HOMEWORK ASSIGNMENT 10

Hand-in deadline: Tuesday 2 July 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 37. (Peierls' argument – Part II) contact: `benedikt.rehle@gmail.com`

In Exercise 31, we used Peierls' contour argument to show that the Ising model on a 2D square lattice with positive boundary conditions exhibits a positive magnetization at sufficiently low temperatures. More concretely, we derived a lower bound for the magnetisation which is independent of the lattice size. In the following exercise, we return to periodic boundary conditions and use our previous result to conclude that the free energy per site is non-analytic in the thermodynamic limit. This establishes the existence of a phase transition in the 2D Ising model.

Consider the Ising model on a square lattice $\Lambda \subseteq \mathbb{R}^2$ – use the notation and the results Exercise 31. For the standard case of periodic boundary conditions, the energy function reads

$$E(S) = -\epsilon \sum_{\langle pq \rangle : p,q \in \Lambda} s_p s_q - B \sum_{p \in \Lambda} s_p,$$

where sites p and q on opposite sides of the square are considered direct neighbours. Define the free energy per site as

$$a_\Lambda(\beta, B) := -\frac{1}{\beta N} \log \sum_S \mathrm{e}^{-\beta E(S)}$$

and, analogously, for positive boundary conditions,

$$a_{\Lambda,+}(\beta, B) := -\frac{1}{\beta N} \log \sum_S \mathrm{e}^{-\beta E_+(S)}.$$

Consider a sequence of $n \times n$ boxes Λ_n. It can be proved that the thermodynamic limit $a(\beta, B) := \lim_{n\to\infty} a_{\Lambda_n}(\beta, B)$ exists for any $\beta > 0, B \in \mathbb{R}$.

(i) Prove that

$$\lim_{n\to\infty} a_{\Lambda_n,+}(\beta, B) \; = \; a(\beta, B).$$

Remark: This means that the boundary conditions have no influence on the asymptotic free energy per site.

(ii) Prove that $B \mapsto a_{\Lambda,+}(\beta, B)$ is a concave function for all $\beta > 0$.

(iii) Let $(f_n)_{n\in\mathbb{N}} \subseteq \mathrm{C}^1(\mathbb{R})$ be concave functions and $f : \mathbb{R} \to \mathbb{R}$ such that $f_n \to f$ pointwise. Prove that for any $h > 0$,

$$\liminf_{n\to\infty} f_n'(x) \; \geq \; \frac{f(x+h) - f(x)}{h}.$$

(iv) Using the identity

$$\frac{\partial}{\partial B} a_{\Lambda,+}(\beta, B)\Big|_{B=0} = -m_{\Lambda,+}(\beta, B=0)$$

and the result from Exercise 31, prove that the asymptotic free energy per site $a(\beta, B)$ is non-analytic at $B = 0$ for sufficiently large β.

Exercise 38. (Application of RG: a quantum flute – or a bosonic string)

Consider a cigar-shaped tube of length π and assume that the pressure inside it can be modelled by a function $p(t,x)$ of the time t and of the coordinate x along the tube. Consider the classical Hamiltonian

$$H = \int_0^\pi \mathrm{d}x \left(\left(\frac{\partial p}{\partial t}\right)^2 + \left(\frac{\partial p}{\partial x}\right)^2 \right).$$

(i) Assume Dirichlet boundary conditions $p(t,0) = p(t,\pi) = 0$. Re-write H in terms of the Fourier transform of $p(t,x)$ with respect to x and prove that H takes this way the form of an infinite sum of classical harmonic oscillators of mass $\frac{1}{2}$,

$$H = \sum_{k=1}^{\infty} h_k, \qquad h_k := \left(\frac{\mathrm{d}p_k}{\mathrm{d}t}\right)^2 + \omega_k\, p_k^2,$$

of which you have to specify the frequency ω_k.

(ii) Consider the quantisation of the Hamiltonian H obtained in (i), consisting of the replacement of each mode p_k with the operator of multiplication times x_k and correspondingly of $\frac{\mathrm{d}p_k}{\mathrm{d}t}$ with the differential operator $-\mathrm{i}\frac{\partial}{\partial x_k}$. Let E_k be the ground state energy of the harmonic oscillator h_k. Prove that $\sum_{k=1}^{\infty} E_k = +\infty$.

(iii) To cure the divergence found in (ii), assume that H can be regularised to some H_{reg} in such a way that each harmonic oscillator h_k has a ground state damped by a factor e^{-a/λ_k}, where a is a reference distance (say, the typical inter-atomic distance) and λ_k is the wave length of the mode k. Correspondingly, consider $\widetilde{E} := \sum_{k=1}^{\infty} E_k e^{-a/\lambda_k}$. Prove the following asymptotics

$$\widetilde{E} = \frac{1}{a^2} - \frac{1}{12} + O(a) \qquad \text{as } a \to 0.$$

(iv) An immediate consequence of (iii) is that re-normalizing H_{reg} by

$$H_{\mathrm{reg}} \mapsto H' := H_{\mathrm{reg}} - \int_0^\pi \mathrm{d}x\, \frac{1}{a^2},$$

namely adding a contribution which is p-independent (thus, not affecting the equation of motion) and preserves locality, the ground state energy of H' stays finite as $a \to 0$. Discuss the value of this ground state in relation to the quantity $\zeta(-1)$, where ζ is the Riemann zeta function.

Exercise 39. (Fermi-Dirac ideal gases: computation of thermodynamic quantities.)

Consider a gas of identical non-interacting spin-$\frac{1}{2}$ particles of mass m confined in a three-dimensional cubic box of size L and hence volume $V = L^3$. Assume periodic boundary conditions, so that the one-particle momentum operator has eigenvalues $\mathbf{p}_\mathbf{l} = \frac{2\pi\hbar}{L}(l_x, l_y, l_z)$ with $l_x, l_y, l_z \in \mathbb{Z}$. Here $\mathbf{l} := (l_x, l_y, l_z)$ labels each possible momentum eigenstate, in which in turn at most two particles can be, one with spin up and one with spin down. Accordingly, the one-particle kinetic energy operator has eigenvalues

$$\varepsilon_\mathbf{l} \ = \ \frac{4\pi^2\hbar^2}{2mL^2}(l_x^2 + l_y^2 + l_z^2)\,.$$

Let $n_{\mathbf{l},\sigma}$ denote the number of particles with quantum numbers $\mathbf{l}$ and spin $\sigma \in \{\uparrow, \downarrow\}$. The grand-partition function at temperature T ($\beta := (k_BT)^{-1}$) and chemical potential μ takes the form

$$Z(T,V,\mu) \ = \ \prod_\mathbf{l}\Big(\sum_{n_{\mathbf{l},\uparrow}=0,1} e^{-\beta n_{\mathbf{l},\uparrow}(\varepsilon_\mathbf{l}-\mu)} \sum_{n_{\mathbf{l},\downarrow}=0,1} e^{-\beta n_{\mathbf{l},\downarrow}(\varepsilon_\mathbf{l}-\mu)}\Big) \ = \ \prod_\mathbf{l}(1+e^{-\beta(\varepsilon_\mathbf{l}-\mu)})^2\,.$$

(i) Prove that the average number of particles in the gas $\langle N\rangle := \Big(\dfrac{\partial(k_BT\ln Z(T,V,\mu))}{\partial\mu}\Big)_{T,V}$ is given by

$$\langle N\rangle \ = \ \sum_\mathbf{l}\langle n_\mathbf{l}\rangle\,, \qquad \langle n_\mathbf{l}\rangle := \frac{2}{e^{\beta(\varepsilon_\mathbf{l}-\mu)}+1} \ = \ \frac{2z}{e^{\beta\varepsilon_\mathbf{l}}+z}\,, \qquad z := e^{\beta\mu}\,.$$

Remark: $\langle n_\mathbf{l}\rangle$ = average number of particles with quantum numbers $\mathbf{l}$; z = fugacity.

(ii) Plot $\langle n_\mathbf{l}\rangle$ as a function of $\varepsilon_\mathbf{l}$ for $T > 0$ and $T = 0$.

(iii) Prove that for large volume V the average particle density $\langle n\rangle := \dfrac{\langle N\rangle}{V}$ can be written as

$$\langle n\rangle \ = \ \frac{2}{\lambda_T^3}f_{3/2}(z)\,,$$

where $\lambda_T := \Big(\dfrac{2\pi\hbar^2}{mk_BT}\Big)^{1/2}$ = "thermal wavelength" and

$$f_{3/2}(z) \ := \ \frac{4}{\sqrt{\pi}}\int_0^{+\infty}\mathrm{d}x\,\frac{z\,x^2}{e^{x^2}+z} \ = \ \sum_{\alpha=1}^{\infty}(-1)^{j+1}\frac{z^\alpha}{\alpha^{3/2}}$$

(*Hint:* for large volume V one can change the summation $\sum_\mathbf{l}$ to an integration, namely $\sum_\mathbf{l} \approx \frac{4\pi V}{(2\pi\hbar)^3}\int_0^{+\infty}p^2\mathrm{d}p$.)

Exercise 40. (Variance of the particle number for a Fermi-Dirac ideal gases)

Same notation as in Exercise 39. Prove that the variance $\langle(N-\langle N\rangle)^2\rangle$ in particle number for a spin-$\frac{1}{2}$ Fermi-Dirac gas when the temperature $T \to 0$ is

$$\langle(N-\langle N\rangle)^2\rangle \ = \ k_BTV\frac{m}{\hbar^2}\Big(\frac{12\langle N\rangle}{4\pi^4V}\Big)^{1/3}.$$

To this aim use the thermodynamic identity

$$\langle(N-\langle N\rangle)^2\rangle \ = \ k_BT\Big(\frac{\partial\langle N\rangle}{\partial\mu}\Big)_{T,V},$$

the result of Exercise 39 (iii), and the asymtpotics (that will be proved in the tutorial)

$$f_{3/2}(z) \ \approx \ \frac{4}{3\sqrt{\pi}}(\ln z)^{3/2} \quad \text{as } z \to +\infty\,.$$

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 37. (i) Compare E and E_+. (ii) Look at derivatives of $a_{\Lambda,+}(\beta, B)$. (iii) Note that for $(a_{ij})_{i\in\mathbb{N},j\in\mathbb{N}} \subseteq \mathbb{R}$, one has $\liminf_i \sup_j a_{ij} \geq \sup_j \liminf_i a_{ij}$. (iv) Put everything together.

Hints for Exercise 38. (i) Fourier-transform with respect to the orthonormal basis $\{\frac{2}{\pi}\sin kx\}_{k=1}^{\infty}$ of $L^2[0,\pi]$. (ii) Recall that the eigenvalues of $h = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2$ are $\hbar\omega(n+\frac{1}{2})$, $n = 0, 1, 2, \dots$. (iii) $\lambda_k = k^{-1}$. Then exchange derivative and summation in the series. Last, Taylor expansion around $a = 0$.

Hints for Exercise 39. (i) Direct computation. (ii) $0 \leqslant \langle n_{\mathbf{l}} \rangle \leqslant 2$, smoothly vanishing at higher temperature; jump at $T = 0$... (iii) For large volume V change the summation $\sum_{\mathbf{l}}$ to an integration, namely $\sum_{\mathbf{l}} \approx \frac{4\pi V}{(2\pi\hbar)^3} \int_0^{+\infty} p^2 \mathrm{d}p$. Then direct computation.

Hints for Exercise 40. Use $\langle n \rangle = \frac{2}{\lambda_T^3} f_{3/2}(z)$ and the asymptotics for $f_{3/2}(z) \approx \frac{4}{3\sqrt{\pi}}(\ln z)^{3/2}$ as $z \to +\infty$ to derive an expression of $\langle N \rangle$ as a function of μ, then take $\frac{\partial}{\partial\mu}$.