Statistical Mechanics (II): Homework 2

Due: October 26, 2006

Problem 3 The Bogoliubov inequality
Let us define

$$(\mathrm{A},\mathrm{B}) = \frac{1}{Z}\sum_{n\neq m}\langle n|\mathrm{A}^{\dagger}|m\rangle\langle m|\mathrm{B}|n\rangle\left(\frac{e^{-E_m/k_BT}-e^{-E_n/k_BT}}{E_n-E_m}\right),$$

where $Z = \mathrm{Tr}[\exp(-H/k_BT)]$ and $\langle\cdot\cdot\rangle = \mathrm{Tr}[\cdot\exp(-H/k_BT)]/\mathrm{Z}$. Verify that it is positive definite, so it can be defined as a scalar product.
(a) Show that

$$(\mathrm{A},\mathrm{B}) \leq \frac{1}{2k_BT}\langle\mathrm{A}^{\dagger}\mathrm{A}+\mathrm{A}\mathrm{A}^{\dagger}\rangle$$

(b) By using the Cauchy-Schwartz inequality $|(\mathrm{A},\mathrm{B})|^2 \leq (\mathrm{A},\mathrm{A})(\mathrm{B},\mathrm{B})$, show that if we take $\mathrm{B} = [\mathrm{C}^{\dagger},\mathrm{H}]$, it implies the Bogoliubov inquality

$$|\langle[\mathrm{C}^{\dagger},\mathrm{A}^{\dagger}]\rangle|^2 \leq \frac{1}{2k_BT}\langle\mathrm{A}^{\dagger}\mathrm{A}+\mathrm{A}\mathrm{A}^{\dagger}\rangle\langle[\mathrm{C}^{\dagger},[\mathrm{H},\mathrm{C}]]\rangle.$$

Problem 4 The Mermin-Wagner theorem
Consider a spin Hamiltonian

$$H = \frac{1}{2}\sum_{i,j}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j - hS^z_{\mathbf{q}}$$

with short-ranged J_{ij} such that

$$\bar{\mathrm{J}} \equiv \frac{1}{2N}\sum_{i,j}|J_{ij}||\mathbf{r}_i-\mathbf{r}_j|^2 < \infty\ .$$

Here N is the number of spins and $S^z_{\mathbf{q}}$ is the Fourier component of S^z_i

$$S^z_{\mathbf{q}} = \sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}S^z_i\ .$$

(a) Take $C = S^x_{\mathbf{k}}$ and $A = S^y_{-\mathbf{k}-\mathbf{q}}$ show that the Bogoliubov inequality implies

$$m^2_{\mathbf{q}} \leq \frac{1}{\hbar^2k_BT}S_{yy}(\mathbf{k}+\mathbf{q})\cdot\frac{1}{N}\langle[S^x_{-\mathbf{k}},[H,S^x_{\mathbf{k}}]]\rangle,$$

where $m_{\mathbf{q}} = \langle S^z_{\mathbf{q}}\rangle/N$ and $S_{yy}(\mathbf{q}) = \langle\mathbf{S^y_q S^y_{-q}}\rangle/\mathbf{N}$.
(b) By going to real space, show that

$$F(k) \equiv \frac{1}{N}\langle[S^x_{-\mathbf{k}},[H,S^x_{\mathbf{k}}]]\rangle = \hbar^2\left(hm_{\mathbf{q}} + \frac{1}{N}\sum_{j,l}J_{jl}(\cos\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_j)-1)\langle S^y_jS^y_l + S^z_jS^z_l\rangle\right).$$

(c) Show that

$$F(k) \leq \hbar^2\left(hm_{\mathbf{q}} + S(S+1)\bar{\mathrm{J}}k^2\right).$$

(d) Combining (a) and (c), one gets

$$S_{yy}(\mathbf{k}+\mathbf{q}) \geq \frac{k_BTm^2_{\mathbf{q}}}{hm_{\mathbf{q}}+S(S+1)\bar{\mathrm{J}}k^2}.$$

By doing the summation $\frac{1}{N}\sum\limits_{k}$ on the above inequality, show that $m_{\mathbf{q}}$ satisfies

$$S(S+1) \geq \frac{k_B T m_{\mathbf{q}}^2}{(2\pi)^d} \int_0^{\Lambda} \frac{S_d k^{d-1} dk}{h m_{\mathbf{q}} + S(S+1)\bar{\mathrm{J}} k^2},$$

where $S_d = 2\pi^{d/2}/\Gamma(d/2)$.

(e) Show that at 2D, the above inequality becomes

$$h m_{\mathbf{q}} \leq C \cdot \frac{S(S+1)\bar{\mathrm{J}}^{1/2}}{T^{1/2}} \frac{1}{\sqrt{\ln|h|}},$$

with C being a numerical constant.

Problem 5 Calculate the three-site correlation function $\langle S_i S_j S_k \rangle$ in the 1D closed Ising chain.

Problem 6 Consider a 1D open Ising chain with the partition function given by

$$\mathrm{Z}_N = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} \exp\left[\mathrm{K} \sum_{i=1}^{N-1} s_i s_{i+1}\right].$$

Show that the summation can be done one by one from s_N to s_1, and it leads to $\mathrm{Z}_N = 2(2\cosh \mathrm{K})^{N-1}$.

Problem 7 Investigate roots of the partition function for the 1D closed Ising chain

$$\mathrm{Z}_N = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} \exp\left[\mathrm{K} \sum_{i=1}^{N} s_i s_{i+1} + \mathrm{h} \sum_{i=1}^{N} (s_i - 1)\right],$$

where $s_{N+1} = s_1$. Show that roots satisfy Yang-Lee unit circle theorem. In particular, show that when $T \to 0$ (i.e., $\mathrm{K} \to \infty$) and $N \to \infty$, a pair of roots approach the positive real axis at $z = \pm 1$.