## Mathematical Statistical Physics

TMP Programme Munich - spring term 2013

HOMEWORK ASSIGNMENT 07
Hand-in deadline: Tuesday 11 June 2013 by 4 p.m. in the "MSP" drop box.
Rules: Each exercise is worth 10 points. Correct answers without proofs are not accepted. Each step should be justified. You can hand in your solutions in German or in English.
Info: www.math.lmu.de/~michel/SS13_MSP.html

Exercise 25. (Representations of the Clifford relations)
Let $\mathcal{M}_{2^{n}}(\mathbb{C})$ denote the space of $2^{n} \times 2^{n}$ complex matrices. A collection $\Gamma_{\alpha} \in \mathcal{M}_{2^{n}}(\mathbb{C})$, $\alpha=1, \ldots, 2 n$, is said to fulfill the Clifford relations if

$$
\begin{equation*}
\Gamma_{\alpha} \Gamma_{\beta}+\Gamma_{\beta} \Gamma_{\alpha}=2 \delta_{\alpha, \beta} \mathbb{1}, \quad \alpha, \beta=1, \ldots, 2 n . \tag{1}
\end{equation*}
$$

(i) For $n=1$, find explicit $\Gamma_{1}, \Gamma_{2}$ that satisfy (1).
(ii) Inductively, one can construct representations of the Clifford relations for arbitrary $n$ : Let $X, Y, Z \in \mathcal{M}_{2}(\mathbb{C})$ denote the Pauli matrices. Assume that $\Gamma_{\alpha} \in \mathcal{M}_{2^{n}}(\mathbb{C}), \alpha=1, \ldots, 2 n$, fulfill the Clifford relations. Prove that the collection $\hat{\Gamma}_{\alpha} \in \mathcal{M}_{2^{n+1}}(\mathbb{C}), \alpha=1, \ldots, 2 n+2$ defined by

$$
\begin{aligned}
& \hat{\Gamma}_{\alpha}=i \Gamma_{\alpha} \otimes X Y, \quad \alpha=1, \ldots, 2 n, \\
& \hat{\Gamma}_{2 n+1}=\mathbb{1}_{2^{n}} \otimes X, \\
& \hat{\Gamma}_{2 n+2}=\mathbb{1}_{2^{n}} \otimes Y,
\end{aligned}
$$

satisfies (1).
Let $\Gamma_{\alpha} \in \mathcal{M}_{2^{n}}(\mathbb{C}), \alpha=1, \ldots, 2 n$, fulfill the Clifford relations.
(iii) Let $S \in \mathcal{M}_{2^{n}}(\mathbb{C})$ be invertible. Prove that the matrices $\widetilde{\Gamma}_{\alpha}:=S \Gamma_{\alpha} S^{-1}$ for $\alpha=1, \ldots, 2 n$ satisfy (1).
(iv) Let $\omega=\left(\omega_{\mu \nu}\right) \in \mathcal{M}_{2 n}(\mathbb{R})$ be orthogonal (i.e. $\omega \omega^{\mathrm{T}}=\mathbb{1}$ ). Prove that the matrices

$$
\Gamma_{\alpha}^{\prime}:=\sum_{\beta=1}^{2 n} \omega_{\alpha \beta} \Gamma_{\beta}, \quad \alpha=1, \ldots, 2 n
$$

satisfy (1).
Let $\Gamma_{\alpha}^{(1)}, \alpha=1, \ldots, 2 n$, and $\Gamma_{\alpha}^{(2)}, \alpha=1, \ldots, 2 n$, be two collections of matrices in $\mathcal{M}_{2^{n}}(\mathbb{C})$ that fulfill the Clifford relations.
(v) Prove that there exists an invertible $S \in \mathcal{M}_{2^{n}}(\mathbb{C})$ such that

$$
\Gamma_{\alpha}^{(1)}=S \Gamma_{\alpha}^{(2)} S^{-1}, \quad \alpha=1, \ldots, 2 n .
$$

Hints: Let $\Gamma_{\alpha} \in \mathcal{M}_{2^{n}}(\mathbb{C}), \alpha=1, \ldots, 2 n$, fulfill the Clifford relations. The generated algebra $\mathcal{A}_{\Gamma}$ is the smallest sub-algebra of $\mathcal{M}_{2^{n}}(\mathbb{C})$ that contains all $\Gamma_{\alpha}$. Convince yourself that it is given by

$$
\mathcal{A}_{\Gamma}=\operatorname{span}\left\{\Gamma_{1}^{x_{1}} \cdots \Gamma_{2 n}^{x_{2 n}} \mid x_{i} \in\{0,1\}, i=1, \ldots, 2 n\right\} \subseteq \mathcal{M}_{2^{n}}(\mathbb{C}) .
$$

You may use the following facts:

- The $\Gamma_{\alpha}$ generate the full algebra, i.e. $\mathcal{A}_{\Gamma}=\mathcal{M}_{2^{n}}(\mathbb{C})$.
- Every algebra automorphism $\phi$ of $\mathcal{M}_{2^{n}}(\mathbb{C})$ is inner, i.e. there exists an invertible $S \in$ $\mathcal{M}_{2^{n}}(\mathbb{C})$ such that $\phi(A)=S A S^{-1}, A \in \mathcal{M}_{2^{n}}(\mathbb{C})$.

Exercise 26. (Spin representation of rotations)
Consider specific rotations $\omega(\alpha \beta \mid \theta) \in \mathcal{M}_{2 n}(\mathbb{R})$ in the $\alpha$ - $\beta$-plane, $\alpha \neq \beta \in\{1, \ldots, 2 n\}$, with angle $\theta \in[0,2 \pi)$. More precisely $\omega(\alpha \beta \mid \theta)$ is defined by

$$
\begin{cases}\omega(\alpha \beta \mid \theta) e_{\lambda}=e_{\lambda}, & \text { if }(\lambda \neq \alpha \text { or } \lambda \neq \beta) \\ \omega(\alpha \beta \mid \theta) e_{\alpha}=e_{\alpha} \cos \theta-e_{\beta} \sin \theta, \\ \omega(\alpha \beta \mid \theta) e_{\beta}=e_{\alpha} \sin \theta+e_{\beta} \cos \theta, & \end{cases}
$$

where $e_{\nu} \in \mathbb{R}^{2 n}$ is the unit vector with entry 1 at index $\nu \in\{1, \ldots, 2 n\}$. Let the collection $\Gamma_{\ell} \in \mathcal{M}_{2^{n}}(\mathbb{C}), \ell=1, \ldots, 2 n$, fulfill the Clifford relations from Exercise 25 and define the matrices

$$
\Gamma_{\mu}^{\prime}=\sum_{\ell=1}^{2 n} \omega(\alpha \beta \mid \theta)_{\mu \ell} \Gamma_{\ell} .
$$

(i) Compute $S(\omega(\alpha \beta \mid \theta))$.
(ii) Conclude that the map $S$ can at best be a projective representation, i.e. a group representation up to a phase (Hint: Prove that the image of a closed path in $O(2 n)$, the orthogonal matrices in $\mathcal{M}_{2 n}(\mathbb{R})$, can be open. It fails to be closed only up to an element of the center.)

Exercise 27. (Maximum Entropy Principle)
Let $\mathcal{A}=\mathcal{M}_{n}(\mathbb{C})$ be the $\mathrm{C}^{*}$-algebra of $n \times n$ complex matrices. Every state on $\mathcal{A}$ is of the form $\omega_{\rho}(A)=\operatorname{Tr}(\rho A), A \in \mathcal{A}$, for some density matrix $\rho \in \mathcal{A}$. For $\omega_{\rho} \in \mathbb{E}_{\mathcal{A}}$, we define the entropy $S\left(\omega_{\rho}\right)$ by

$$
S\left(\omega_{\rho}\right)=-\operatorname{Tr}(\rho \log \rho) .
$$

Given a Hamiltonian, i.e. a self-adjoint $H \in \mathcal{A}$, and an inverse temperature $\beta>0$, we can define the free energy of a state $\omega$ as

$$
F(\omega)=\omega(H)-\frac{1}{\beta} S(\omega)
$$

(i) Prove that the free energy of a state $\omega_{\rho}$ can be written as

$$
F\left(\omega_{\rho}\right)=-\frac{1}{\beta} \log \operatorname{Tr}\left(\mathrm{e}^{-\beta H}\right)+\frac{1}{\beta} \operatorname{Tr}\left(\rho \log \rho-\rho \log \rho_{\beta H}\right)
$$

where $\rho_{\beta H}$ is the Gibbs state at inverse temperature $\beta$, i.e.

$$
\rho_{\beta H}=\frac{\mathrm{e}^{-\beta H}}{\operatorname{Tr}\left(\mathrm{e}^{-\beta H}\right)} .
$$

(ii) Prove that for any Hermitian $A, B \in \mathcal{A}, A \geqslant 0, B>0$ (i.e. $B$ has strictly positive spectrum), the following convexity inequality holds:

$$
\operatorname{Tr}(A \log A-A \log B) \geqslant \operatorname{Tr}(A-B)
$$

(iii) Conclude that the Gibbs state $\omega_{\rho_{\beta H}}$ is a minimizer for the free energy F, and determine its minimal value.

Remark: In fact, the Gibbs state $\omega_{\rho_{\beta H}}$ is the unique minimizer for the free energy.

The purpose of the next exercise is to recapitulate the mean-field solution of the Ising model. The earliest theories of phase transitions, the Weiss molecular field theory and the Van der Waals theory of liquid-gas phase transitions, are examples of what is now generically called "mean field theory". As it turns out, the mean field approximation for the Ising model yields a ferromagnetic state for temperatures $0<T<T_{c}$, with $T_{c}$ being the critical temperature. The results for critical exponents and scaling functions within this scheme are qualitatively correct in spatial dimensions $d>4$.

Exercise 28. (Ising model in mean field approximation)
Let $p_{\max } \in \mathbb{N}, \Lambda:=\left\{p \in \mathbb{Z}^{d} \mid 0 \leqslant p_{i} \leqslant p_{\max }\right\}$, and $N:=|\Lambda|:=$ number of lattice sites in $\Lambda$. Assign to each $p \in \Lambda$ a spin variable $s_{p} \in\{-1,+1\}$ (spin up / spin down). Define the energy of an Ising ferromagnet $\mathcal{E}(S)$ associated with a configuration $S: p \mapsto s_{p}$ of the system by

$$
\mathcal{E}(S):=-\epsilon \sum_{\langle p, q\rangle} s_{p} s_{q}-B \sum_{p=1}^{N} s_{p}
$$

where $\sum_{\langle p, q\rangle}$ denotes the sum over all distinct nearest neighbour pairs (each lattice point has $c=2 d$ nearest neighbors), $\epsilon>0$ denotes the ferromagnetic interaction energy, and $B \in \mathbb{R}$ is the external magnetic field.
(i) Compute the partition function $Q_{N}(B, T):=\sum_{S} e^{-\beta \mathcal{E}(S)}$, with $\beta:=1 /\left(k_{B} T\right), T \geqslant 0$ in the mean-field approximation.
The mean field approach assumes that each spin sees a mean magnetization field $m$ due to all its neighbours such that we can write $s_{p}=m+\left(s_{p}-m\right)=m+\delta s_{p}$, where $\delta s_{p}$ denotes the fluctuation of the spin $s_{p}$ around the mean field $m$. Use this expression for $s_{p}$ to simplify the Hamiltonian by neglecting terms of order $\delta s_{p} \delta s_{q}$, i.e., by neglecting fluctuations ( $=$ mean field approximation).
(ii) Compute the free energy density in the limit $N \rightarrow \infty: a(B, T):=\lim _{N \rightarrow \infty} a_{N}(B, T)$ where $a_{N}(B, T):=-\frac{1}{\beta N} \log Q_{N}(B, T)$.
(iii) So far, the mean field $m$ has been a variational parameter which is still to be determined. To this end, compute the mean magnetization field $m(B, T):=\lim _{N \rightarrow \infty}\left\langle\frac{1}{N} \sum_{p=1}^{N} s_{p}\right\rangle$, where $\langle\cdot\rangle$ denotes the average over all possible configurations, and derive a consistency relation for the mean field $m$.
(iv) Discuss the number of solutions of this consistency relation for the mean magnetization field $m$ in dependence of the temperature $T$ in the case of a vanishing external magnetic field. A graphical sketch might be helpful. You should argue from this plot that the system is ferromagnetic for positive temperatures below a critical temperature $T_{c}$.

## Hints

Recommendation: try first to solve the exercises with the only amount of information provided in their formulation. I.e., try to understand the question, to identify what the involved notions from class are, to structure a potentially successful solving strategy. Go through these additional hints only if you get completely stuck in your first attempts.

## Hints for Exercise 25.

(i) A well-known example. (ii) - (iv) Straightforward computations. (v) Define a map $\phi$ : $\mathcal{M}_{2^{n}}(\mathbb{C}) \rightarrow \mathcal{M}_{2^{n}}(\mathbb{C})$ by requiring $\Gamma_{\alpha}^{(1)} \mapsto \Gamma_{\alpha}^{(2)}, \alpha=1, \ldots, 2 n$, and extending it to all of $\mathcal{M}_{2^{n}}(\mathbb{C})$. Prove that $\phi$ is an automorphism, and use that any automorphism is inner.

## Hints for Exercise 26.

(i) We call $S(\omega)$ a spin representation of the rotation $\omega$ when $\sum_{\ell=1}^{2 n} \omega_{\mu \ell} \Gamma_{\ell}=S(\omega) \Gamma_{\mu} S(\omega)^{-1}$ for $\omega \in \mathcal{M}_{2 n}(\mathbb{R})$ orthogonal, and $S(\omega) \in \mathcal{M}_{2^{n}}(\mathbb{C})$ invertible. Try $S(\omega(\alpha \beta \mid \theta))=e^{\frac{\theta}{2} \Gamma_{\alpha} \Gamma_{\beta}}$ as a spin representation of $\omega(\alpha \beta \mid \theta)$ for $\alpha \neq \beta \in\{1, \ldots, 2 n\}$. More specifically, prove that $\Gamma_{\mu}^{\prime}=\sum_{\ell=1}^{2 n} \omega(\alpha \beta \mid \theta)_{\mu \ell} \Gamma_{\ell}=e^{\frac{\theta}{2} \Gamma_{\alpha} \Gamma_{\beta}} \Gamma_{\mu}\left(e^{\frac{\theta}{2} \Gamma_{\alpha} \Gamma_{\beta}}\right)^{-1}$ by making use of the Clifford relations and trigonometric identities. (ii) Compute $S(\omega(\alpha \beta \mid 2 \pi))$.

## Hints for Exercise 27.

(i) Straightforward computation. (ii) The Spectral Theorem for Hermitian matrices implies that there are complete sets of eigenvalues $\left\{a_{i}\right\}_{i=1, \ldots, n}$ and $\left\{b_{i}\right\}_{i=1, \ldots, n}$ with corresponding orthonormal eigenvectors $\left\{\psi_{i}^{A}\right\}_{i=1, \ldots, n}$ and $\left\{\psi_{i}^{B}\right\}_{i=1, \ldots, n}$ for $A$ and $B$, respectively. Evaluate the trace in $\operatorname{Tr}(A \log A-A \log B)$ in the basis $\left\{\psi_{i}^{A}\right\}_{i=1, \ldots, n}$. Prove that by convexity of $x \mapsto \log x$, one has $\sum_{j=1}^{n}\left|\left\langle\psi_{i}^{A}, \psi_{j}^{B}\right\rangle\right|^{2} \log b_{j} \leq \log \left\langle\psi_{i}^{A}, B \psi_{i}^{A}\right\rangle$. Use this, together with $x \log x \geq x-1$, to conclude that $\operatorname{Tr}(A \log A-A \log B) \geq \operatorname{Tr}(A-B)$. (iii) Apply the result from (ii) to the expression from (i).

Hints for Exercise 28. (i) Insert $s_{p}=m+\delta s_{p}$ into the energy function, neglect terms of order $\delta s_{p} \delta s_{q}$ and express the energy again in terms of $s_{p}$. The energy of the Ising ferromagnet in this mean field approximation is effectively the energy of a paramagnet where only interactions between the spins and the external magnetic field are present. (iii) Note that $m(B, T)=$ $-\partial a(B, T) / \partial B$. (iv) Plot the left hand side and the right hand side of the consistency relation as functions of the mean magnetization $m$ into one diagram and discuss the different behavior of intersection points for different values of the temperature $T$.

