sum_{\{\sigma_i^z\}} \sum_{j=1}^N \mu \sigma_j^z \exp \left[ \frac{J}{k_B T} \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z + \frac{\mu H}{k_B T} \sum_{i=1}^N \sigma_i^z \right],$$

wobei

$$Z(H, N) = \sum_{\{\sigma_i^z\}} \exp \left[ \frac{J}{k_B T} \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z + \frac{\mu H}{k_B T} \sum_{i=1}^N \sigma_i^z \right].$$

Wenn  $\mu H \ll k_B T$ ,

$$\exp \left[ \frac{\mu H}{k_B T} \sigma_i^z \right] \approx 1 + \frac{\mu H}{k_B T} \sigma_i^z,$$

und  $Z(H, N) \approx Z(N)$ .

Dann

$$M = \chi H,$$

mit

$$\chi = \frac{\mu^2}{k_B T} \sum_{i=1}^N \sum_{j=1}^N \langle \sigma_i^z \sigma_j^z \rangle.$$

$$\langle \sigma_i^z \sigma_j^z \rangle = \frac{1}{Z} \sum_{\{\sigma_i^z\}} \sigma_i^z \sigma_j^z \exp \left[ \frac{J}{k_B T} \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z \right] = \left[ \tanh \frac{J}{k_B T} \right]^{|i-j|}.$$

Für  $N = 3$  [sehen Sie (1)]:

$$\langle (\sigma_i^z)^2 \rangle = 1,$$

$$\langle \sigma_1^z \sigma_2^z \rangle = \langle \sigma_2^z \sigma_3^z \rangle = \frac{1}{Z(3)} 2^3 \cosh \frac{J}{k_B T} \sinh \frac{J}{k_B T} = \tanh \frac{J}{k_B T},$$

$$\langle \sigma_1^z \sigma_3^z \rangle = \frac{1}{Z(3)} 2^3 \sinh^2 \frac{J}{k_B T} = \tanh^2 \frac{J}{k_B T}.$$

$$\sum_{i=1}^N \sum_{j=1}^N \langle \sigma_i^z \sigma_j^z \rangle = 3 + 2 (\langle \sigma_1^z \sigma_2^z \rangle + \langle \sigma_2^z \sigma_3^z \rangle + \langle \sigma_1^z \sigma_3^z \rangle) = 3 + 2 \left( 2 \tanh \frac{J}{k_B T} + \tanh^2 \frac{J}{k_B T} \right).$$

$$M = \frac{\mu^2 H}{k_B T} \left[ 1 + 2 \left( 1 + \tanh \frac{J}{k_B T} \right)^2 \right].$$

(f)

$$\chi = \frac{\mu^2}{k_B T} \left[ 1 + 2 \left( 1 + \tanh \frac{J}{k_B T} \right)^2 \right].$$

## 2. Harmonische Oszillator:

(a)

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

$$Z = \int dx dp e^{-\beta H} = \underbrace{\int dp e^{-\frac{\beta}{2m}p^2}}_{\left(\frac{2\pi m}{\beta}\right)^{1/2}} \underbrace{\int dx e^{-\beta \frac{m}{2}\omega^2 x^2}}_{\left(\frac{2\pi}{\beta m \omega^2}\right)^{1/2}}$$

$$\Rightarrow \boxed{Z = \frac{2\pi k_B T}{\omega}}$$

$$F = -k_B T \ln Z \quad \Rightarrow \quad \boxed{F = -k_B T \ln \frac{2\pi k_B T}{\omega}}$$

$$S = -\frac{\partial F}{\partial T} \quad \Rightarrow \quad \boxed{S = k_B \ln \frac{2\pi k_B T}{\omega} + k_B}$$

$$U = F + TS \quad \Rightarrow \quad \boxed{U = k_B T}$$

$$c_V = \left(\frac{\partial U}{\partial T}\right)_V \quad \Rightarrow \quad \boxed{c_V = k_B}$$

(b)

$$H = \hbar\omega \left(a^+ a + \frac{1}{2}\right)$$

$$Z = Z_1 = \sum_{n=0}^{\infty} e^{-\beta \hbar \omega (n+1/2)} = e^{-\beta \hbar \omega / 2} \frac{1}{1 - e^{-\beta \hbar \omega}} = \boxed{\left[2 \sinh \left(\frac{\beta \hbar \omega}{2}\right)\right]^{-1} = Z}$$

$$F = -k_B T \ln Z \quad \Rightarrow \quad \boxed{F = k_B T \ln \left[2 \sinh \left(\frac{\hbar \omega}{2k_B T}\right)\right]}$$

$$S = -\frac{\partial F}{\partial T} \quad \Rightarrow \quad \boxed{S = -k_B \ln \left[2 \sinh \left(\frac{\hbar \omega}{2k_B T}\right)\right] + \frac{\hbar \omega}{2T} \coth \left(\frac{\hbar \omega}{2k_B T}\right)}$$

$$U = F + TS \quad \Rightarrow \quad \boxed{U = \frac{\hbar \omega}{2} \coth \left(\frac{\hbar \omega}{2k_B T}\right)}$$

$$c_V = \left( \frac{\partial U}{\partial T} \right)_V \Rightarrow \boxed{c_V = \frac{1}{k_B} \left( \frac{\hbar\omega}{2T} \right)^2 \frac{1}{\sinh^2 \left( \frac{\hbar\omega}{2k_B T} \right)}}$$

$$T \rightarrow \infty \quad : \quad U = k_B T, \quad c_V = k_B \quad \text{wie klassisch}$$

$$T \rightarrow 0 \quad : \quad U = \frac{\hbar\omega}{2} \quad \text{Nullpunktsenergie}$$

$$c_V = \frac{1}{k_B} \left( \frac{\hbar\omega}{2T} \right)^2 e^{-\frac{\hbar\omega}{k_B T}} \propto \frac{\Delta^2}{T^2} e^{-\Delta/k_B T}, \quad \Delta = \hbar\omega = \text{Energiespalte}$$