Homework #3. Due: Tuesday, 21 February 2006

This homework has two problems. The goal of the first problem is to derive the *gap equation*, which is a necessary condition on the single-spin density matrix in the mean field approximation for quantum spin systems. In the second problem you are asked to solve the gap equation for the lattice BCS model, aka the XY model in a magnetic field.

Problem 1. Consider a quantum spin model on $\mathbb{Z}^d$, $d \geq 1$, with a n-dimensional single-site Hilbert spaces for each site (spin) in the lattice: $\mathcal{H}_{\{x\}} = \mathbb{C}^n$, for all $x \in \mathbb{Z}^d$, and with $n \geq 2$. Let $A_x \in \mathcal{A}_{\{x\}}$ and $B_{xy} \in \mathcal{A}_{\{x,y\}}$ be copies of given hermitian matrices A and B. The local Hamiltonians of our model are defined, for any finite subset $\Lambda \subset \mathbb{Z}^d$, by

$$H_\Lambda = \sum_{x\in\Lambda} A_x + \sum_{x,y\in\Lambda,|x-y|=1} B_{xy}\,.$$

For any $n \times n$ density matrix ρ we can define state ω_ρ on $\mathcal{A}$, i.e., the algebra of quasiloical observables of the infinite system, by continuous extension of the the product state defined on local elements of the form $A_{x_1}A_{x_2}\cdots A_{x_k}$, where $k \geq 1$, $x_1, \ldots, x_k$ are distinct sites in $\mathbb{Z}^d$, and $A_{x_i} \in \mathcal{A}_{\{x_i\}}$, for $1 \leq i \leq k$, by

$$\omega_\rho(A_{x_1}A_{x_2}\cdots A_{x_k}) = \prod_{i=1}^{k} \operatorname{Tr} \rho A_{x_i}\,.$$

Let $\beta \geq 0$ be the inverse temperature and recall the mean field approximation is given by the product states ω_ρ that minimize the free energy density (i.e., the free energy per spin) of the system.

a) Show that the free-energy density functional is given by

$$f_\beta(\rho) = \operatorname{Tr} \rho h_\rho + \beta^{-1} \operatorname{Tr} \rho \log \rho\,.$$

where h_ρ is the $n \times n$ matrix given by

$$A + d \operatorname{Tr}_2(\mathbb{1} \otimes \rho)B\,.$$

b) Use the Entropy-Energy Balance (aka Local Thermodynamic Equilibrium) inequalities with $X \in \mathcal{A}_{\{x\}}$ to prove that any ρ minimizing f_β must satisfy

$$\rho = \frac{e^{-\beta h_\rho}}{\operatorname{Tr} e^{-\beta h_\rho}}\,. \tag{1}$$

Equation (1) is sometimes called the gap equation for historical reasons having to do with the application in Problem 2.

Problem 2. The lattice BCS model is an example of the class of Hamiltonians described in Problem 1. It is a spin 1/2 model, so $n = 2$. For simplicity consider $d = 1$. A and B are given by

$$A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad B = -\lambda(C^* \otimes C + C \otimes C^*), \quad \text{where } C = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

a) Show that the set of all 2×2 density matrices ρ can be parametrized as follows:

$$\rho = \begin{pmatrix} \frac{1}{2} + r & \mu \\ \overline{\mu} & \frac{1}{2} - r \end{pmatrix},$$

with $r \in \mathbb{R}$ and $\mu \in \mathbb{C}$ satisfying

$$r^2 + |\mu|^2 \leq 1/4\,.$$

b) Calculate h_ρ.

c) Calculate $e^{-\beta h_\rho}$.

d) Solve the gap equation (1) for this model (find all solutions for all $\beta \geq 0$). It is useful to graph the parameters r and $|\mu|$ of the solutions as a function of β.

e) Determine which of the solutions found in part d actually minimize f_β.