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PHY452H1S Basic Statistical Mechanics. Lecture 13: Interacting spin. Taught by Prof. Arun Paramekanti

1.1 Disclaimer

Peeter's lecture notes from class. May not be entirely coherent.

1.2 Interacting spin

For these notes

$$\boxed{\hbar = k_{\mathrm{B}} = 1}$$

This lecture requires concepts from phy456 [1].

We'll look at pairs of spins as a toy model of interacting spins as depicted in fig. 1.1.

Figure 1.1: Pairs of interacting spins

Example: Simple atomic system, with the nucleus and the electron can interact with each other (hyper-fine interaction).

Consider two interacting spin $1/2$ operators $\mathbf{S}$ each with components $\hat{S}^x$, $\hat{S}^y$, $\hat{S}^z$

$$H = J\mathbf{S}_1 \cdot \mathbf{S}_2 - B(\hat{S}_1^z + \hat{S}_2^z) \tag{1.1}$$

$$\hat{S}_1^z + \hat{S}_2^z \propto \text{magnetization along } \hat{\mathbf{z}} \tag{1.2}$$

We rewrite the dot product term of the Hamiltonian in terms of just the squares of the spin operators

$$H = J\frac{(\mathbf{S}_1 + \mathbf{S}_2)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2}{2} - B(\hat{S}_1^z + \hat{S}_2^z) \tag{1.3}$$

The squares $\mathbf{S}_1^2$, $\mathbf{S}_2^2$, $(\mathbf{S}_1 + \mathbf{S}_2)^2$ can be thought of as "length"s of the respective angular momentum vectors.

We write

$$\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2, \tag{1.4}$$

for the total angular momentum. We recall that we have

$$\hat{S}_2^z = \hat{S}_1^z = S(S+1), \tag{1.5}$$

where $S = 1/2$, and $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ implies that $S_{\text{total}} \in \{0, 2\}$.

$S_{\text{total}} = 0$ (singlet)

$S_{\text{total}} = 1$. Triplet: $(-1, 0, +1)$

$S_{\text{total}} = 0$ state For $m = 0$

$$\frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) \tag{1.6}$$

energies

$$J\frac{-3/4 - 3/4}{2} = -\frac{3}{4}J \tag{1.7}$$

For $m = 1$

$$\frac{1}{\sqrt{2}}(\uparrow\uparrow) \tag{1.8}$$

energies

$$J\left(1 - \frac{3}{4}\right) - B \to \frac{J}{4} - B \tag{1.9}$$

$S_{\text{total}} = 1$ *state* For $m = 0$

$$\frac{1}{\sqrt{2}} (\uparrow\downarrow + \downarrow\uparrow) \tag{1.10}$$

energies

$$\frac{J}{4} \tag{1.11}$$

For $m = 1$

$$\frac{1}{\sqrt{2}} (\downarrow\downarrow) \tag{1.12}$$

energies

$$\frac{J}{4} + B. \tag{1.13}$$

These are illustrated schematically in fig. 1.2.

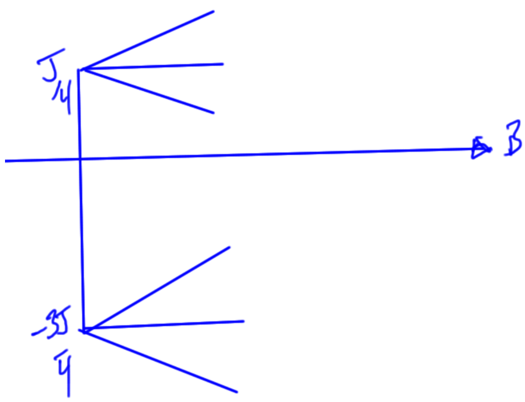

Figure 1.2: Energy levels for two interacting spins as a function of magnetic field

Our single pair partition function is

$$Z_1 = e^{+\beta 3J/4} + e^{-\beta(J/4-B)} e^{-\beta 3J/4} + e^{-\beta(J/4+B)} \tag{1.14}$$

So for N pairs our partition function is

$$Z = Z_1^N = \left(e^{+\beta 3J/4} + e^{-\beta(J/4-B)} e^{-\beta 3J/4} + e^{-\beta(J/4+B)} \right)^N. \tag{1.15}$$

Our free energy

$$F = -T \ln Z = -TN \ln Z_1. \tag{1.16}$$

$$-\frac{\partial F}{\partial \beta} = TN \frac{\partial}{\partial \beta} \ln Z_1. \tag{1.17}$$

Our magnetization μ is

$$\mu = \frac{TN}{Z_1}\left(\beta e^{-\beta(J/4-B)} - \beta e^{-\beta(J/4+B)}\right) \tag{1.18}$$

The moment per particle, after $T\beta$ cancellation, is

$$\begin{aligned} m &= \frac{\mu}{N} \\ &= \frac{1}{Z_1}\left(e^{-\beta(J/4-B)} - e^{-\beta(J/4+B)}\right) \\ &= 2\frac{e^{-\beta J/4}}{Z_1} \sinh\left(\frac{B}{T}\right). \end{aligned} \tag{1.19}$$

Low temperatures, small B ($T \ll J, B \ll J$) The $e^{3\beta J/4}$ term will dominate.

$$Z_1 \approx e^{3J\beta/4} \tag{1.20}$$

$$m \approx 2e^{-\beta J} \sinh\left(\frac{B}{T}\right). \tag{1.21}$$

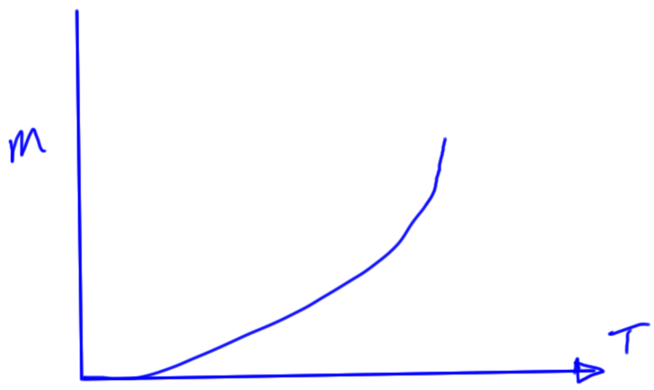

Figure 1.3: magnetic moment

The specific heat has a similar behavior

$$C_V \sim e^{-\beta J}. \tag{1.22}$$

Considering a single spin $1/2$ system, we have energies as illustrated in fig. 1.4.

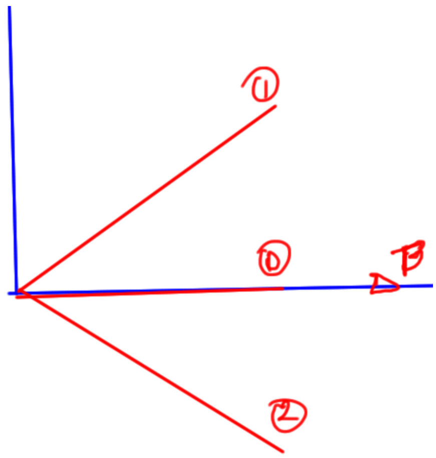

Figure 1.4: Single particle spin energies as a function of magnetic field

At zero temperatures we have a finite non-zero magnetization as illustrated in fig. 1.5, but as we heat the system up, the state of the system will randomly switch between the 1, and 2 states. The partition function democratically averages over all such possible states.

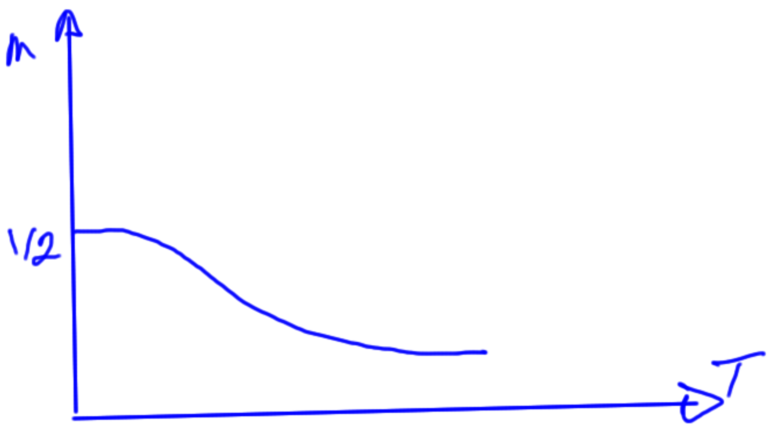

Figure 1.5: Single spin magnetization

Once the system heats up, the spins are democratically populated within the entire set of possible states.

We contrast this to this interacting spins problem which has a magnetization of the form fig. 1.6.

For the single particle specific heat we have specific heat of the form fig. 1.7.

We'll see the same kind of specific heat distribution with temperature for the interacting spins problem, but the peak will be found at an energy that's given by the difference in energies of the two states as illustrated in fig. 1.8.

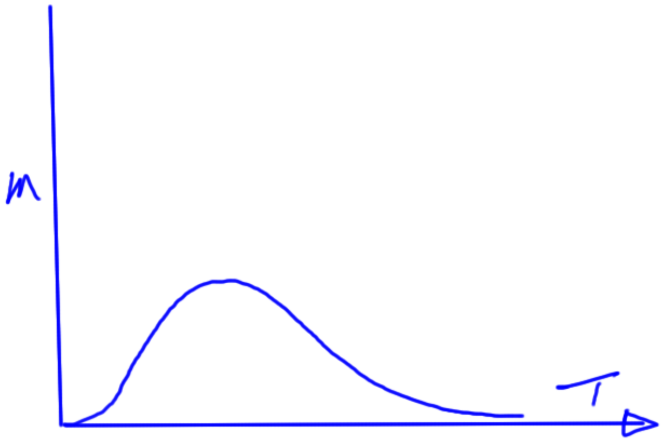

Figure 1.6: Interacting spin magnetization

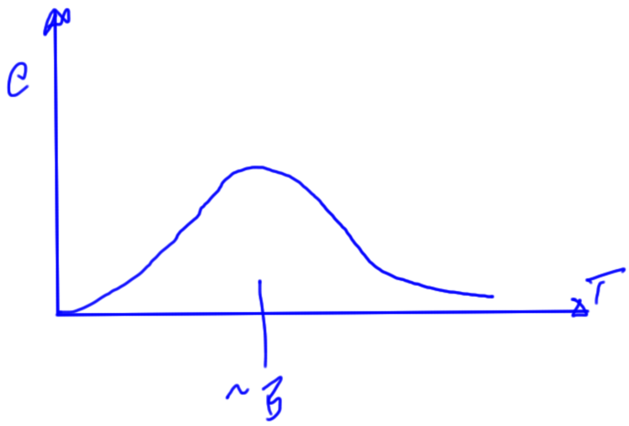

Figure 1.7: Single particle specific heat

$$\Delta E = \frac{J}{4} - \frac{-3J}{4} = J \tag{1.23}$$

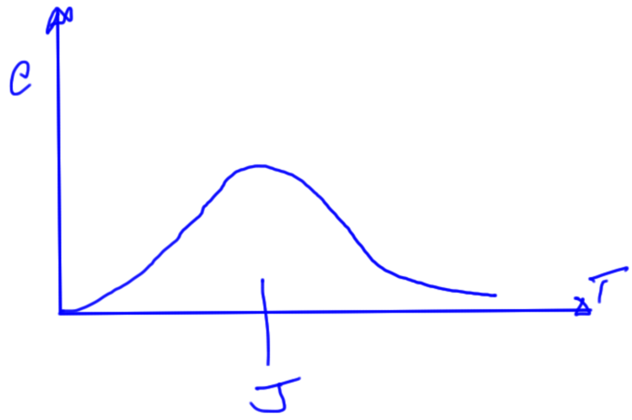

Figure 1.8: Magnetization for interacting spins

Bibliography

[1] Peeter Joot. *Quantum Mechanics II.*, chapter Two spin systems, angular momentum, and Clebsch-Gordon convention. URL http://sites.google.com/site/peeterjoot2/math2011/phy456.pdf. 1.2