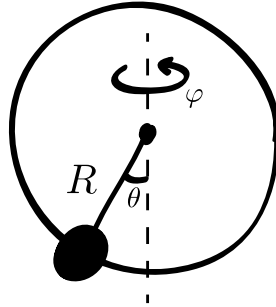


**Exercise 1. Free Rotors**

We consider  $N$  independent free rotors (fixed on a lattice) which are free to point in any direction in space, with the moment of inertia  $I = mR^2$  (see figure).



- (a) Classical rotors: we use the Hamiltonian for each independent rotor expressed by momenta in spherical coordinates,

$$\mathcal{H} = \frac{1}{2I} \left( p_\theta^2 + \frac{p_\varphi^2}{\sin^2 \theta} \right) . \quad (1)$$

Calculate the (canonical) partition function, the internal energy and the heat capacity.

First a note: how the Hamiltonian (1) is derived.

Let's start from the Lagrangian of the rotor in cartesian coordinates

$$\mathcal{L} = \frac{1}{2} m |\vec{v}|^2 , \quad \text{with } \vec{v} = \frac{d\vec{r}}{dt} . \quad (2)$$

In spherical coordinates with  $|\vec{r}| = R$ , we have

$$d\vec{r} = R (d\theta \vec{e}_\theta + \sin \theta d\varphi \vec{e}_\varphi) , \quad (3)$$

and thus

$$\mathcal{L}(\theta, \varphi) = \frac{1}{2} m R^2 (\dot{\theta}^2 + \sin^2 \theta \dot{\varphi}^2) . \quad (4)$$

The conjugate momenta are then

$$p_\theta = \frac{\partial \mathcal{L}}{\partial \dot{\theta}} = m R^2 \dot{\theta} \quad \Rightarrow \quad \dot{\theta} = \frac{p_\theta}{m R^2} ; \quad (5)$$

$$p_\varphi = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}} = m R^2 \sin^2 \theta \dot{\varphi} \quad \Rightarrow \quad \dot{\varphi} = \frac{p_\varphi}{m R^2 \sin^2 \theta} . \quad (6)$$

Then

$$\mathcal{H} = \dot{\theta} p_\theta + \dot{\varphi} p_\varphi - \mathcal{L} = \frac{1}{2} \left[ \frac{p_\theta^2}{m R^2} + \frac{p_\varphi^2}{m R^2 \sin^2 \theta} \right] = \frac{1}{2I} \left[ p_\theta^2 + \frac{p_\varphi^2}{\sin^2 \theta} \right] . \quad (7)$$

Also, for when we will calculate the partition function later, we need to determine the correct measure to integrate on the variables  $\theta$ ,  $\varphi$ ,  $p_\theta$  and  $p_\varphi$ . If you do the calculation explicitly (using in particular Eqs. (5) and (6)), one can see that the correct integration measure is simply  $d\theta d\varphi dp_\theta dp_\varphi$ .

- (b) Quantum rotors: we use the equivalent Hamiltonian for the free rotors expressed by the angular momentum,

$$H = \frac{\mathbf{L}^2}{2mR^2} = \frac{\mathbf{L}^2}{2I} . \quad (8)$$

Calculate the (canonical) partition function. Determine the entropy, the internal energy, and the heat capacity. Calculate the average value of the magnitude of the angular momentum,  $\langle \mathbf{L}^2 \rangle$  and the  $z$ -axis component,  $\langle L_z \rangle$ . Compute them numerically and study the high and low temperature limits. It is useful to define  $\theta_{\text{rot}}$  by  $k_B \theta_{\text{rot}} = 1/I$ .

*Hint.* If  $f^{(n)}(\infty) \rightarrow 0, \forall n \in \mathbb{N}$  then the Euler–Maclaurin formula could be simplified to:

$$\sum_{l=0}^{\infty} f(l) = \int_0^{\infty} dl f(l) + \frac{1}{2} f(0) - \sum_{k=2}^{\infty} \frac{(-1)^k b_k}{(k)!} f^{(k-1)}(0) + R_{\infty} \quad (9)$$

where  $R_{\infty}$  is a small correction and  $b_k$  are the Bernoulli numbers  $b_2 = 1/6, b_3 = 0, b_4 = -1/30, \dots$ .  
<http://people.csail.mit.edu/kuat/courses/euler-maclaurin.pdf>

### Solution.

(a) The partition function of an individual rotor is

$$Z_1 = \int d\Theta d\phi dp_{\Theta} dp_{\phi} \exp\left\{-\beta\left[\frac{1}{2I}(p_{\Theta}^2 + \frac{p_{\phi}^2}{\sin^2 \Theta})\right]\right\} \quad (S.1)$$

$$= 2\pi \int dp_{\Theta} e^{-\frac{\beta}{2I} p_{\Theta}^2} \int d\Theta \int dp_{\phi} e^{-\frac{\beta}{2I} \frac{p_{\phi}^2}{\sin^2 \Theta}} \quad (S.2)$$

$$= 2\pi \sqrt{\frac{2\pi I}{\beta}} \int d\Theta \sqrt{\frac{2\pi I \sin^2 \Theta}{\beta}} \quad (S.3)$$

$$= \frac{4\pi^2 I}{\beta} \int_0^{\pi} d\Theta \sin \Theta \quad (S.4)$$

$$= \frac{8\pi^2 I}{\beta}. \quad (S.5)$$

Then the partition function of  $N$  rotors is

$$Z = \left(\frac{8\pi^2 I}{\beta}\right)^N = Z_0^N \quad (S.6)$$

and the free energy is

$$F = -k_B T \ln Z = -N k_B T \ln \frac{8\pi^2 I}{\beta}. \quad (S.7)$$

The internal energy is then given by

$$U = -\frac{\partial \ln Z}{\partial \beta} = -\frac{\partial \{N \ln(\frac{8\pi^2 I}{\beta})\}}{\partial \beta} = \frac{N}{\beta} = k_B T N \quad (S.8)$$

and the heat capacity is just

$$C = \frac{\partial U}{\partial T} = N k_B. \quad (S.9)$$

Note that the system just corresponds to a free particle on the surface of a sphere: the internal energy and heat capacity are thus as expected from the equipartition law for a system with two degrees of freedom.

(b) Is it useful to work in the eigenbasis  $|l, m\rangle$  defined by  $\mathbf{L}^2 |l, m\rangle = l(l+1) |l, m\rangle, L_z |l, m\rangle = m |l, m\rangle$  where  $l = 0 \dots \infty$  and  $m = -l \dots l$ . The partition function is  $Z = Z_1^N$  where

$$Z_1 = \sum_{l=0}^{\infty} \sum_{m=-l}^l e^{-\beta l(l+1)/(2I)} = \sum_{l=0}^{\infty} (2l+1) e^{-\beta l(l+1)/(2I)} = \sum_{l=0}^{\infty} (2l+1) e^{-l(l+1)\theta_{\text{rot}}/(2T)} \quad (S.10)$$

The high (low) temperature limits correspond to  $\frac{\theta_{\text{rot}}}{T} \rightarrow 0$  ( $\frac{\theta_{\text{rot}}}{T} \rightarrow \infty$ ). For low temperature limit we keep only first two terms in the sum. For the high temperature limit we use Euler-Maclaurin formula up to  $k = 4$  and collect the dominant terms.

$$\int_0^{\infty} dl (2l+1) e^{-l(l+1)\theta_{\text{rot}}/(2T)} = -\frac{2T}{\theta_{\text{rot}}} \int_0^{\infty} dl \frac{d}{dl} e^{-l(l+1)\theta_{\text{rot}}/(2T)} = \frac{2T}{\theta_{\text{rot}}} \quad (S.11)$$

In the two limits the results become:

$$Z_1 = \begin{cases} \frac{2T}{\theta_{\text{rot}}} + \frac{1}{3} + \frac{\theta_{\text{rot}}}{30T} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow 0 \\ 1 + 3e^{-\theta_{\text{rot}}/T} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow \infty \end{cases}. \quad (\text{S.12})$$

The internal energy is:

$$U = -\frac{\partial \ln Z}{\partial \beta} = k_B T^2 \frac{\partial \ln Z}{\partial T} = \begin{cases} Nk_B \left( \frac{2T^2}{\theta_{\text{rot}}} - \frac{\theta_{\text{rot}}}{30} \right) \left( \frac{2T}{\theta_{\text{rot}}} + \frac{1}{3} + \frac{\theta_{\text{rot}}}{30T} \right)^{-1} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow 0 \\ 3Nk_B \theta_{\text{rot}} e^{-\theta_{\text{rot}}/T} \left( 1 + 3e^{-\theta_{\text{rot}}/T} \right)^{-1} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow \infty \end{cases} \quad (\text{S.13})$$

$$\approx \begin{cases} Nk_B \left( T - \frac{\theta_{\text{rot}}}{6} - \frac{\theta_{\text{rot}}^2}{180T} \right) & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow 0 \\ 3Nk_B \theta_{\text{rot}} e^{-\theta_{\text{rot}}/T} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow \infty \end{cases}. \quad (\text{S.14})$$

The entropy is:

$$S - S_0 = -\frac{\partial F}{\partial T} = \frac{\partial k_B T \ln Z}{\partial T} = Nk_B \left( \ln Z_1 + T \frac{\partial \ln Z_1}{\partial T} \right) = Nk_B \ln Z_1 + \frac{U}{T} \quad (\text{S.15})$$

$$\approx \begin{cases} Nk_B \left( \ln \left( \frac{2T}{\theta_{\text{rot}}} + \frac{1}{3} + \frac{\theta_{\text{rot}}}{30T} \right) + 1 - \frac{\theta_{\text{rot}}}{6T} - \frac{\theta_{\text{rot}}^2}{180T^2} \right) & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow 0 \\ Nk_B \left( \ln \left( 1 + 3e^{-\theta_{\text{rot}}/T} \right) + 3 \frac{\theta_{\text{rot}}}{T} e^{-\theta_{\text{rot}}/T} \right) & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow \infty \end{cases}. \quad (\text{S.16})$$

It is clear that  $S(T=0) = 0$ .

By symmetry, the projection of the angular momentum is 0.

The specific heat is:

$$C_V = \frac{\partial U}{\partial T} \approx \begin{cases} Nk_B \left( 1 + \frac{1}{180} \left( \frac{\theta_{\text{rot}}}{T} \right)^2 \right) & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow 0 \\ 3Nk_B \left( \frac{\theta_{\text{rot}}}{T} \right)^2 e^{-\theta_{\text{rot}}/T} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow \infty \end{cases}. \quad (\text{S.17})$$

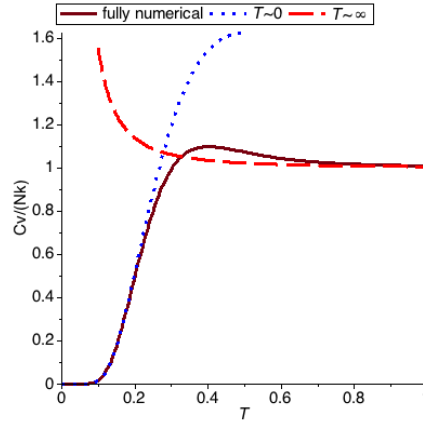


Figure 1: The two analytic approximations and the fully numerical solution for the specific heat as a function of temperature ( $\theta_{\text{rot}} = 1$ ).

## Exercise 2. Independent Dimers in a Magnetic Field. Quantum vs Ising.

We consider a system of  $N$  independent dimers of two spins,  $s = 1/2$ , described by the Hamiltonian

$$\mathcal{H}_0^{\text{quantum}} = J \sum_i \left( \vec{S}_{i,1} \cdot \vec{S}_{i,2} \right), \quad (10)$$



where  $i$  is the dimer index.  $\vec{S}_{i,1}$  and  $\vec{S}_{i,2}$  are the spin operators of the first and second particle of the dimer, respectively. Both spins have size  $s = 1/2$ . For simplicity, we use  $\hbar = 1$ . To this quantum system corresponds a classical Ising dimer, described by:

$$\mathcal{H}_0^{\text{Ising}} = \frac{1}{2} J \sum_i \left( \sigma_{i,1} \cdot \sigma_{i,2} - \frac{1}{2} \right), \quad (11)$$

where  $\sigma_{i,m} = \pm 1$ . The spins are aligned along the  $z$  axis. We will use eigenstates and eigenenergies to denote also the classical states and energies.

- (a) What are the eigenstates and the eigenenergies of a single dimer for the two cases?
- (b) For both cases consider the macroscopic system and determine the Helmholtz free energy, the entropy, the internal energy and the specific heat as a function of temperature and  $N$ . Discuss the limit  $T \rightarrow 0$  and  $T \rightarrow \infty$  for both signs of  $J$  (antiferromagnetic and ferromagnetic case).
- (c\*) We now apply a magnetic field along  $z$  direction leading to an additional term in the Hamiltonian,

$$\mathcal{H}_{\text{mag}}^{\text{quantum}} = -g\mu_B H \sum_{i,m} S_{i,m}^z \quad (12a)$$

$$\mathcal{H}_{\text{mag}}^{\text{Ising}} = -g\mu_B H \sum_{i,m} \frac{\sigma_{i,m}}{2}. \quad (12b)$$

How do the eigenenergies change? Sketch the energies with respect to the applied field  $H$ , the partition functions and determine the ground state for both cases. For the antiferromagnetic case you should notice a critical field. What differences do you notice between the classical and quantum system when the critical field is reached? For the quantum case discuss in this context the entropy per dimer in the limit  $T \rightarrow 0$ .

- (d\*) Calculate the magnetization  $m$  for the two cases. In which limit are they the same? Moreover compute the magnetic susceptibility  $\chi$  for the quantum case and discuss its dependence on  $H$  for different temperatures.

### Solution.

- (a) For the *Quantum case* we may write the Hamiltonian in terms of the total dimer spin  $\vec{S}_i = \vec{S}_{i,1} + \vec{S}_{i,2}$  as

$$\mathcal{H}_0^{\text{quantum}} = \frac{J}{2} \sum_i \left( \vec{S}_i^2 - \vec{S}_{i,1}^2 - \vec{S}_{i,2}^2 \right) = \frac{J}{2} \sum_i \left( \vec{S}_i^2 - \frac{3}{2} \right). \quad (S.18)$$

Clearly, the eigenstates of a single dimer are the spin singlets and triplets:

- The singlet  $\Psi^s = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$  has total spin 0 and, thus, eigenvalue  $E^s = -\frac{3}{4}J$ .
- The triplet states are  $\Psi_0^t = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ ,  $\Psi_1^t = |\uparrow\uparrow\rangle$  and  $\Psi_{-1}^t = |\downarrow\downarrow\rangle$ . They have total spin 1,  $\vec{S}_i^2 = 2$  and eigenvalue  $E^t = \frac{1}{4}J$ .

The *Ising case* has also four states:

- The doublet states  $\Phi_{up}^{anti} = |\uparrow\downarrow\rangle$ ,  $\Phi_{down}^{anti} = |\downarrow\uparrow\rangle$  have total spin 0 and the eigenvalue  $E^s = -\frac{3}{4}J$ .
- The doublet state  $\Phi_1 = |\uparrow\uparrow\rangle$ ,  $\Phi_{-1} = |\downarrow\downarrow\rangle$  have total spin magnitude 1 and the eigenvalue  $E^t = \frac{1}{4}J$ .

The two systems have the same eigenvalues but with different degeneracies.

(b) The partition function for the two cases is

$$Z^{\text{quantum}} = \left( 3e^{-\frac{J}{4k_B T}} + e^{\frac{3J}{4k_B T}} \right)^N \quad (\text{S.19a})$$

$$Z^{\text{Ising}} = \left( 2e^{-\frac{J}{4k_B T}} + 2e^{\frac{3J}{4k_B T}} \right)^N, \quad (\text{S.19b})$$

so we could write them as

$$Z = \left( ae^{-\frac{J}{4k_B T}} + be^{\frac{3J}{4k_B T}} \right)^N, \quad (\text{S.20})$$

where  $a = 3, b = 1$  for the quantum case and  $a = b = 2$  for the Ising one.

The connection to thermodynamics is made via the Helmholtz free energy:

$$F(T, N) = -\frac{1}{\beta} \ln Z = \frac{JN}{4} - \frac{N}{\beta} \ln \left( a + be^{\beta J} \right), \quad (\text{S.21})$$

where  $\beta = \frac{1}{k_B T}$ . The entropy is given by

$$\begin{aligned} S(T, N) &= -\frac{\partial F}{\partial T} = -\frac{\partial F}{\partial \beta} \cdot \frac{\partial \beta}{\partial T} = k_B \beta^2 \frac{\partial F}{\partial \beta} \\ &= k_B \beta^2 \left( \frac{N}{\beta^2} \ln \left( a + be^{\beta J} \right) - \frac{N}{\beta} \frac{bJ e^{\beta J}}{a + be^{\beta J}} \right) \\ &= Nk_B \ln \left( a + be^{\beta J} \right) - Nk_B \beta \frac{bJ e^{\beta J}}{a + be^{\beta J}}. \end{aligned} \quad (\text{S.22})$$

The internal energy is given by

$$U(T, N) = -\frac{\partial}{\partial \beta} \ln Z = JN \left( \frac{1}{4} - \frac{be^{\beta J}}{a + be^{\beta J}} \right), \quad (\text{S.23})$$

and, finally, the specific heat evaluates to

$$c(T, N) = \frac{1}{N} \frac{\partial U}{\partial T} = -\frac{k_B \beta^2}{N} \frac{\partial U}{\partial \beta} = abk_B J^2 \frac{\beta^2 e^{\beta J}}{(a + be^{\beta J})^2}. \quad (\text{S.24})$$

Note here that the specific heat vanishes in the limit of low and high temperatures independent of the sign of  $J$ . For the *quantum case* the internal energy vanishes for large temperatures (independent of the sign of  $J$ ) and reaches  $N$  times the ground state energy for  $T \rightarrow 0$  (for  $J > 0$  singlets are preferred and we get  $U \rightarrow -\frac{3}{4}JN$ , whereas for  $J < 0$  we get the triplets and  $U \rightarrow JN\frac{1}{4}$ ). On the other hand for the *Ising case*  $U \rightarrow -\frac{1}{4}JN$  for large temperature independent of the sign of  $J$ , while for  $T \rightarrow 0$  we get the minimum energy state ( $U \rightarrow -\frac{3}{4}JN$  for  $J > 0$  and  $U \rightarrow JN\frac{1}{4}$  for  $J < 0$ ).

- (c) The z-component of the magnetic moment vanishes for  $\Psi^s$  and  $\Psi_0^t$  and therefore their energy does not change. However, the  $\Psi_{\pm 1}^t$  do have a nonvanishing z-component of  $\pm g\mu_B$ , which leads to a new energy  $E_{\pm 1}^t = \frac{1}{4}J \mp g\mu_B H$  (Figure 2).

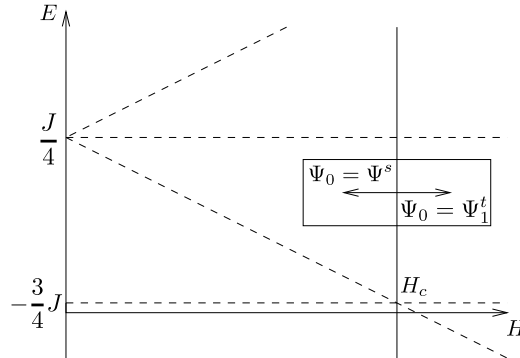


Figure 2: The energy for the four states of the quantum dimer as a function of the magnetic field for  $J > 0$  (the antiferromagnetic case).

For the classical system the total magnetic moment for  $\Phi^{anti}$  is zero so the corresponding energy is unchanged when the magnetic field is applied, while for  $\Phi$  we have the same energy dependence like for the

quantum case. Therefore only the energy for states with parallel spins is split, the other one remaining degenerate.

To calculate the entropy per dimer for the quantum case (it is known as the von Neumann entropy<sup>1</sup>) we start with the thermal state (in the basis of its eigenstates) and the partition function (per dimer) is:

$$\rho = \frac{1}{Z} \begin{pmatrix} e^{\beta J} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{-\beta g \mu_B H} & 0 \\ 0 & 0 & 0 & e^{\beta g \mu_B H} \end{pmatrix} \quad \text{and} \quad (\text{S.25})$$

$$Z^{\text{quantum}} = \text{tr}(Z\rho) = e^{\beta J} + 1 + 2 \cosh(\beta g \mu_B H), \quad (\text{S.26})$$

where we have introduced an energy offset of  $\frac{J}{4}$  (the triplet and singlet energies become  $E_{\text{offset}}^s = -J, E_{\text{offset}}^t = 0$ ). Note that  $\rho$  is independent of the offset since we normalize it to  $\text{tr} \rho = 1$ . The von Neumann entropy per dimer is given by

$$\begin{aligned} \frac{s(T, H)}{k_B} &= -\text{tr}(\rho \log \rho) \\ &= \log Z - \frac{\beta}{Z} \frac{\partial Z}{\partial \beta} \\ &= \log(e^{\beta J} + 1 + 2 \cosh(\beta g \mu_B H)) - \frac{2\beta g \mu_B H \sinh(\beta g \mu_B H) + \beta J e^{\beta J}}{e^{\beta J} + 1 + 2 \cosh(\beta g \mu_B H)}. \end{aligned} \quad (\text{S.27})$$

The expression corresponds to the result we got in b) in the limit  $H \rightarrow 0$ .

Let us first consider the case  $J > 0$ . Here, the singlet state is preferable at low fields  $|H| < H_c$  and we get  $s(T; H) \rightarrow 0$  for  $T \rightarrow 0$ . At  $|H| = H_c$  we have a two-fold degeneracy in the ground state ( $s(T; H) \rightarrow k_B \log 2$  for  $T \rightarrow 0$ ) and with  $H > H_c$  the ground state is unique again ( $s(T; H) \rightarrow 0$  for  $T \rightarrow 0$ ). This is illustrated in Figure 2 and Figure 3.

If  $J < 0$  the triplet state is energetically favorable. If  $|H| = 0$  then the ground state is three-fold degenerate ( $s(T; H) \rightarrow k_B \log 3$  for  $T \rightarrow 0$ ). Finite fields break this symmetry and we get ( $s(T; H) \rightarrow 0$  for  $T \rightarrow 0$ ) if  $|H| > 0$ .

For the Ising case the partition function is given by:

$$Z^{\text{Ising}} = e^{-\frac{\beta J}{4}} \left( 2e^{\beta J} + 2 \cosh(\beta g \mu_B H) \right). \quad (\text{S.28})$$

For  $J > 0$  in the limit  $T \rightarrow 0$  the doublet state is the minimum one as long  $|H| < H_c$  and for  $|H| = H_c$  it has three-fold degeneracy while for  $|H| > H_c$  a unique state is obtained.

The description for  $J < 0$  is the same as for the quantum system.

- (d) For the quantum system using the free energy per dimer,

$$f(T, H) = -\frac{1}{\beta} \log Z = -\frac{1}{\beta} \log \left( e^{\beta J} + 1 + 2 \cosh(\beta g \mu_B H) \right) \quad (\text{S.29})$$

we find for the magnetization

$$m^{\text{quantum}}(T, H) = -\left( \frac{\partial f(T, H)}{\partial H} \right)_T = \frac{2g \mu_B \sinh(\beta g \mu_B H)}{e^{\beta J} + 1 + 2 \cosh(\beta g \mu_B H)} \quad (\text{S.30})$$

For the Ising system

$$m^{\text{Ising}}(T, H) = \frac{2g \mu_B \sinh(\beta g \mu_B H)}{2e^{\beta J} + 2 \cosh(\beta g \mu_B H)}, \quad (\text{S.31})$$

so for  $e^{\beta J} \sim 1$  it is the same with the one for the quantum case. This correspond to the high temperature limit  $\beta \rightarrow 0$ .

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<sup>1</sup> This is equivalent to calculating the Helmholtz free energy per dimer and taking the derivative with regards to temperature as is done in (a). To see this, note that

$$\begin{aligned} s(T, H) &= -\frac{\partial F}{\partial T} = -k_B \beta^2 \frac{\partial}{\partial \beta} \frac{1}{\beta} \log Z = k_B \log Z - k_B \beta \frac{\partial}{\partial \beta} \log Z = k_B \log Z - \frac{k_B \beta}{Z} \frac{\partial}{\partial \beta} \text{tr} e^{-\beta \mathcal{H}} \\ &= k_B \log Z + \frac{k_B \beta}{Z} \frac{\partial}{\partial \beta} \text{tr} \rho Z = k_B \log Z - \frac{k_B \beta}{Z} \frac{1}{\beta} \text{tr}(\rho Z \log \rho Z) = k_B \log Z - k_B \text{tr}(\rho [\log \rho + \log Z]) \\ &= k_B \log Z - k_B \text{tr}(\rho \log \rho) - k_B \text{tr}(\rho) \log Z = -k_B \text{tr}(\rho \log \rho) \quad , \end{aligned}$$

where we used that  $\rho Z$  is of the form  $\rho Z = e^{-\beta \mathcal{H}}$  (and thus  $\frac{\partial}{\partial \beta}(\rho Z) = \frac{1}{\beta} \rho Z \log(\rho Z)$ ), and that  $\text{tr} \rho = 1$ . Don't forget also that  $Z$  is a scalar, not an operator.

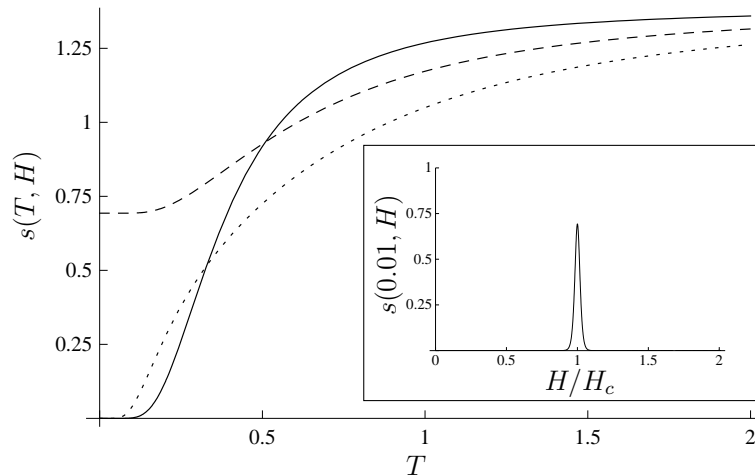


Figure 3: Entropy per dimer ( $J > 0$ ) as a function of temperature for zero field (solid line), critical field (dashed line) and for higher field (dotted line). The inset shows the entropy at low temperature as a function of the field, peaked around the critical field.

The susceptibility for the quantum case is given by:

$$\chi(T, H) = \frac{\partial m(T, H)}{\partial H} = 2\beta\mu_B^2 g^2 \frac{2 + (1 + e^{\beta J}) \cosh(\beta g\mu_B H)}{(1 + e^{\beta J} + 2 \cosh(\beta g\mu_B H))^2}. \quad (\text{S.32})$$

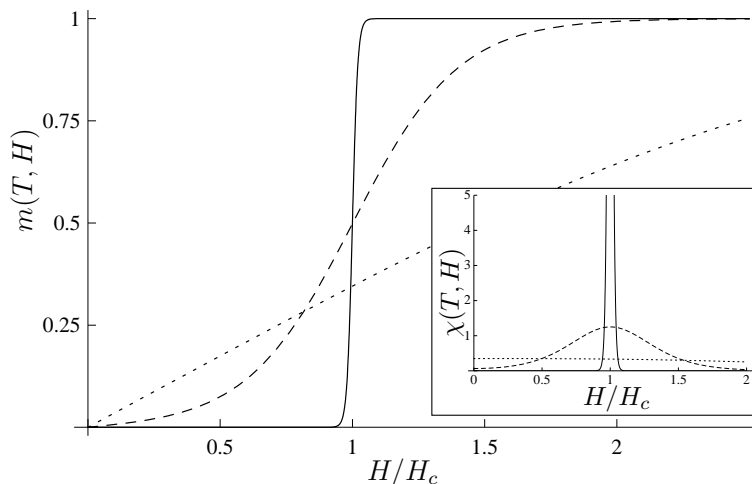


Figure 4: Magnetization as a function of applied field for small temperature (solid line), intermediate temperature (dashed line) and  $T \sim J$ . The inset shows the susceptibility for the corresponding temperatures. For  $T \rightarrow 0$ , the susceptibility diverges at  $H = H_c$ .

Let  $J > 0$ . If we plot the result for different temperatures (Figure 4), we see that for very small temperatures, the magnetization has a sudden increase at  $H_c$ , which follows directly from the fact that at this field strength, the ground-state of the system becomes magnetized. For higher temperatures,  $k_B T \sim J$ , the system behaves as if it was a simple paramagnet, i.e. we have a linear dependence on the magnetic field. In this regime, the relevant energy scale is given by the temperature and thus the system is not ordered anymore but fluctuations dominate.