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Übungen zu Theoretische Physik IV

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http://www.th.physik.uni-bonn.de/people/forste/exercises/ws1213/tp4

–In-Class Exercises–

A 5.1 Quantum mechanical Virial theorem

In the lecture, the classical virial theorem for interacting particles

$$PV = \frac{2}{3}\langle E_{\text{kin}}\rangle - \frac{1}{6}\sum_{m,n}\left\langle (x_m - x_n)\frac{\partial v(|x_m - x_n|)}{\partial (x_m - x_n)}\right\rangle$$

was shown. Here we want to discuss the quantum mechanical version of it. Consider a system of N particles in a cube with volume V and length L. The Hamilton operator is given by

$$H = \sum_n \frac{p_n^2}{2m} + \sum_n V(x_n - x_{\text{Wand}}) + \frac{1}{2}\sum_{n,m} v(x_n - x_m)\ ,$$

where $V(x_n - x_{\text{Wand}})$ is the wall potential and $v(x_n - x_m)$ describes the interaction of the particles.

Use the fact, that $\langle\Psi|\,[H, x_n\cdot p_n]\,|\Psi\rangle = 0$ for energy eigenstates Ψ, to show

$$2\langle E_{\text{kin}}\rangle - \left\langle \sum_n x_n\cdot\nabla_n V(x_n - x_{\text{Wand}})\right\rangle - \left\langle \sum_n\sum_{n\neq m} x_n\cdot\nabla_n v(x_n - x_m)\right\rangle = 0\,,$$

where $\nabla_n = \left(\frac{\partial}{\partial x_{n,1}}\ \frac{\partial}{\partial x_{n,1}}\ \frac{\partial}{\partial x_{n,3}}\right)^{\text{T}}$.

Analogously to the classical case, from the form of the wall potential

$$V_{\text{Wand}} = V_\infty \sum_{n=1}^{\infty}\sum_{i=1}^{3}\Theta(x_{n,i} - L)\,,$$

one sees that $PV = \frac{1}{3}\langle\sum_n x_n\cdot\nabla_n V(x_n - x_{\text{Wand}})\rangle$. Plugging this in yields the quantum mechanical virial theorem

$$2\langle E_{\text{kin}}\rangle - 3PV - \frac{1}{2}\left\langle \sum_n\sum_m (x_n - x_m)\cdot\nabla v(x_n - x_m)\right\rangle = 0\,.$$

A 5.2 Ising-model

The Ising-model is a statistical model for ferromagnetism in solids. The facts, that it shows a phase transition in $D \geq 2$ dimensions and that it is one of the few models with this behaviour which can be solved without huge numerical efforts, makes it one of the most studied models in statistical physics.

The model contains a spin lattice in an external magnetic field in which only the interactions of next neighbours is considered. The Hamilton operator is given by

$$H = -J \sum_{\langle i,j \rangle}^{N} \sigma_i \sigma_j - \mu B \sum_{j=1}^{N} \sigma_j \,.$$

Here σ_i denotes the z-component of the spin at the position i in the lattice and can take the values ± 1. B is the external magnetic field, μ the magnetic moment of the spins and J describes the strength of interaction of the spins. $\langle i, j \rangle$ means, that the sum is only over the q next neighbours of i and q depends on the lattice. We will calculate the one dimensional case, i.e. $q = 2$, in exercise H 5.1 exactly, in general however there is no analytically exact solution of the model. Hence we will employ the *mean field approximation* in which the interaction of a spin σ_i with its next neighbours is replaced by the mean field $\langle \sigma \rangle$ of the other spins. Using the identity

$$\sigma_i \sigma_j = \sigma_i \langle \sigma_j \rangle + \langle \sigma_i \rangle \sigma_j - \langle \sigma_i \rangle \langle \sigma_j \rangle + (\sigma_i - \langle \sigma_i \rangle)(\sigma_j - \langle \sigma_j \rangle) \,,$$

one can bring H to the form

$$H = -J \left(q \langle \sigma \rangle \sum_{j=1}^{N} \sigma_j - \frac{q}{2} N \langle \sigma \rangle^2 + \sum_{\langle i,j \rangle} (\sigma_i - \langle \sigma_i \rangle)(\sigma_j - \langle \sigma_j \rangle) \right) - \mu B \sum_{j=1}^{N} \sigma_j \,.$$

Here we used, that because of translational invariance of the lattice, the mean spin $\langle \sigma_i \rangle$ cannot depend on the index i. Now, in the mean field approximation, the term $\sum_{\langle i,j \rangle} (\sigma_i - \langle \sigma_i \rangle)(\sigma_j - \langle \sigma_j \rangle)$, which describes the variation of a certain spin from the mean value, is neglected. Hence we find for the Hamilton operator

$$H_{\mathrm{MF}} = J \frac{q}{2} N \langle \sigma \rangle^2 - \mu \left(B_{\mathrm{MF}} + B \right) \sum_{j=1}^{N} \sigma_j \,,$$

where the magnetic field

$$B_{\mathrm{MF}} = q \frac{J \langle \sigma \rangle}{\mu}$$

is caused by the spins.

(a) One can find two expressions for the mean magnetization. On the one hand

$$\langle D \rangle = \mu \left\langle \sum_{j=1}^{N} \sigma_j \right\rangle = N \mu \langle \sigma \rangle \;.$$

On the other hand we can use the general expression

$$\langle D \rangle = - \left(\frac{\partial F}{\partial B} \right)_{N,T} \,.$$

Calculate the canonical partition function and the free energy in the mean field approximation. Use your result to deduce the consistency condidion

$$\langle\sigma\rangle = \tanh\left[\beta\mu\left(\frac{qJ}{\mu}\langle\sigma\rangle + B\right)\right] ,$$

which can be used to determine $\langle\sigma\rangle$.

Now, substitute $x = \beta qJ\langle\sigma\rangle + \beta\mu B$. Then the consistency condition becomes

$$\frac{1}{\beta qJ}(x - \beta\mu B) = \tanh x .$$

The solutions to this equation are given by the intersections of the line $\frac{1}{\beta qJ}(x - \beta\mu B)$ with the function $\tanh x$.

(b) Consider the case $B = 0$. How many solutions can you find for x above and below the critical temperature $T_c = \frac{qJ}{k}$? What does this mean for the possible values of B_{MF}?

–Homework–

H 5.1 One dimensional Ising-model *(3+3+3+3=12) Points*

Here we want to consider the one dimensional version of the Ising-model. The Hamilton operator is given by

$$H = -J\sum_{j=1}^{N}\sigma_j\sigma_{j+1} - \mu B\sum_{j=1}^{N}\sigma_j .$$

To keep things simple, the linear lattice is compatified to a circle with periodic boundary condition, i.e. $\sigma_{N+1} = \sigma_1$.

(a) The matrix elements of the *transfer matrix* T are defined as

$$\langle\sigma_i|T|\sigma_j\rangle = \exp\left(\beta\left[J\sigma_i\sigma_j + \frac{\mu B}{2}(\sigma_i + \sigma_j)\right]\right) .$$

Show that the canonical partition function $Z = \sum_{\{\sigma_i=\pm 1\}}\exp[-\beta H(\{\sigma_i\})]$ is given by

$$Z = \sum_{\sigma_1=\pm 1}\langle\sigma_1|T^N|\sigma_1\rangle = \mathrm{Sp}\left(T^N\right) .$$

Hint: The states $|\pm 1\rangle$ fulfill the closure relation $\sum_{\sigma=\pm 1}|\sigma\rangle\langle\sigma| = 1$.

(b) Assign the unit vector $\begin{pmatrix}1\\0\end{pmatrix}$ to the spin $\sigma = 1$ and the unit vector $\begin{pmatrix}0\\1\end{pmatrix}$ to the spin $\sigma = -1$, such that T takes the form

$$T = \begin{pmatrix}\exp\{\beta(J+\mu B)\} & \exp\{-\beta J\}\\ \exp\{-\beta J\} & \exp\{\beta(J-\mu B)\}\end{pmatrix} .$$

Calculate the eigenvalues of T and calculate the partition function Z explicitly.

(c) The *mean magnetization* is defined by

$$\langle D \rangle = -\left(\frac{\partial F}{\partial B}\right)_{T,N} .$$

Calculate the free energy F and show, that the system is paramagnetic in the absence of an external magnetic field, i.e. the mean magnetization vanishes in this case, when the interaction of the spins is switched off. How does the mean magnetization behave in the limits $T \to 0$ and $T \to \infty$ if the external B field is switched on?

(d) Show, that if the interactions are switched on, the mean magnetization is given by

$$\langle D \rangle = N\mu \frac{\sinh \beta\mu B}{\sqrt{\exp\{-4\beta J\} + \sinh^2 \beta\mu B}} \frac{\lambda_1^N - \lambda_2^N}{\lambda_1^N + \lambda_2^N} ,$$

where $\lambda_{1,2}$ are the eigenvalues of T, which were determined in (b). How does $\langle D \rangle$ behave in the limit $(\beta\mu B) \to 0$?

H 5.2 Ultrarelativistic Gas *(5+3=8) Points*

We want to determine the thermodynamical properties of an ultrarelativistic ideal classical gas using the canonical ensemble. Such a gas consists of massless particles moving with the speed of light such that the relativistic energy momentum relation

$$\epsilon = \sqrt{p^2c^2 + m^2c^4} = |p|c$$

holds. The Hamilton function is given by

$$H(\{q_i\}, \{p_i\}) = \sum_{i=1}^{N} |p_i|c$$

and the canonial partition function is

$$Z(T, V, N) = \frac{1}{N! h^{3N}} \int \mathrm{d}^{3N}q \, \mathrm{d}^{3N}p \exp\left\{-\beta \sum_{i=1}^{N} |p_i|c\right\} .$$

(a) Show, that

$$Z(T, V, N) = \frac{1}{N!}\left(8\pi V \left(\frac{kT}{hc}\right)^3\right)^N .$$

Hint: Remember the integral representation of the gamma function from sheet 2: $\Gamma(n) = \int_0^\infty t^{n-1}\mathrm{e}^{-t}\mathrm{d}t$

(b) Use Stirlings formula to calculate the free Energy F as well as the chemical potential μ and show the equations of state of the ultrarelativistic gas

$$pV = NkT ,$$
$$E = 3NkT .$$