

Theorie der Kondensierten Materie I WS 2015/16

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Blatt 5

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1. Mathematical preliminaries: from a sum to an integral

(5 + 5 = 10 Punkte)

(a) Euler-Maclaurin expansion.

We write the integral in question as

$$\int_a^b F(\lambda x) dx = \sum_{n=a}^{b-1} \int_n^{n+1} F(\lambda x) dx \quad (1)$$

and use the identity proposed in the exercise to get

$$\begin{aligned} \int_a^b F(\lambda x) dx &= \frac{1}{2} \sum_{n=a}^{b-1} [F(\lambda(n+1)) + F(\lambda n)] - \lambda \sum_{n=a}^{b-1} \int_n^{n+1} dx F'(\lambda x) \left[(x-n) - \frac{1}{2} \right] \\ &= \sum_{n=a+1}^b F(\lambda n) + \frac{1}{2} [F(\lambda a) - F(\lambda b)] - \lambda \sum_{n=a}^{b-1} \int_n^{n+1} dx F'(\lambda x) \left[(x-n) - \frac{1}{2} \right] \quad (2) \end{aligned}$$

Note that the second term in this expression is of the order of λ at small λ , while the third term is of the order of λ^2 because

$$\int_n^{n+1} \left[(x-n) - \frac{1}{2} \right] = 0. \quad (3)$$

We thus get

$$\int_a^b dx F(\lambda x) = \sum_{n=a+1}^b F(\lambda n) + \frac{1}{2} [F(\lambda a) - F(\lambda b)] + O(\lambda^2). \quad (4)$$

We now proceed from Eq. (2) using

$$d \left[(x-n)^2 - (x-n) + \frac{1}{6} \right] = 2 \left[(x-n) - \frac{1}{2} \right] \quad (5)$$

and integrating by parts. We get

$$\begin{aligned} \int_a^b F(\lambda x) dx &= \sum_{n=a+1}^b F(\lambda n) + \frac{1}{2} [F(\lambda a) - F(\lambda b)] - \frac{\lambda}{12} \sum_{n=a}^{b-1} [F'(\lambda(n+1)) - F'(\lambda n)] \\ &\quad + \frac{\lambda^2}{2} \sum_{n=a}^{b-1} \int_n^{n+1} dx F''(\lambda x) \left[(x-n)^2 - (x-n) + \frac{1}{6} \right] \quad (6) \end{aligned}$$

Note that the integration constant $(1/6)$ in Eq. (4) was not occasional. Due to this choice of the integration constant

$$\int_n^{n+1} dx \left[(x-n)^2 - (x-n) + \frac{1}{6} \right] = 0. \quad (7)$$

Thus, the last term in Eq. (6) has the order λ^3 and we can write

$$\int_a^b dx F(\lambda x) = \sum_{n=a+1}^b F(\lambda n) + \frac{1}{2} [F(\lambda a) - F(\lambda b)] + \frac{\lambda}{12} [F'(\lambda a) - F'(\lambda b)] + O(\lambda^3). \quad (8)$$

Let us now send b to infinity assuming that $F(\infty) = 0$. We also take $a = 0$. We get

$$\begin{aligned} \int_0^\infty dx F(\lambda x) &= \sum_{n=1}^\infty F(\lambda n) + \frac{1}{2} F(0) + \frac{\lambda}{12} F'(0) + O(\lambda^2) = \\ &= \sum_{n=0}^\infty F\left(\lambda \left(n + \frac{1}{2}\right) + \frac{\lambda}{2}\right) + \frac{1}{2} F(0) + \frac{\lambda}{12} F'(0) + O(\lambda^2) = \\ &= \sum_{n=0}^\infty \left[F\left(\lambda \left(n + \frac{1}{2}\right)\right) + \frac{\lambda}{2} F'\left(\lambda \left(n + \frac{1}{2}\right)\right) + \frac{\lambda^2}{8} F''\left(\lambda \left(n + \frac{1}{2}\right)\right) \right] \\ &\quad + \frac{1}{2} F(0) + \frac{\lambda}{12} F'(0) + O(\lambda^2) \\ &= \sum_{n=0}^\infty \left[F\left(\lambda \left(n + \frac{1}{2}\right)\right) + \frac{\lambda}{2} F'(\lambda n) + \frac{3\lambda^2}{8} F''(\lambda n) \right] + \frac{1}{2} F(0) + \frac{\lambda}{12} F'(0) + O(\lambda^2). \end{aligned} \quad (9)$$

We now use

$$\begin{aligned} \sum_{n=0}^\infty F'(\lambda n) &= F'(0) + \sum_{n=1}^\infty F'(\lambda n) = F'(0) + \int_0^\infty dx F'(\lambda x) - \frac{1}{2} F'(0) + O(\lambda) \\ &= \frac{1}{2} F'(0) - \frac{1}{\lambda} F(0) + O(\lambda), \end{aligned} \quad (10)$$

$$\sum_{n=0}^\infty F''(\lambda n) = \int_0^\infty dx F''(\lambda x) + O(1) = -\frac{1}{\lambda} F'(0) + O(1). \quad (11)$$

to get

$$\begin{aligned} \int_0^\infty dx F(\lambda x) &= \sum_{n=0}^\infty F\left(\lambda \left(n + \frac{1}{2}\right)\right) - \frac{1}{2} F(0) + \frac{\lambda}{4} F'(0) - \frac{3\lambda}{8} F'(0) + \frac{1}{2} F(0) + \frac{\lambda}{12} F'(0) + O(\lambda^2) \\ &= \sum_{n=0}^\infty F\left(\lambda \left(n + \frac{1}{2}\right)\right) - \frac{\lambda}{24} F'(0) + O(\lambda^2) \end{aligned} \quad (12)$$

This is exactly what we were looking for.

(b) **Poisson summation formula.**

The function

$$\sum_{n=1}^{\infty} \delta(x - n) \quad (13)$$

is a periodic function of x with period 1. As such it can be expanded into Fourier series over functions $e^{2\pi i k x}$. The expansion coefficients

$$\int_{-1/2}^{1/2} \sum_{n=1}^{\infty} \delta(x - n) e^{-2\pi i k x} = 1. \quad (14)$$

Thus

$$\sum_{n=1}^{\infty} \delta(x - n) = \sum_k e^{2\pi i k x} \quad (15)$$

We multiply both sides of Eq. (15) by arbitrary $f(x)$ and integrate over x from $-\infty$ to ∞ . We get the statement of the exercise.

2. Fermionic density in magnetic field

(5 + 5 + 5 = 15 Punkte)

We consider spinless electrons of mass m in magnetic field H .

(a) In 3D the eigenenergies of an electron in magnetic field are given by

$$\epsilon = \omega_c \left(n + \frac{1}{2} \right) + \frac{p_z^2}{2m}, \quad \omega_c = eB/mc. \quad (16)$$

Due to the degeneracy of Landau levels the number of states per unit volume in the given n -th Landau level and with the momentum p_z in the interval $(p_z, p_z + dp_z)$ is given by

$$dN_n = \frac{B}{\Phi_0} \frac{dp_z}{2\pi} = \frac{B}{\Phi_0} \frac{dp_z}{2\pi}, \quad \Phi_0 = \frac{2\pi\hbar c}{e}. \quad (17)$$

We now use that within the given Landau level $p_z = \pm \sqrt{2m(\epsilon - \omega_c(n + 1/2))}$. Thus

$$dN_n = 2 \frac{B}{\Phi_0} \frac{d\epsilon}{4\pi} \sqrt{\frac{2m}{\epsilon - \omega_c(n + 1/2)}} \quad (18)$$

At given ϵ the Landau levels with $n \leq n_{\max}(\epsilon) \equiv [\epsilon/\omega_c - 1/2]$ will contribute to the density of states. Here $[x]$ stands for the largest integer smaller than x . Thus

$$\nu_{3D}(\epsilon) = \frac{B}{2\pi\Phi_0} \sum_{n=0}^{n_{\max}(\epsilon)} \sqrt{\frac{2m}{\epsilon - \omega_c(n + 1/2)}}. \quad (19)$$

In the 2D case the only possible energies of an electron in magnetic field are $\omega_c(n + 1/2)$. Taking into account the degeneracy of Landau levels we get

$$\nu_{2D}(\epsilon) = \frac{B}{\Phi_0} \sum_{n=0}^{\infty} \delta(\epsilon - \omega_c(n + 1/2)). \quad (20)$$

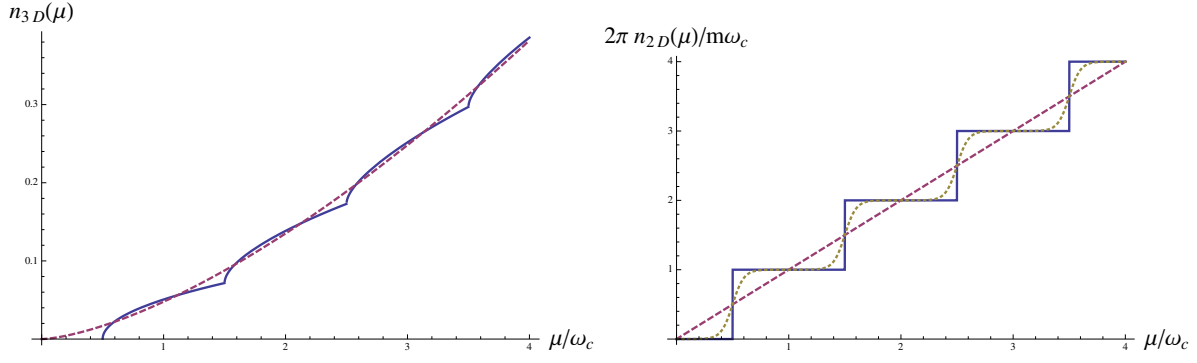


Abbildung 1: The dependence of the particle density on chemical potential. In 2D case n_{2D} is normalized to the density $m\omega_c/2\pi$ corresponding to a completely filled Landau level.

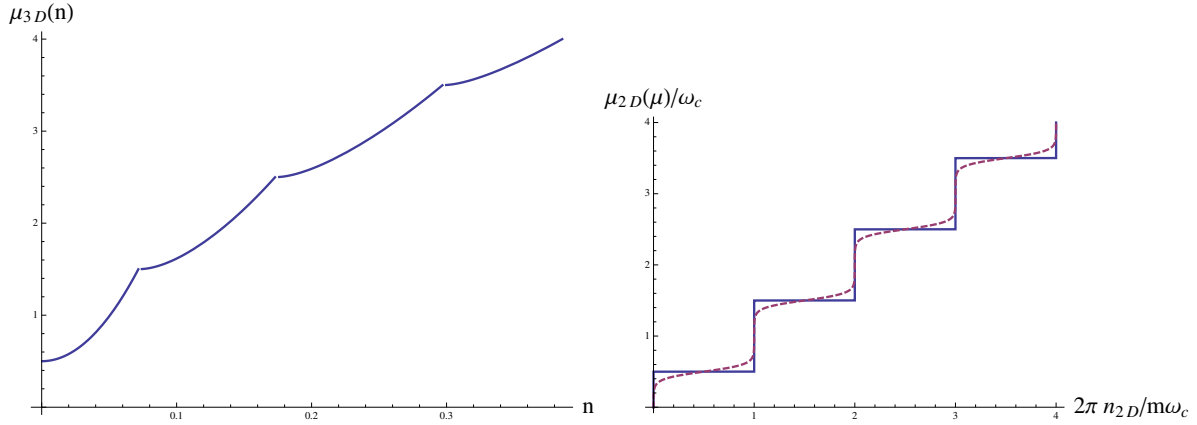


Abbildung 2: The dependence of chemical potential on the particle density. In 2D case n_{2D} is normalized to the density $m\omega_c/2\pi$ corresponding to a completely filled Landau level.

- (b) The density as a function of chemical potential can be now found by straightforward integration of the density of states with the fermi function. We get at $T = 0$

$$n_{3D}(\mu) = \int_0^\mu d\epsilon \nu_{3D}(\epsilon) = \frac{B}{\pi\Phi_0} \sum_{n=0}^{n_{\max}(\mu)} \sqrt{2m(\mu - \omega_c(n + 1/2))} \quad (21)$$

$$n_{2D}(\mu) = \int_0^\mu d\epsilon \nu_{2D}(\epsilon) = \frac{B}{\Phi_0} (n_{\max}(\mu) + 1) \quad (22)$$

At large μ we get

$$n_{3D}(\mu) \approx \frac{B}{\pi\Phi_0} \int_0^{\mu/\omega_c} dn \sqrt{2m(\epsilon - \omega_c n)} = \frac{B}{\pi\Phi_0} \frac{2\sqrt{2m}\mu^{3/2}}{3\omega_c} = \frac{\sqrt{2m}m\mu^{3/2}}{3\pi^2}, \quad (23)$$

$$n_{2D}(\mu) \approx \frac{B}{\Phi_0} n_{\max}(\mu) \approx \frac{B}{\Phi_0} \frac{\mu}{\omega_c} = \frac{m\mu}{2\pi}. \quad (24)$$

These results correspond to n_μ in the absence of magnetic field. The behaviour of n_μ in 3D and 2D is shown in Fig. 1. Dashed lines show $n(\mu, B = 0)$. Finite temperature smoothes the singularities in $n(\mu)$. It is especially important in 2D where the function $n_{2D}(\mu, T = 0)$ has jumps. At finite temperature $n_{2D}(\mu, T)$ is continuous (see dotted line in Fig. 1b).

- (c) The dependences $\mu(n)$ can be obtained from Fig. 1 just by exchanging the axes. The result is shown in Fig. 2. The effect of finite temperature is again especially

important for 2D case. At zero temperature μ_{2D} is always pinned to the Landau levels and only jump between them at integer $2\pi n_{2D}/m\omega_c$. Finite temperature makes $\mu_{2D}(n)$ continuous.

3. de Haas - van Alphen effect in two dimensions

(5 + 5 = 10 Punkte)

The de Haas - van Alphen effect is particularly simple in two dimensions. In this exercise we consider spinless electron gas in two dimensions and at zero temperature.

- (a) Let us fix H and S (magnetic field and area of the sample) and vary N . For small N all the fermions can be put into the first Landau level and will energy equal to simply $\omega_c/2$. This means the

$$E(N, S, H, T = 0) = N\omega_c/2, \quad N < HS/\Phi_0. \quad (25)$$

Equation (25) is valid however only for $N < HS/\Phi_0$, i.e. when there are enough states in the lowest Landau level to accommodate all the electrons.

When $HS/\Phi_0 < N < 2HS/\Phi_0$ the lowest Landau level is completely filled and extra electrons are accommodate at the second Landau level where the energy is $3\omega_c/2$. Thus

$$E(N, S, H, T = 0) = \frac{\omega_c}{2} \frac{HS}{\Phi_0} + \frac{3\omega_c}{2} \left(N - \frac{HS}{\Phi_0} \right), \quad \frac{HS}{\Phi_0} < N < \frac{2HS}{\Phi_0} \quad (26)$$

It is now easy to write down the general formula.

$$E(N, S, H, T = 0) = \sum_{p=0}^{n-1} \omega_c \left(p + \frac{1}{2} \right) \frac{HS}{\Phi_0} + \omega_c \left(n + \frac{1}{2} \right) \left(N - \frac{HSn}{\Phi_0} \right), \quad (27)$$

$$\frac{HS}{\Phi_0} n < N < \frac{HS}{\Phi_0} (n+1). \quad (28)$$

Here n takes values $0, 1, 2, \dots$

We can simplify Eq. (28) as

$$E(N, S, H, T = 0) = -\frac{\omega_c HS}{2\Phi_0} n(n+1) + \omega_c \left(n + \frac{1}{2} \right) N, \quad \frac{HS}{\Phi_0} n < N < \frac{HS}{\Phi_0} (n+1). \quad (29)$$

Taking into account $\omega_c = eH/mc$ we find

$$E(N, S, H, T = 0) = -\frac{e^2 H^2 S}{4\pi mc^2} n(n+1) + \frac{eH}{mc} \left(n + \frac{1}{2} \right) N, \quad \frac{S}{N\Phi_0} n < \frac{1}{H} < \frac{S}{\Phi_0 N} (n+1). \quad (30)$$

Here we have rewritten the inequality $\frac{HS}{\Phi_0} n < N < \frac{HS}{\Phi_0} (n+1)$ in an equivalent form. We see that that the energy of the system is a piece-wise parabolic function of the magnetic field.

- (b) We now differentiate energy with respect to the magnetic field to get the magnetization.

$$M/S = -\partial_H E = \frac{e^2 H}{2\pi mc^2} n(n+1) - \frac{e}{mc} \left(n + \frac{1}{2} \right) N/S, \quad \frac{S}{N\Phi_0} n < \frac{1}{H} < \frac{S}{\Phi_0 N} (n+1). \quad (31)$$

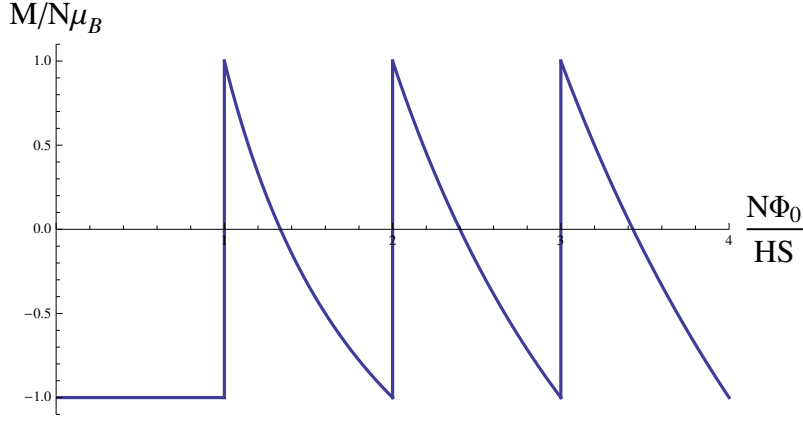


Abbildung 3: Magnetization as a function of $1/H$.

Magnetization is piece-wise linear function of magnetic field. It has jumps at the points $1/H = Sn/N\Phi_0$ with integer n . Indeed,

$$\left. \frac{M}{S} \right|_{\frac{1}{H} = \frac{S_n}{N\Phi_0} + 0} = \frac{e^2 N \Phi_0}{2\pi m c^2 n S} n(n+1) - \frac{e}{mc} \left(n + \frac{1}{2} \right) N/S = \frac{eN}{2mcS} = \frac{\mu_B N}{S}, \quad (32)$$

$$\left. \frac{M}{S} \right|_{\frac{1}{H} = \frac{S_n}{N\Phi_0} - 0} = \frac{e^2 N \Phi_0}{2\pi m c^2 n S} (n-1)n - \frac{e}{mc} \left(n - 1 + \frac{1}{2} \right) N/S = \frac{eN}{2mcS} = -\frac{\mu_B N}{S}. \quad (33)$$

It is also easy to see that on each of the intervals $\frac{S}{N\Phi_0}n < \frac{1}{H} < \frac{S}{\Phi_0 N}(n+1)$ the magnetization is a monotonous function of H . It is now easy to sketch the graph of M . Just as in the 3D case magnetization experiences oscillations as function of $1/H$.