Physikalisches Institut

Universität Bonn

Theoretische Physik

Übungsblatt 3

26. Oktober 2012

WS 12/13

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 3.1 Derivatives in multidimensional Analysis

In this exercise, we want to remind ourselves of some important notions from (real) multidimensional analysis. Consider a vector-valued map $f(x^1, x^2, \ldots, x^n)$ with l components $f^a(x^1, x^2, \ldots, x^n)$, which depends on n real real variables, i.e. a map $f : \mathbb{R}^n \to \mathbb{R}^l$. The simplest and most natural generalization of the notion of a derivative in one-dimensional analysis is the *partial derivative*,

$$\frac{\partial}{\partial x^i} f^a(x^1, \ldots, x^n) \equiv \lim_{h \to 0} \frac{f^a(x^1, \ldots, x^i + h, \ldots, x^n) - f^a(x^1, \ldots, x^i, \ldots, x^n)}{h},$$

in which one looks at the variation of one of the map's components in the direction of a single coordinate, while all other coordinates are kept constant.[1] If we now consider a second map $g : \mathbb{R}^m \to \mathbb{R}^n$, as well as the concatonation $h = f \circ g : \mathbb{R}^m \to \mathbb{R}^l$ of f and g, we can use the *chain rule*

$$\frac{\partial h^i}{\partial x^j}(p) = \sum_{k=1}^n \frac{\partial f^i}{\partial y^k}(g(p)) \frac{\partial g^k}{\partial x^j}(p), \qquad i = 1, \ldots, l, \ j = 1, \ldots, m,$$

to determine the partial derivatives of h. Henceforth we will be especially interested in the case $l = 4$, i.e. for real-valued functions $f(x^1, x^2, \ldots, x^n)$.

In general one is not interested in the variation of a map along just one component, but in the direction of any given vector. For that purpose one defines the *directional derivative* along a unit vector $v \in \mathbb{R}^n$,

$$D_v f(p) \equiv \left. \frac{\mathrm{d}}{\mathrm{d}t} f(p + tv) \right|_{t=0}.$$

(a) Show that $D_v f(p) = \sum_{k=1}^n \frac{\partial f}{\partial x^k}(p) v^k$.

Now we want to define the total differential of the function f which plays a central role in thermodynamics. In order to do that, though, we have to first introduce the notion of a linear for. Consider a vector space V over the field $\mathbb{R}$. A map $f : V \to \mathbb{R}$ is called *linear form*, if the identities

$$f(x + y) = f(x) + f(y), \qquad \forall x, y \in V \qquad \text{und}$$
$$f(\alpha x) = \alpha f(x), \qquad \forall \alpha \in \mathbb{R}, x \in V$$

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[1]This, of course, only works if this limit exists, which we will always assume. In the context of thermodynamics the functions we consider are, up to certain interesting examples, always smooth.

are satisfied. The set of all linear forms over an n-dimensional vector space V is itself an n-dimensional vector space, called the *dual space V^**. If $\{x_i\}$ $(i = 1, \ldots, n)$ is a basis of V, the set $\{dx^i\}$, where

$$dx^i(x_j) = \delta^i_j$$

is a basis of V^*. Keep in mind, that the dx^i are themselves maps from V to $\mathbb{R}$.

(b) Show, by a proper definition of addition and scalar multiplication, that V^* is itself an $\mathbb{R}$ vector space and that $\{dx^i\}$ is a basis of this vector space.

Consider now an open subspace M of $\mathbb{R}^n$ and a differentiable function $f : M \to \mathbb{R}$. The *total derivative* of f is then defined as the map

$$df(p): \begin{array}{ccc} \mathbb{R}^n & \to & \mathbb{R} \\ v & \mapsto & D_v f(p) \end{array},$$

which maps a vector v, to the directional derivative $D_v f(p)$ of the function f at the point p in the direction of v. Because of the linearity of the directional derivative, $df(p)$ is a linear form and we can write

$$df(p) = \sum_{k=1}^{n} \frac{\partial f}{\partial x^k}(p) \, dx^k.$$

By definition every total derivative is a linear form. On the other hand, not every linear form A is a total derivative of a function. If the linear form satisfies the *integrability condition* $dA = 0$ (one then calls A closed), though, one can at least in the neighbourhood of every point find a function f, such that $A = df$. If the domain of a linear form is the whole $\mathbb{R}^n$, or, more generally a star domain, then this *integral f* of A even exists globally[2].

In the context of thermodynamics it often happens, that a system is completely determined by a certain number of functions of state, though one has a bigger number of functions of state at hand. Of course in this case the functions of state are not independend from each other and can be seen as functions of each other. To illustrate that, let us look at a function $f : S^2 \to \mathbb{R}$, where S^2 denotes the two dimensional unit sphere. We parameterize the S^2 via its canonical embedding into the $\mathbb{R}^3$, that means using the euclidean coordinates (x, y, z) which depend on each other via the relation $1 = x^2 + y^2 + z^2$.

(c) Let $f(x, y) = x^2 + y^2$. Write down $df(x, y)$. What is $df(x, z(x, y))$?

In such cases one sometimes explicitly indicate the variables that are kept constant. For instance one writes

$$\frac{\partial}{\partial x} f(x, y) = \left(\frac{\partial f(x, y)}{\partial x} \right)_y = \left(\frac{\partial f}{\partial x} \right)_y.$$

(d) Calculate $\left(\frac{\partial f}{\partial x} \right)_y$ as well as $\left(\frac{\partial f}{\partial x} \right)_z$ for the function $f(x, y) = x^2 + y^2$.

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[2]For general manifolds the existence of global integrals of closed forms depends on the de-Rham cohomology group of the manifold.

(e) Show the relation

$$\left(\frac{\partial f}{\partial x}\right)_z = \left(\frac{\partial f}{\partial x}\right)_y + \left(\frac{\partial f}{\partial y}\right)_x \left(\frac{\partial y}{\partial x}\right)_z .$$

(f) Finally consider three dependend variables $u(v, w)$, $v(u, w)$, $w(u, v)$, that means we can imagine these three variables as coordinates on a two-dimensional space. First, show that

$$\left(\frac{\partial u}{\partial v}\right)_w = \frac{1}{\left(\frac{\partial v}{\partial u}\right)_w} .$$

Use this relation to show the chain rule

$$\left(\frac{\partial u}{\partial v}\right)_w \left(\frac{\partial v}{\partial w}\right)_u \left(\frac{\partial w}{\partial u}\right)_v = -1 ,$$

by using a *curve* in the (v, w) space along which u is constant, such that $du = 0$.

$-$HOMEWORK$-$

H 3.1 Temperature of the Spin Ensemble   *(2+1+2=5) Points*
Consider the spin ensemle from exercise H 2.2.

(a) From exercise H 2.2b) one can see, that $\omega(E, \delta E)$ is approximately given by

$$\log \omega(E, \delta E) = -\frac{1}{2}\left(N - \frac{E}{\mu B}\right)\log\left(\frac{1}{2} - \frac{E}{2N\mu B}\right) - \frac{1}{2}\left(N + \frac{E}{\mu B}\right)\log\left(\frac{1}{2} + \frac{E}{2N\mu B}\right) ,$$

where we neglected the irrelevant term $\log(\delta E / 2\mu B)$. Express the energy E in terms of its temperature T.

(b) In which cases is T negative?

(c) Express the magnetization $M = \mu(n_1 - n_2)$ in terms of the temperature.

H 3.2 Two Spin Ensembles   *(4+4+2=10) Points*
Consider two copies of the spin ensemble from exercise H 2.2 in a magnetic field B. We denote the number of particles and magnetic moment of the first ensemble by N and μ, those of the second ensemble by N' and μ'. The energies of the ensembles are then given by $bN\mu B$ and $b'N'\mu'B$ respectively, where $b = 1 - \frac{2n_1}{N}$ and $b' = 1 - \frac{2n_1'}{N'}$. Let $|b|, |b'| \ll 1$, such that the expressions for the densities of states ω that were deduced in exercise H 2.2d) are valid.

(a) Show that in the thermodynamical equilibrium, that means in the most probable con-figuration of the system, the entropies $\tilde{E}$ and $\tilde{E}'$ of the two subsystems are related by

$$\frac{\tilde{E}}{\mu^2 N} = \frac{\tilde{E}'}{\mu'^2 N'}$$

and calculate $\tilde{E}$.

Hint: Neglect terms involving $\delta E^{(\prime)}$.

(b) The probability $P(E)\mathrm{d}E$ for the first ensemble to have an energy between E and $E + \mathrm{d}E$ in the equilibrium configuration is proportional to the number of states in the equilibrium configuration of the total system in which the first ensemble has this energy. Show, that

$$P(E)\mathrm{d}E = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(E-\tilde{E})^2}{\sigma^2}} \mathrm{d}E\,,$$

where $\sigma^2 = \frac{\mu^2 \mu'^2 B^2 N N'}{\mu^2 N + \mu'^2 N'}$.

Hint: What is $\int_{-\infty}^{\infty} P(E)\mathrm{d}E$?

(c) Calculate the variance $(\Delta E)^2$.

H 3.3 Ideal Gas   *(2+3=5) Points*
In the limit of a very big and fixed number of particles, the entropy of an ideal gas is given by

$$S(E,V) = kN \log \left[\frac{V}{N} \left(\frac{4\pi mE}{3Nh^2} \right)^{\frac{3}{2}} e^{\frac{5}{2}} \right].$$

(a) Express the energy E in terms of the temperature.

(b) The pressure is defined as

$$P = T \left(\frac{\partial S}{\partial V} \right)_E.$$

Calculate P and deduce the thermal equation of state of the ideal gas, that means express its pressure in terms of V and T.