Physics 204B, Winter 2011, Problem Set 2

[1.] (a) Generalize the in-class discussion of N independent spin-1/2 particles in a magnetic field in the z direction to find the partition function of spin-1, $\hat{H} = -B\mu_{\rm B}\sum_i \hat{S}_i^z$. (Here S_i^z is an angular momentum operator for spin-1.) What is $\langle \hat{H} \rangle$ and what happens as $T \to 0$ and $T \to \infty$? What changes if the field is in the x or y directions?

(b) The *free energy* and *entropy* are given by $F = -T \ln Z$ and $F = \langle E \rangle - TS$. Write an expression for S and evaluate it at low and high T. Do your results make sense in terms of the statement that the entropy has something to do with the logarithm of the number of states accessible to the system?

[2.] In class we computed the partition function of the "planar rotator model" (PRM) in $d = 1$. In the $d = 1$ PRM we had a chain of "spins" which were represented by a lattice of unit vectors $\vec{S}_i$ in the plane whose energy $E = -J\sum_i \vec{S}_i \cdot \vec{S}_{i+1} = -J\sum_i \cos(\theta_i - \theta_{i+1})$, where the angle θ_i represents the orientation of $\vec{S}_i$ with respect to some fixed axis. As you recall, the calculation involved the eigenvalues of an infinite dimensional matrix which turned out to be related to Bessel functions.

Now do the (far easier!) problem of the computation of the partition function of the "Ising model" in $d = 1$. In the Ising model, instead of having a continuous spin $\vec{S}_i$ the variable $S_i = \pm 1$ can take on only two discrete values and $E = -J\sum_i S_i S_{i+1}$. The idea is the exact same as for the PRM, except the matrices now are much simpler.

[3.] (a) In a certain basis, a quantum mechanical system has a Hamiltonian and an observable represented by the matrices,

$$\hat{H} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} \qquad \hat{V} = \begin{pmatrix} 1 & 1 & 0 & 8 \\ 1 & 1 & 5 & 0 \\ 0 & 5 & 7 & 0 \\ 8 & 0 & 0 & -3 \end{pmatrix}$$

respectively. Compute the expectation value of the energy as a function of temperature, $\langle H \rangle(T)$. What are the high and low tenperature limits?

(b) Compute $\langle \hat{V} \rangle(T)$ and its high and low temperature limits.

[4.] A hollow sphere of radius a contains standing sound waves. Given the fact that the waves satisfy,

$$\nabla^2\psi = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \qquad \left.\frac{\partial\psi}{\partial r}\right|_{r=a} = 0$$

find the minimum frequency. Note: These are Neumann boundary conditions. In class we did a similar problem with Dirichlet boundary conditions, $\psi(r = a) = 0$ in studying the energy levels of a quantum particle confined to a sphere. Question: Why are Neumann boundary conditions appropriate here?!

1-1

$\mathcal{H} = \sum B S_i^z \Rightarrow N$ identical terms like $\begin{pmatrix} -B & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & B \end{pmatrix}$

$$Z = \left[e^{\beta B} + 1 + e^{-\beta B}\right]^N$$

$$\langle E \rangle = N \frac{-Be^{\beta B} + Be^{-\beta B}}{e^{\beta B} + 1 + e^{-\beta B}} \rightarrow \begin{cases} -B & \text{at low } T \\ 0 & \text{at high } T \end{cases}$$

$$\frac{1}{N} S = \beta\left[\langle E \rangle - F\right] \frac{1}{N}$$

$$= \frac{-\beta B e^{\beta B} + \beta B e^{-\beta B}}{e^{\beta B} + 1 + e^{-\beta B}} + \ln\left[e^{\beta B} + 1 + e^{-\beta B}\right]$$

As $T \to \infty$ $(\beta \to 0)$ $\qquad S \to N \ln 3$

As $T \to 0$ $(\beta \to \infty)$ $\qquad \frac{1}{N} S \to -\beta B + \beta B = 0$

Results do not change if field is in another direction (x or y). This is obvious physically (by symmetry). Mathematically, eigenvalues of S_x and S_y are identical to those of S_z.

$$Z = \mathrm{Tr}\, e^{-\beta E} = \mathrm{Tr}\, e^{+\beta J \sum \sigma_\ell \sigma_{\ell+1}}$$

$$= \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_N=\pm 1} e^{\beta J \sigma_1 \sigma_2} e^{\beta J \sigma_2 \sigma_3} \cdots e^{\beta J \sigma_{N-1}\sigma_N}$$

$$\equiv M(\sigma_1,\sigma_2) \rightarrow \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix}$$

$$= \sum_{\sigma_1} \sum_{\sigma_2} \cdots \sum_{\sigma_N} M(\sigma_1\sigma_2) M(\sigma_2\sigma_3) \cdots M(\sigma_{N-1}\sigma_N)$$

Add $M(\sigma_N \sigma_1)$ periodic b.c. term

$$M^2(\sigma_1\sigma_3)$$

$$\Rightarrow \sum_{\sigma_1} M^N(\sigma_1\sigma_1) = \mathrm{Tr}\, M^N$$

Eigenvalues of M are $(e^{\beta J} - \lambda)^2 = e^{-2\beta J}$

$$\lambda = e^{\beta J} \pm e^{-\beta J} = \begin{matrix} 2\cosh \beta J \\ 2\sinh \beta J \end{matrix}$$

$$\therefore Z = (2\cosh\beta J)^N + (2\sinh\beta J)^N$$

$$= (2\cosh\beta J)^N \left[1 + (\tanh\beta J)^N \right]$$

$(\tanh\beta J)^N \rightarrow 0$ as $N \rightarrow \infty$

3-1

a) $H = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix}$

Eigenvalues $-1, 1, 2, 3$

Eigenvectors $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}$ $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$ $\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$ $\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$ respectively.

Partition Function

$$Z = e^{\beta} + e^{-\beta} + e^{-2\beta} + e^{-3\beta}$$

$$\langle H \rangle = \frac{\left(-1 e^{\beta} + e^{-\beta} + 2e^{-2\beta} + 3e^{-3\beta}\right)}{e^{\beta} + e^{-\beta} + e^{-2\beta} + e^{-3\beta}}$$

low T limit $\langle H \rangle \to -1$ (ground state)

high T limit $\langle H \rangle \to 5/4$ (all states equally likely)

b) $\langle V \rangle = Z^{-1}\left(V_{-1} e^{+\beta} + V_1 e^{-\beta} + V_2 e^{-2\beta} + V_3 e^{-3\beta}\right)$

where $V_1 = \langle \psi_1 | V | \psi_1 \rangle$ etc.

$$V_1 = \frac{1}{\sqrt{2}}(1\ {-1}\ 0\ 0)\begin{pmatrix} 1 & 1 & 0 & 8 \\ 1 & 1 & 5 & 0 \\ 0 & 5 & 7 & 0 \\ 8 & 0 & 0 & -3 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2}(1\ {-1}\ 0\ 0)\begin{pmatrix} 0 \\ 0 \\ -5 \\ 8 \end{pmatrix} = 0$$

3-2

$$V_2 = \frac{1}{\sqrt{2}}(1\,1\,0\,0)\begin{pmatrix} 1 & 1 & 0 & 8 \\ 1 & 1 & 5 & 0 \\ 0 & 5 & 7 & 0 \\ 8 & 0 & 0 & -3 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2}(1\,1\,0\,0)\begin{pmatrix} 2 \\ 2 \\ 5 \\ 8 \end{pmatrix} = 2$$

V_3 and V_4 are $\vartheta_{33} = 7$ and $\vartheta_{44} = -3$

Thus $\langle V \rangle = z^{-1}\left(2e^{-\beta} + 7e^{-2\beta} - 3e^{-3\beta}\right)$

As $T \to 0$ $\langle V \rangle \to 0$

$T \to \infty$ $\langle V \rangle \to 3/2$.