

8. Bosonic systems

8.1. Bose condensate

Number of particles

The average number of particles is

$$\begin{aligned}\bar{N} &= \langle N \rangle = - \left(\frac{\partial \Omega}{\partial \mu} \right)_T \\ &= \sum_l \frac{1}{e^{\beta(\epsilon_l - \mu)} - 1}\end{aligned}$$

or

$$\bar{N} = \sum_l \bar{n}_l.$$

We denote

$$z = e^{\beta\mu} = \text{fugacity},$$

so

$$\bar{n}_l = \frac{1}{e^{\beta\epsilon_l} z^{-1} - 1}.$$

Let us consider free non-interacting gas when density is large. Then

$$\epsilon_l = \frac{\hbar^2 k_l^2}{2m} = \frac{\mathbf{p}_l^2}{2m},$$

and

$$1 \leq e^{\beta\epsilon_l} < \infty.$$

Because stability requires $\partial \bar{N} / \partial \mu > 0$, the fugacity is restricted to lie between

$$0 \leq z < 1$$

or $\mu < 0$.

We treat the state $\mathbf{p} = 0$ separately, since the corresponding occupation number \bar{n}_0 can become macroscopic:

$$\bar{n}_0 = \frac{z}{1-z} \rightarrow_{z \rightarrow 1} \infty.$$

We write the grand potential as

$$\begin{aligned}\Omega_{\text{BE}} &= k_B T \ln [1 - e^{\beta\mu}] \\ &+ k_B T \sum_{\mathbf{k} \neq 0} \ln \left[1 - e^{\beta\mu} e^{-\beta \frac{\hbar^2 k^2}{2m}} \right].\end{aligned}$$

Let us define function $g_\alpha(z)$ so that

$$g_\alpha(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^\alpha}.$$

Then (homework!)

$$\Omega_{\text{BE}} = k_B T \ln(1-z) - \frac{V k_B T}{\lambda_T^3} g_{5/2}(z).$$

where $\lambda_T = \sqrt{2\pi\hbar^2/(mk_B T)}$. For the number of particles we get

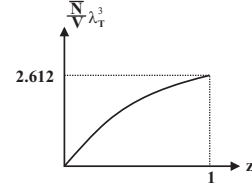
$$\bar{N} = \bar{n}_0 + \frac{V}{\lambda_T^3} g_{3/2}(z).$$

When the temperature is high or the density low, the term $\frac{\bar{n}_0}{V}$ is negligible as compared with $\frac{g_{3/2}(z)}{\lambda_T^3}$, i.e.

$$\frac{\bar{N}}{V} \lambda_T^3 = g_{3/2}(z).$$

Now $g_{3/2}(z)$ is a positive monotonically increasing function and

$$\begin{aligned}\left(\frac{\bar{N}}{V} \lambda_T^3 \right)_{z=0} &= g_{3/2}(0) = 0 \\ \left(\frac{\bar{N}}{V} \lambda_T^3 \right)_{z=1} &= g_{3/2}(1) = \zeta(3/2) = 2.612.\end{aligned}$$



Let us choose the density $\rho = \frac{\bar{N}}{V}$ ja T so that

$$\frac{\bar{N}}{V} \lambda_T^3 = 2.612,$$

and $z = 1$. If we still increase the density or decrease the temperature the increase of the term $\frac{\bar{N}}{V} \lambda_T^3$ must originate from $\frac{\bar{n}_0}{V} \lambda_T^3$, since $z \leq 1$, i.e.

$$\frac{\bar{N}}{V} \lambda_T^3 = g_{3/2}(z), \quad \text{when } \frac{\bar{N}}{V} \lambda_T^3 < 2.612$$

$$\frac{\bar{N}}{V} \lambda_T^3 = \frac{\bar{n}_0}{V} \lambda_T^3 + g_{3/2}(1), \quad \text{when } \frac{\bar{N}}{V} \lambda_T^3 \geq 2.612.$$

When

$$\lambda_T^3 \geq 2.612 \frac{V}{\bar{N}},$$

the state $\mathbf{p} = 0$ will be occupied macroscopically forming the *Bose-Einstein condensate*. The formation starts when the temperature is less than the *critical temperature*

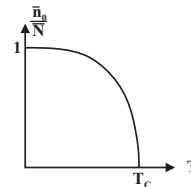
$$T_c = \left(\frac{2\pi\hbar^2}{mk_B} \right) \left(\frac{\rho}{2.612} \right)^{2/3}$$

or the density greater than the *critical density*

$$\rho_c = 2.612 \left(\frac{mk_B T}{2\pi\hbar^2} \right)^{3/2}.$$

When $T < T_c$, the relative fraction of the condensate is

$$\frac{\bar{n}_0}{\bar{N}} = 1 - \frac{2.612}{\lambda_T^3} \frac{V}{\bar{N}} = 1 - \left(\frac{T}{T_c} \right)^{3/2}.$$



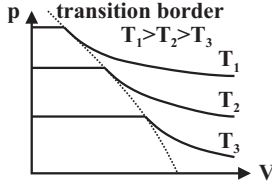
Pressure

With the help of the grand potential the pressure is

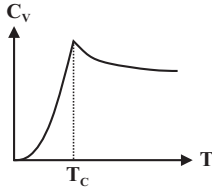
$$p = - \left(\frac{\partial \Omega}{\partial V} \right)_{T,N} = \frac{k_B T}{\lambda_T^3} g_{5/2}(z),$$

so

$$p = \begin{cases} \frac{k_B T}{\lambda_T^3} g_{5/2}(z) & \text{above the} \\ & \text{critical point} \\ \frac{k_B T}{\lambda_T^3} g_{5/2}(1) = 1.342 \frac{k_B T}{\lambda_T^3} & \text{below the} \\ & \text{critical point.} \end{cases}$$



This is a 2nd order phase transition ($d^2\Omega/dV^2$ discontinuous)

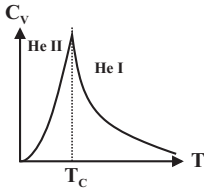


⁴He liquid

A *second order* phase transition to a *super liquid state* at the temperature $T_c = 2.17\text{K}$. The expression given above,

$$T_c = \frac{2\pi\hbar^2}{mk_B} \left(\frac{\rho}{2.612} \right)^{2/3},$$

results in $T_c = 3.13\text{K}$, which is close to the experimental value.



This is called a λ -transition.

Two-liquid model

When $T < T_c$, we assume that ⁴He is a “mixture” of two components: superfluid and normal fluid. Then

$$\begin{aligned} \rho &= \rho_s + \rho_n \\ \mathbf{j} &= \mathbf{j}_s + \mathbf{j}_n \\ &\vdots \end{aligned}$$

When $T \rightarrow 0$, then $\frac{\rho_s}{\rho} \rightarrow 1$, but $\frac{\bar{n}_0}{N} \rightarrow \sim 0.1$.

This is due to the fact that ⁴He is *not* an ideal liquid: between ⁴He atoms there is

- a strong repulsion at short distances,
- an attraction at longer distances.

8.2. Black body radiation (photon gas)

The *photon* is a relativistic massless *boson*, whose spin is $S = 1$, so $g = 2S + 1 = 3$. In the vacuum only transverse polarisation exists, so that $g = 2$.

The energy of a photon is

$$\begin{aligned} \epsilon(p) &= \sqrt{(m_0 c^2)^2 + (pc)^2} \\ &= pc = \hbar kc. \end{aligned}$$

Using frequency f or angular velocity ω , the energy becomes

$$\epsilon = \hbar\omega = \hbar 2\pi f = hf.$$

Since the wavelength λ is

$$\lambda = \frac{2\pi}{k},$$

we have

$$\begin{aligned} f &= \frac{c}{\lambda} \\ \omega &= ck. \end{aligned}$$

Density of states

Employing the periodic boundary conditions the wave vector is

$$\mathbf{k} = \frac{2\pi}{L} (n_x, n_y, n_z),$$

so the number of states in the vicinity of \mathbf{k} is

$$\begin{aligned} dN_{\mathbf{k}} &= g \left(\frac{L}{2\pi} \right)^3 d\mathbf{k} \\ &= g \frac{V}{(2\pi)^3} 4\pi k^2 dk. \end{aligned}$$

With the help of the angular velocity this is

$$\begin{aligned} dN_{\mathbf{k}} &= dN_{\omega} = g \frac{V}{(2\pi)^3} 4\pi \frac{\omega^2}{c^2} \frac{d\omega}{c} \\ &= g \frac{V\omega^2 d\omega}{2\pi^2 c^3}. \end{aligned}$$

We denote now

$$dN_{\omega} = f(\omega) d\omega,$$

so

$$f(\omega) d\omega = V \frac{\omega^2 d\omega}{\pi^2 c^3}.$$

The sum over quantum states can be replaced by the integration like

$$\sum_l \dots = \sum_{\mathbf{k}, \lambda} \dots = \int_0^{\infty} d\omega f(\omega) \dots$$

Here \mathbf{k} is the wave vector and

$$\lambda = \begin{cases} L, & \text{left} \\ R, & \text{right} \end{cases}$$

is the polarization.

Photons obey the *Bose-Einstein statistics*

In field theory the photon modes are equivalent to independent harmonic oscillators, and the Hamiltonian of the system can be written as

$$\hat{H} = \sum_{\mathbf{k}, \lambda} (\hbar c k) \left(a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda} + \frac{1}{2} \right).$$

Here the eigenvalues of $\hat{n} = a^\dagger a$ are $0, 1, \dots$; thus, the energy of individual mode is

$$E = \left(n + \frac{1}{2} \right) \hbar \omega = n \hbar \omega + 0\text{-point motion.}$$

Because the number of photons in a photon gas is not an independent degree of freedom (depends on E), μ does not appear as a Lagrange multiplier. Thus, according to the Bose-Einstein distribution the occupation of the energy state $\epsilon(\omega)$ (*Planck distribution*) is

$$\bar{n}(\omega) = \frac{1}{e^{\beta \hbar \omega} - 1}.$$

The *total energy* is

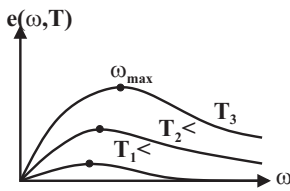
$$E = \int_0^\infty d\omega f(\omega) \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1}.$$

The *energy density* will be

$$\begin{aligned} \frac{E}{V} &= e(T) = \frac{\hbar}{\pi^2 c^3} \int_0^\infty d\omega \frac{\omega^3}{e^{\beta \hbar \omega} - 1} \\ &= \int_0^\infty d\omega e(\omega, T), \end{aligned}$$

where the energy density at the given angular velocity obeys *Planck's law of radiation*

$$e(\omega, T) = \frac{\hbar \omega^3}{\pi^2 c^3 (e^{\beta \hbar \omega} - 1)}.$$



We can see that the maximum of the intensity follows the *Wien displacement law*

$$\omega_{\max} = \text{constant} \times T.$$

At the long wavelength limit, $\lambda \gg \frac{hc}{k_B T}$ or $\omega \ll \frac{k_B T}{\hbar}$, the energy density obeys the *Rayleigh-Jeans law*

$$e(\omega, T) = \text{const.} \times \omega^2 T.$$

At a given temperature the energy density will be

$$\begin{aligned} e(T) &= \int_0^\infty d\omega \frac{\hbar \omega^3}{\pi^2 c^3 (e^{\beta \hbar \omega} - 1)} \\ &= \frac{\hbar}{\pi^2 c^3} \frac{1}{(\beta \hbar)^4} \int_0^\infty dx \frac{x^3}{e^x - 1} \\ &= \frac{k_B^4 T^4}{\pi^2 c^3 \hbar^3} \frac{\pi^4}{15}, \end{aligned}$$

where

$$\begin{aligned} \int_0^\infty dx \frac{x^3}{e^x - 1} &= \sum_{n=1}^\infty \int_0^\infty dx x^3 e^{-nx} \\ &= \Gamma(4) \left(1 + \frac{1}{2^4} + \frac{1}{3^4} \dots \right) = 6 \times \zeta(4) = \frac{\pi^4}{15} \end{aligned}$$

Thus the energy density obeys the *Stefan-Boltzmann law*

$$e(T) = \frac{4}{c} \sigma T^4,$$

where σ is the *Stefan-Boltzmann constant*

$$\sigma = \frac{\pi^2 k_B^4}{60 \hbar^3 c^2} = 5.67 \cdot 10^{-8} \frac{\text{W}}{\text{m}^2 \text{K}^4}.$$

Thermodynamics

Now

$$\Omega = F - \mu N = F,$$

because $\mu = 0$. Thus the free energy is

$$\begin{aligned} F &= k_B T \int_0^\infty d\omega f(\omega) \ln [1 - e^{-\beta \hbar \omega}] \\ &= \frac{V}{\pi^2 c^3} k_B T \int_0^\infty d\omega \omega^2 \ln [1 - e^{-\beta \hbar \omega}] \\ &= \frac{V k_B T}{\pi^2 c^3 (\beta \hbar)^3} \int_0^\infty dx x^2 \ln [1 - e^{-x}] \\ &= -V \frac{k_B^4 T^4}{\pi^2 c^3 \hbar^3} \frac{\pi^4}{45}, \end{aligned}$$

or

$$F = -\frac{4}{3} \frac{\sigma}{c} V T^4 = -\frac{1}{3} E.$$

Here

$$E = e(T) V$$

is the total energy.

The *entropy* is

$$S = -\frac{\partial F}{\partial T}$$

or

$$S = \frac{16}{3} \frac{\sigma}{c} V T^3.$$

The *pressure* is

$$p = -\frac{\partial F}{\partial V}$$

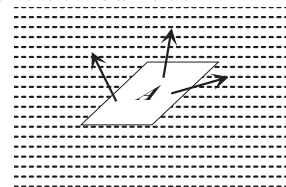
or

$$p = \frac{4}{3} \frac{\sigma}{c} T^4.$$

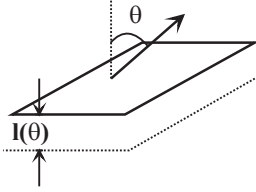
We see that the photon gas satisfies the relation

$$p = \frac{1}{3} e.$$

Radiation of a black surface



We can think that the emitting surface is a hole on a hollow container filled with isotropic black body radiation. The radiation power can be determined by counting the number of photons escaping through the hole per time interval.



In the time interval τ the photons escaping to the direction θ originate from the region whose depth is

$$\ell(\theta) = c\tau \cos \theta.$$

The total energy of photons going into the spherical angle element $d\Omega$ is

$$e(T)Ac\tau \cos \theta \frac{d\Omega}{4\pi}.$$

Thus, the total energy of the radiation escaping in time τ is

$$\begin{aligned} E_{\text{rad}} &= e(T)Ac\tau \int_{\theta=0}^{\pi/2} \cos \theta \frac{d\Omega}{4\pi} \\ &= e(T)Ac\tau \frac{1}{2} \int_0^{\pi/2} d\theta \sin \theta \cos \theta \\ &= \frac{1}{4} Ae(T)c\tau. \end{aligned}$$

The radiation power per unit area (intensity) is

$$\begin{aligned} I &= \frac{E_{\text{rad}}}{A\tau} = \frac{1}{4} ce(T) \\ &= \sigma T^4. \end{aligned}$$

If the radiation arrives from a fixed direction (e.g. solar radiation) with intensity I , then the absorbed radiation power is naturally

$$P = IA_{\perp}$$

where A_{\perp} is the projected area perpendicular to the radiation.

8.3. Phonons

Classical harmonic lattice

We let the ions of a crystal to oscillate in the vicinity of their equilibrium position. We assume that

1. At the average equilibrium position the crystal is a Bravais lattice. With every point \mathbf{R} of the lattice we can thus associate an atom. The vector \mathbf{R} , however, represents only the average position of the ion.
2. Typical deviations from the equilibrium positions are small as compared with the interatomic distances.

According to the hypothesis 1 the atoms of the crystal can be identified with the Bravais lattice points \mathbf{R} ; e.g. $\mathbf{r}(\mathbf{R})$ stands for the actual position of the ion associated

with the lattice point \mathbf{R} . If $\mathbf{u}(\mathbf{R})$ is the deviation of the ion \mathbf{R} from its equilibrium then

$$\mathbf{r}_R = \mathbf{R} + \mathbf{u}_R.$$

Let $\phi(\mathbf{r})$ be the potential energy of two ions separated by the distance \mathbf{r} . The energy of the whole lattice is then

$$\begin{aligned} U &= \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} \phi(\mathbf{r}_R - \mathbf{r}_{R'}) \\ &= \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} \phi(\mathbf{R} - \mathbf{R}' + \mathbf{u}_R - \mathbf{u}_{R'}). \end{aligned}$$

When we use the notation \mathbf{P}_R for the momentum of the ion \mathbf{R} the total Hamiltonian is

$$H = \sum_{\mathbf{R}} \frac{\mathbf{P}_R^2}{2m} + U.$$

Harmonic approximation

Because $u_R \ll$ interatomic distances, we can approximate U as a Taylor series:

$$\begin{aligned} U &= \frac{N}{2} \sum_{\mathbf{R}} \phi(\mathbf{R}) \\ &+ \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} (\mathbf{u}_R - \mathbf{u}_{R'}) \cdot \nabla \phi(\mathbf{R} - \mathbf{R}') \\ &+ \frac{1}{4} \sum_{\mathbf{R}\mathbf{R}'} [(\mathbf{u}_R - \mathbf{u}_{R'}) \cdot \nabla]^2 \phi(\mathbf{R} - \mathbf{R}') \\ &+ \mathcal{O}(u^3). \end{aligned}$$

In the equilibrium the total force due to other ions affecting the ion \mathbf{R} is

$$\mathbf{F} = - \sum_{\mathbf{R}'} \nabla \phi(\mathbf{R} - \mathbf{R}').$$

Since we are at an equilibrium this force must be zero. Thus the linear term in the series expansion of U vanishes. Up to the second order we are left with

$$U = U^{\text{eq}} + U^{\text{harm}},$$

where U^{eq} is the potential energy of the equilibrium and

$$\begin{aligned} U^{\text{harm}} &= \frac{1}{4} \sum_{\substack{\mathbf{R}\mathbf{R}' \\ \mu, \nu = x, y, z}} [u_{R, \mu} - u_{R', \mu}] \phi_{\mu\nu}(\mathbf{R} - \mathbf{R}') \\ &\quad \times [u_{R, \nu} - u_{R', \nu}] \\ \phi_{\mu\nu}(\mathbf{r}) &= \frac{\partial^2 \phi(\mathbf{r})}{\partial r_{\mu} \partial r_{\nu}}. \end{aligned}$$

If we are not interested in the quantities related to the equilibrium of the crystal (total energy, total volume, total compressibility, ...) we can forget the term U^{eq} . The harmonic potential is usually written more generally as

$$U^{\text{harm}} = \frac{1}{2} \sum_{\substack{\mathbf{R}\mathbf{R}' \\ \mu\nu}} u_{R, \mu} D_{\mu\nu}(\mathbf{R} - \mathbf{R}') u_{R', \nu}.$$

The former expression can be obtained by setting

$$D_{\mu\nu}(\mathbf{R} - \mathbf{R}') = \delta_{\mathbf{R}\mathbf{R}'} \sum_{\mathbf{R}''} \phi_{\mu\nu}(\mathbf{R} - \mathbf{R}'') - \phi_{\mu\nu}(\mathbf{R} - \mathbf{R}').$$

The heat capacity of classical lattice

The classical ideal gas gives a good description for a real gases at high enough temperatures. However, the classical description for solid crystal heat capacity is not well described by classical dynamics.

The volume element of the the $3N$ dimensional classical phase space formed by the N ions of the lattice is

$$d\Gamma = \prod_{\mathbf{R}} \frac{1}{h} d\mathbf{u}_{\mathbf{R}} d\mathbf{P}_{\mathbf{R}} = \prod_{\mathbf{R},\mu} \frac{1}{h} du_{R,\mu} dP_{R,\mu}$$

and the canonical partition sum is

$$Z = \int d\Gamma e^{-\beta H}.$$

The total energy E is then

$$E = \frac{1}{Z} \int d\Gamma e^{-\beta H} H = -\frac{\partial}{\partial \beta} \ln Z.$$

When we change variables,

$$\begin{aligned} \mathbf{u}_{\mathbf{R}} &= \beta^{-1/2} \bar{\mathbf{u}}_{\mathbf{R}} \\ \mathbf{P}_{\mathbf{R}} &= \beta^{-1/2} \bar{\mathbf{P}}_{\mathbf{R}}, \end{aligned}$$

the partion function can be written as

$$\begin{aligned} Z &= \int d\Gamma \exp \left[-\beta \left(\sum \frac{\mathbf{P}_{\mathbf{R}}^2}{2M} + U^{\text{eq}} + U^{\text{harm}} \right) \right] \\ &= e^{-\beta U^{\text{eq}}} \beta^{-3N} \int \prod_{\mathbf{R}} \frac{1}{h} d\bar{\mathbf{u}}_{\mathbf{R}} d\bar{\mathbf{P}}_{\mathbf{R}} \times \\ &\quad \exp \left[-\sum \frac{\bar{\mathbf{P}}_{\mathbf{R}}^2}{2M} - \frac{1}{2} \sum \bar{u}_{R,\mu} D_{\mu\nu}(\mathbf{R} - \mathbf{R}') \bar{u}_{R',\nu} \right] \end{aligned}$$

Because all dependence on the temperature is outside of the integral the energy can be calculated easily

$$\begin{aligned} E &= -\frac{\partial}{\partial \beta} \ln(e^{-\beta U^{\text{eq}}} \beta^{-3N} \times \text{const.}) \\ &= U^{\text{eq}} + 3Nk_B T. \end{aligned}$$

The heat capacity is

$$C_v = \frac{\partial E}{\partial T} = 3Nk_B.$$

This expression for heat capacity, due to the lattice vibrations, is known as *Dulong-Petit's law*.

Experimentally

- at low temperatures the heat capacity is smaller than the one obtained from the Dulong-Petit law. When we approach the temperature $T = 0$ the heat capacity tends to zero, due to quantum effects.

- even at higher temperatures the measured heat capacities do not approach the Dulong-Petit limit.

Einstein's model

Let us assume that every ion of the crystal moves in a similar harmonic potential well independently of each other. Then we can quantize the harmonic oscillators:

$$H = \sum_{\mathbf{x}_s} \hbar \omega_E (a_{\mathbf{x}_s}^\dagger a_{\mathbf{x}_s} + \frac{1}{2}),$$

where the parameter

$$\omega_E \equiv \frac{k_B T_E}{\hbar}$$

is the *Einstein frequency* common for all $3N$ oscillators and T_E the corresponding *Einstein temperature*.

The partition function of one single harmonic oscillator is

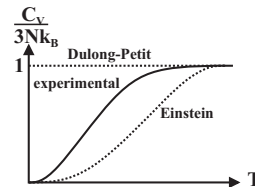
$$\begin{aligned} Z_{\text{harm}}(\omega) &= \text{Tr} e^{-\beta \hbar \omega (a^\dagger a + \frac{1}{2})} = \sum_{n=0}^{\infty} e^{-\beta \hbar \omega (n + \frac{1}{2})} \\ &= e^{-\frac{1}{2} \beta \hbar \omega} \sum_n (e^{-\beta \hbar \omega})^n = \frac{e^{-\frac{1}{2} \beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}} \\ &= \frac{1}{2 \sinh(\frac{1}{2} \beta \hbar \omega)}. \end{aligned}$$

Since the number of modes is $3N$ the canonical partition function is

$$\begin{aligned} Z &= \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \dots \sum_{n_{3N}=1}^{\infty} e^{-\beta \hbar \omega_E \sum_{j=1}^{3N} (n_j + \frac{1}{2})} \\ &= \prod_{j=1}^{3N} \sum_{n=0}^{\infty} e^{-\beta \hbar \omega_E (n + \frac{1}{2})} = Z_{\text{harm}}^{3N}(\omega_E) \\ &= \left[2 \sinh\left(\frac{T_E}{2T}\right) \right]^{-3N}. \end{aligned}$$

The heat capacity is

$$\begin{aligned} C_V &= \frac{\partial E}{\partial T} = -\frac{\partial}{\partial T} \frac{\partial}{\partial \beta} \ln Z = \frac{\partial}{\partial T} \left(k_B T^2 \frac{\partial \ln Z}{\partial T} \right) \\ &= k_B T \frac{\partial^2}{\partial T^2} T \ln Z = 3Nk_B \frac{(T_E/2T)^2}{\sinh^2(T_E/2T)}. \end{aligned}$$



Normal modes of the harmonic crystal

One-dimensional Bravais lattice

If the separation of the lattice points in the one dimensional Bravais lattice is a the lattice points are na , n an integer. Every lattice point na is associated with one atom.

We assume that in this one dimensional lattice only the nearest neighbours interact. Using the notation

$$K = \phi''(x),$$

the harmonic potential of the lattice is

$$U^{\text{harm}} = \frac{1}{2}K \sum_n [u(na) - u((n+1)a)]^2.$$

The classical equations of motion are

$$\begin{aligned} M\ddot{u}(na) &= -\frac{\partial U^{\text{harm}}}{\partial u(na)} \\ &= -K[2u(na) - u((n-1)a) - u((n+1)a)]. \end{aligned}$$

We assume that the N points of the lattice form a ring, i.e. the deviations satisfy the boundary conditions

$$u((N+1)a) = u(a); \quad u(0) = u(Na).$$

We seek solutions of the form

$$u(na, t) \propto e^{i(kna - \omega t)}$$

To satisfy the boundary conditions we must have

$$e^{ikNa} = 1.$$

We see that the allowed values for k are

$$k = \frac{2\pi}{a} \frac{n}{N}, \quad n \text{ integer.}$$

Substituting the exponential trial into the equation of motion we see that the angular velocity ω must satisfy

$$\omega(k) = \sqrt{\frac{2K(1 - \cos ka)}{M}} = 2\sqrt{\frac{K}{M}} \left| \sin \frac{1}{2}ka \right|.$$

The solutions represent a wave advancing in the ring with the phase velocity $c = \omega/k$ and with the group velocity $v = \partial\omega/\partial k$. Clearly, $\omega(k)$ is invertible only if $-\pi < ka < \pi$, i.e. we are within the *Brillouin zone*.

If the wavelength is large or the wave vector k small then the dispersion relation

$$\omega = \left(a\sqrt{\frac{K}{M}} \right) k$$

is linear and the phase and group velocities equal.

One dimensional lattice with base

We assume that in the primitive cell there are two atoms. Let the equilibrium positions of the ions to be na and $na + d$, where $d \leq a/2$. We denote the deviations of the ions these equilibrium positions by $u_1(na)$ and $u_2(na)$. For the simplicity we assume that the masses of the atoms are equal. The harmonic interaction due to the nearest neighbours is

$$\begin{aligned} U^{\text{harm}} &= \frac{K}{2} \sum_n [u_1(na) - u_2(na)]^2 \\ &\quad + \frac{G}{2} \sum_n [u_2(na) - u_1((n+1)a)]^2, \end{aligned}$$

where K describes the interaction of the ions na and $na + d$, and G the interaction of $na + d$ and $(n+1)a$. The classical equations of motion are

$$\begin{aligned} M\ddot{u}_1(na) &= -\frac{\partial U^{\text{harm}}}{\partial u_1(na)} \\ &= -K[u_1(na) - u_2(na)] \\ &\quad -G[u_1(na) - u_2((n-1)a)] \\ M\ddot{u}_2(na) &= -\frac{\partial U^{\text{harm}}}{\partial u_2(na)} \\ &= -K[u_2(na) - u_1(na)] \\ &\quad -G[u_2(na) - u_1((n+1)a)]. \end{aligned}$$

Again we look for a solution of the form

$$\begin{aligned} u_1(na) &= \epsilon_1 e^{i(kna - \omega t)} \\ u_2(na) &= \epsilon_2 e^{i(kna - \omega t)}. \end{aligned}$$

Substituting these into the equations of motion we end up with the linear homogenous simultaneous equations

$$\begin{aligned} [M\omega^2 - (K + G)]\epsilon_1 + (K + Ge^{-ika})\epsilon_2 &= 0 \\ (K + Ge^{ika})\epsilon_1 + [M\omega^2 - (K + G)]\epsilon_2 &= 0. \end{aligned}$$

This system has a non-trivial solution only if the coefficient determinant vanishes. From this we obtain

$$\omega^2 = \frac{K + G}{M} \pm \frac{1}{M} \sqrt{K^2 + G^2 + 2KG \cos ka}.$$

The ratio of the amplitudes is

$$\frac{\epsilon_1}{\epsilon_2} = \mp \frac{K + Ge^{ika}}{|K + Ge^{ika}|}.$$

For every allowed wave vector k (counting N) we get *two* solutions. Altogether the number of the normal modes is now $2N$. We consider couple of limiting cases.

Case 1. $k \ll \pi/a$

The angular velocities of the modes are now

$$\begin{aligned} \omega &= \sqrt{\frac{2(K + G)}{M}} - \mathcal{O}((ka)^2) \\ \omega &= \sqrt{\frac{KG}{2M(K + G)}}(ka). \end{aligned}$$

Since the latter dispersion relation is linear the corresponding mode is called *acoustic*. In the former mode $\omega = \sqrt{2(K + G)/M}$, when $k = 0$. Since at the long wavelength limit this mode can couple with electromagnetic radiation it is called the *optical branch*. At the long wavelength limit, when $k \approx 0$, the amplitudes satisfy

$$\epsilon_1 = \mp \epsilon_2$$

the upper sign corresponding to the optical mode and the lower sign to the acoustic mode. *Case 2. $k = \pi/a$* At the border of the Brillouin zone the modes are

$$\begin{aligned} \omega &= \sqrt{\frac{2K}{M}}, \text{ optical branch} \\ \omega &= \sqrt{\frac{2G}{M}}, \text{ acoustical branch.} \end{aligned}$$

Correspondingly for the amplitudes

$$\epsilon_1 = \mp \epsilon_2.$$

Case 3. $K \gg G$

The dispersion relations are now

$$\begin{aligned}\omega &= \sqrt{\frac{2K}{M}} \left[1 + \mathcal{O}\left(\frac{G}{K}\right) \right] \\ \omega &= \sqrt{\frac{2G}{M}} \sin \frac{1}{2}ka \left[1 + \mathcal{O}\left(\frac{G}{K}\right) \right],\end{aligned}$$

and the amplitudes satisfy

$$\epsilon_1 \approx \mp \epsilon_2.$$

The frequency of the optical branch is now independent on the wave vector. Its magnitude corresponds to the vibration frequency of a molecule of two atoms with equal masses and coupled with the spring constant K .

On the other hand, the acoustical branch is the same as in the case of the linear chain.

Case 4. $K = G$

Now we have a Bravais lattice formed by single atoms with the primitive cell length $a/2$.

Extra: Three dimensional Bravais lattice of single atoms

Using the matrix notation the harmonic potential can be written more compactly

$$U^{\text{harm}} = \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} \mathbf{u}_R \mathbf{D}(\mathbf{R} - \mathbf{R}') \mathbf{u}_{R'}.$$

Independent on the interionic forces the matrix

$\mathbf{D}(\mathbf{R} - \mathbf{R}')$ obeys certain symmetries:

1. $D_{\mu\nu}(\mathbf{R} - \mathbf{R}') = D_{\nu\mu}(\mathbf{R}' - \mathbf{R})$

This property can be verified by exchanging the order of differentiations in the definitions of the elements of \mathbf{D} :

$$D_{\mu\nu}(\mathbf{R} - \mathbf{R}') = \left. \frac{\partial^2 U}{\partial u_\mu(\mathbf{R}) \partial u_\nu(\mathbf{R}')} \right|_{\mathbf{u}=\mathbf{o}}.$$

2. $\mathbf{D}(\mathbf{R}) = \mathbf{D}(-\mathbf{R})$

Let us consider a lattice where the displacements from the equilibrium are \mathbf{u}_R . In the corresponding reversal lattice the displacements are $-\mathbf{u}_{-R}$. Since every Bravais lattice has the inversion symmetry the energies of both lattices must be equal, no matter what the deviations \mathbf{u}_R are, i.e.

$$\begin{aligned}U^{\text{harm}} &= \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} \mathbf{u}_R \mathbf{D}(\mathbf{R} - \mathbf{R}') \mathbf{u}_{R'} \\ &= \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} (-\mathbf{u}_{-R}) \mathbf{D}(\mathbf{R} - \mathbf{R}') (-\mathbf{u}_{-R'}) \\ &= \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} \mathbf{u}_R \mathbf{D}(\mathbf{R}' - \mathbf{R}) \mathbf{u}_{R'},\end{aligned}$$

for an arbitrary \mathbf{u}_R . This can be valid only if

$$\mathbf{D}(\mathbf{R} - \mathbf{R}') = \mathbf{D}(\mathbf{R}' - \mathbf{R}).$$

In addition, according to the symmetry 1, we have

$$D_{\mu\nu}(\mathbf{R} - \mathbf{R}') = D_{\nu\mu}(\mathbf{R} - \mathbf{R}'),$$

so the matrix \mathbf{D} is symmetric. 3. $\sum_{\mathbf{R}} \mathbf{D}(\mathbf{R}) = 0$

We move every ion \mathbf{R} to $\mathbf{R} + \mathbf{d}$. This is equivalent with translating the whole lattice by the amount \mathbf{d} . The potential energies of the original and the translated lattices are equal; in particular at the equilibrium 0, i.e.

$$\begin{aligned}0 &= \sum_{\substack{\mathbf{R}\mathbf{R}' \\ \mu\nu}} d_\mu D_{\mu\nu}(\mathbf{R} - \mathbf{R}') d_\nu \\ &= \sum_{\mu\nu} N d_\mu d_\nu \left(\sum_{\mathbf{R}} D_{\mu\nu}(\mathbf{R}) \right).\end{aligned}$$

Since the vector \mathbf{d} is arbitrary we must have

$$\sum_{\mathbf{R}} \mathbf{D}(\mathbf{R}) = \mathbf{o}.$$

The classical equations of motion

$$M \ddot{u}_{R,\mu} = - \frac{\partial U^{\text{harm}}}{\partial u_{R,\mu}} = - \sum_{\mathbf{R}'} D_{\mu\nu}(\mathbf{R} - \mathbf{R}') u_{R',\nu},$$

or in the matrix notation

$$M \ddot{\mathbf{u}}_R = - \sum_{\mathbf{R}'} \mathbf{D}(\mathbf{R} - \mathbf{R}') \mathbf{u}_{R'}$$

form a system of $3N$ equations. Again we seek solutions of the form

$$\mathbf{u}_R = \boldsymbol{\epsilon} e^{i(\mathbf{k} \cdot \mathbf{R} - \omega t)}.$$

Here the *polarisation vector* $\boldsymbol{\epsilon}$ tells us the direction of the motion of the ions. Furthermore we require that for every primitive vector \mathbf{a}_i the solutions satisfy the Born-von Karman boundary conditions

$$\mathbf{u}(\mathbf{R} + N_i \mathbf{a}_i) = \mathbf{u}(\mathbf{R}),$$

when the total number of primitive cells is $N = N_1 N_2 N_3$. These conditions can be satisfied only if the wave vector \mathbf{k} is of form

$$\mathbf{k} = \frac{n_1}{N_1} \mathbf{b}_1 + \frac{n_2}{N_2} \mathbf{b}_2 + \frac{n_3}{N_3} \mathbf{b}_3.$$

Here \mathbf{b}_i are vectors in the reciprocal lattice and n_i integers. We see that we get different solution only if \mathbf{k} is restricted into the 1st Brillouin zone, i.e. there are exactly N allowed values for the wave vector.

We substitute the trial into the equations of motion and end up with

$$M \omega^2 \boldsymbol{\epsilon} = \mathbf{D}(\mathbf{k}) \boldsymbol{\epsilon}, \quad (*)$$

where

$$\mathbf{D}(\mathbf{k}) = \sum_{\mathbf{R}} \mathbf{D}(\mathbf{R}) e^{-i\mathbf{k} \cdot \mathbf{R}}$$

is so called *dynamical matrix*. For every allowed \mathbf{k} we have as the solution of (*) three eigenvalues and vectors. The number of normal modes is therefore $3N$.

Employing symmetry properties of $D(\mathbf{R})$ we can rewrite the dynamical matrix as

$$\begin{aligned} D(\mathbf{k}) &= \frac{1}{2} \sum_{\mathbf{R}} D(\mathbf{R}) [e^{-i\mathbf{k}\cdot\mathbf{R}} + e^{i\mathbf{k}\cdot\mathbf{R}} - 2] \\ &= \sum_{\mathbf{R}} D(\mathbf{R}) [\cos(\mathbf{k}\cdot\mathbf{R}) - 1]. \end{aligned}$$

Thus the dynamical matrix is

$$D(\mathbf{k}) = -2 \sum_{\mathbf{R}} D(\mathbf{R}) \sin^2\left(\frac{1}{2}\mathbf{k}\cdot\mathbf{R}\right).$$

We see that $D(\mathbf{k})$ is a real and symmetric function of \mathbf{k} . Since $D(\mathbf{R})$ is symmetric $D(\mathbf{k})$ is also symmetric. We rewrite the equation (*) as

$$D(\mathbf{k})\epsilon_s(\mathbf{k}) = \lambda_s(\mathbf{k})\epsilon_s(\mathbf{k}).$$

As the eigenvalues of a real and symmetric matrix $\lambda_s(\mathbf{k})$ are real and the eigenvectors $\epsilon_s(\mathbf{k})$ can be orthonormalized, i.e.

$$\epsilon_s(\mathbf{k}) \cdot \epsilon_{s'}(\mathbf{k}) = \delta_{ss'}, \quad s, s' = 1, 2, 3.$$

The polarizations of three normal modes are $\epsilon_s(\mathbf{k})$ and the angular velocities correspondingly

$$\omega_s(\mathbf{k}) = \sqrt{\frac{\lambda_s(\mathbf{k})}{M}}.$$

Let us assume now that the mutual interaction of the ions decreases rapidly with the increasing separation. Strictly speaking we assume that

$$\lim_{\mathbf{R} \rightarrow \infty} D(\mathbf{R}) = \mathcal{O}(R^{-5}).$$

Then, at long wavelength, i.e. when $\mathbf{k} \approx \mathbf{0}$, we have

$$\sin^2\left(\frac{1}{2}\mathbf{k}\cdot\mathbf{R}\right) \approx \left(\frac{1}{2}\mathbf{k}\cdot\mathbf{R}\right)^2$$

and

$$D(\mathbf{k}) \approx -\frac{k^2}{2} \sum_{\mathbf{R}} (\hat{\mathbf{k}}\cdot\mathbf{R})^2 D(\mathbf{R}).$$

Let $c_s(\hat{\mathbf{k}})^2$ be the eigenvalues of the matrix

$$-\frac{1}{2M} \sum_{\mathbf{R}} (\hat{\mathbf{k}}\cdot\mathbf{R})^2 D(\mathbf{R}).$$

We see that at small wave vectors the frequency is

$$\omega_s(\mathbf{k}) = c_s(\hat{\mathbf{k}})k.$$

Thus the dispersion of all three modes is a linear function of k so all three modes are acoustical. In general $c_s(\hat{\mathbf{k}})$, together with $\omega_s(\mathbf{k})$, depend also on the direction $\hat{\mathbf{k}}$ of the propagation in addition to the mode s .

Extra: Three dimensional lattice with base

We proceed exactly like in the case the one dimensional lattice with base. We assume that there are p ions in the

primitive cell. Every ion in the primitive cell adds one degree of freedom so the total number of modes at a given wave vector \mathbf{k} is $3p$. The corresponding frequencies are $\omega_s^i(\mathbf{k})$, where now $s = 1, 2, 3$ and $i = 1, 2, \dots, p$. The corresponding displacements are

$$\mathbf{u}_s^i(\mathbf{R}, t) = \epsilon_s^i(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{R} - \omega_s^i(\mathbf{k})t)}.$$

The polarizations are no more orthogonal but satisfy

$$\sum_{i=1}^p \epsilon_s^{i*}(\mathbf{k}) \cdot \epsilon_{s'}^i(\mathbf{k}) = \delta_{ss'}.$$

Analogically with one dimensional lattice 3 of the modes are now acoustical and the rest $3(p-1)$ modes optical.

Extra: Quantum mechanical treatment

Let us consider the harmonic Hamiltonian

$$\begin{aligned} H^{\text{harm}} &= \sum_{\mathbf{R}} \frac{1}{2M} P_{\mathbf{R}}^2 \\ &\quad + \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} \mathbf{u}_{\mathbf{R}} D(\mathbf{R} - \mathbf{R}') \mathbf{u}_{\mathbf{R}'} \end{aligned}$$

describing the lattice. Let $\omega_s(\mathbf{k})$ and $\epsilon_s(\mathbf{k})$ be the frequencies and polarizations in the corresponding classical lattice. We define the operator $a_{\mathbf{k}s}$ so that

$$\begin{aligned} a_{\mathbf{k}s} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot\mathbf{R}} \epsilon_s(\mathbf{k}) \cdot \\ &\quad \left[\sqrt{\frac{M\omega_s(\mathbf{k})}{2\hbar}} \mathbf{u}_{\mathbf{R}} + i \sqrt{\frac{1}{2\hbar M\omega_s(\mathbf{k})}} P_{\mathbf{R}} \right]. \end{aligned}$$

The Hermitean conjugate $a_{\mathbf{k}s}^\dagger$ of the operator $a_{\mathbf{k}s}$ is

$$\begin{aligned} a_{\mathbf{k}s}^\dagger &= \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \epsilon_s(\mathbf{k}) \cdot \\ &\quad \left[\sqrt{\frac{M\omega_s(\mathbf{k})}{2\hbar}} \mathbf{u}_{\mathbf{R}} - i \sqrt{\frac{1}{2\hbar M\omega_s(\mathbf{k})}} P_{\mathbf{R}} \right]. \end{aligned}$$

The operator $a_{\mathbf{k}s}^\dagger$ is called the phonon creation operator and $a_{\mathbf{k}s}$ the phonon annihilation operator.

We employ the canonical commutation relations for the position and momentum

$$\begin{aligned} [u_{\mathbf{R},\mu}, P_{\mathbf{R}',\nu}] &= i\hbar \delta_{\mu\nu} \delta_{\mathbf{R}\mathbf{R}'} \\ [u_{\mathbf{R},\mu}, u_{\mathbf{R}',\nu}] &= [P_{\mathbf{R},\mu}, P_{\mathbf{R}',\nu}] = 0, \end{aligned}$$

the identities

$$\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} = \begin{cases} 0, & \mathbf{k} \text{ is not a reciprocal vector} \\ N, & \mathbf{k} \text{ is a reciprocal vector} \end{cases}$$

and

$$\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} = 0, \quad \mathbf{R} \neq \mathbf{0}$$

together with the property of an orthogonal vector set

$$\sum_{s=1}^3 [\epsilon_s(\mathbf{k})]_{\mu} [\epsilon_s(\mathbf{k})]_{\nu} = \delta_{\mu\nu}.$$

One can easily show that the creation and annihilation operators obey the commutation relations

$$\begin{aligned} [a_{\mathbf{k}_s}, a_{\mathbf{k}'_s'}^\dagger] &= \delta_{\mathbf{k}\mathbf{k}'}\delta_{ss'} \\ [a_{\mathbf{k}_s}, a_{\mathbf{k}'_s'}] &= [a_{\mathbf{k}_s}^\dagger, a_{\mathbf{k}'_s'}^\dagger] = 0. \end{aligned}$$

With the help of the creation and annihilation operators the operators \mathbf{u}_R and \mathbf{P}_R can be written as

$$\begin{aligned} \mathbf{u}_R &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}_s} \sqrt{\frac{\hbar}{2M\omega_s(\mathbf{k})}} (a_{\mathbf{k}_s} + a_{-\mathbf{k}_s}^\dagger) \times \\ &\quad \boldsymbol{\epsilon}_s(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{R}} \\ \mathbf{P}_R &= \frac{-i}{\sqrt{N}} \sum_{\mathbf{k}_s} \sqrt{\frac{\hbar M\omega_s(\mathbf{k})}{2}} (a_{\mathbf{k}_s} - a_{-\mathbf{k}_s}^\dagger) \times \\ &\quad \boldsymbol{\epsilon}_s(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{R}}. \end{aligned}$$

The Hamiltonian is now

$$H = \sum_{\mathbf{k}_s} \hbar\omega_s(\mathbf{k}) (a_{\mathbf{k}_s}^\dagger a_{\mathbf{k}_s} + \frac{1}{2}).$$

This is simply the Hamiltonian of the system of $3N$ independent harmonic oscillators whose energies are correspondingly

$$E = \sum_{\mathbf{k}_s} (n_{\mathbf{k}_s} + \frac{1}{2}) \hbar\omega_s(\mathbf{k}).$$

Here $n_{\mathbf{k}_s}$ the eigenvalues of the occupation number operator $\hat{n}_{\mathbf{k}_s} = a_{\mathbf{k}_s}^\dagger a_{\mathbf{k}_s}$, i.e. $n_{\mathbf{k}_s} = 0, 1, 2, \dots$

Debye's model

It is always possible to diagonalize a harmonic Hamiltonian (D symmetric). This is most convenient in momentum space, where different lattice momenta \mathbf{k} become independent. Harmonic potential gives rise to harmonic oscillators, and in order to get the exact solution we should evaluate the partition function

$$\begin{aligned} Z &= \text{Tr} e^{-\beta \sum_{\mathbf{k}_s} \hbar\omega_s(\mathbf{k}) (a_{\mathbf{k}_s}^\dagger a_{\mathbf{k}_s} + \frac{1}{2})} \\ &= \sum_{\{n_{\mathbf{k}_s=0}\}} e^{-\beta \sum_{\mathbf{k}_s} \hbar\omega_s(\mathbf{k}) (n_{\mathbf{k}_s} + \frac{1}{2})}. \end{aligned}$$

The \mathbf{k} -summation goes over all lattice momenta, $\mathbf{k} = \mathbf{n}2\pi/(Na)$, where we assume lattice size $V = (aN)^3$ and periodic boundary conditions.

In the first Brillouin zone there are $3N$ modes, $n_i = 0 \dots (N-1)$.

The solution requires the knowledge of the dispersion relation $\omega_s(\mathbf{k})$. A reasonable realistic and analytical approximation is provided by the *Debye's model*:

- At low temperatures only the contribution of the low energetic phonons is prominent, so we take into account only the acoustic modes: 2 transverse and 1 longitudinal polarisations.
- we assume that the small k dispersion relation holds:

$$\begin{aligned} \omega_l(k) &= c_l k \\ \omega_t(k) &= c_t k. \end{aligned}$$

- We cut the spectra at the *Debye frequency*

$$\omega_D \equiv \frac{k_B T_D}{\hbar},$$

where T_D is the corresponding *Debye temperature*, and which is chosen so that the number of modes equals the number of modes within the first Brillouin zone.

In each mode j the density of states is

$$dN_j = \left(\frac{L}{2\pi}\right)^3 4\pi k^2 dk = \frac{V}{2\pi^2 c_j^3} \omega^2 d\omega.$$

Thus the total density is

$$dN = \frac{V}{2\pi^2} \left(\frac{2}{c_t^3} + \frac{1}{c_l^3}\right) \omega^2 d\omega.$$

Because the total number of modes is

$$3N = \int_{\omega=0}^{\omega_D} dN = \frac{V}{6\pi^2} \left(\frac{2}{c_t^3} + \frac{1}{c_l^3}\right) \omega_D^3$$

we get as the Debye frequency

$$\omega_D^3 = \frac{N}{V} 18\pi^2 \left(\frac{2}{c_t^3} + \frac{1}{c_l^3}\right)^{-1}$$

and correspondingly as the density of states

$$dN(\omega) = \frac{9N}{\omega_D^3} \omega^2 d\omega \quad (\omega < \omega_D).$$

The canonical partition function is

$$\begin{aligned} Z &= \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \dots \sum_{n_{3N}=0}^{\infty} e^{-\beta \sum_{\mathbf{k}_s} \hbar\omega_s(\mathbf{k}) (n_{\mathbf{k}_s} + \frac{1}{2})} \\ &= \prod_{\mathbf{k}_s} \frac{e^{-\frac{1}{2}\beta\hbar\omega_s(\mathbf{k})}}{1 - e^{-\beta\hbar\omega_s(\mathbf{k})}}, \end{aligned}$$

from which we can derive as the free energy

$$F = \underbrace{\sum_{\mathbf{k}_s} \frac{1}{2} \hbar\omega_s(\mathbf{k})}_{\text{0-point energy}} + k_B T \sum_{\mathbf{k}_s} \ln \left[1 - e^{-\beta\hbar\omega_s(\mathbf{k})} \right]$$

or

$$F = F_0 + k_B T \frac{9N}{\omega_D^3} \int_0^{\omega_D} d\omega \omega^2 \ln(1 - e^{-\beta\hbar\omega}).$$

Because $S = -\frac{\partial F}{\partial T}$ and $C_V = T \frac{\partial S}{\partial T}$, we have $C_V = -T \frac{\partial^2 F}{\partial T^2}$, and we obtain

$$C_V = 3N k_B f_D \left(\frac{T_D}{T}\right).$$

Here

$$f_D(x) = \frac{3}{x^3} \int_0^x dy \frac{y^4 e^y}{(e^y - 1)^2}$$

is the so-called *Debye function*. Typical Debye temperatures

	T_D
Au	170
Cu	315
Fe	420
Cr	460
B	1250
C (diamond)	1860

Note: The higher T_D the stiffer, harder crystal.

Behaviour of C_V :

$T \rightarrow \infty$

Because

$$f_D(x) \xrightarrow{x \rightarrow 0} \frac{3}{x^3} \int_0^x dy y^2 = 1,$$

we have

$$C_V \rightarrow 3Nk_B,$$

and we end up with the Dulong-Petit heat capacity.

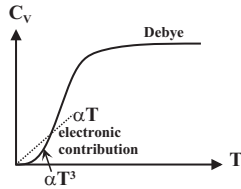
$T \rightarrow 0$

Because

$$f_D(x) \xrightarrow{x \rightarrow \infty} \frac{3}{x^3} \int_0^\infty dy \frac{y^4 e^y}{(e^y - 1)^2} = \frac{\text{constant}}{x^3},$$

we get

$$C_V(T) \rightarrow \text{const.} \times T^3 = \frac{12\pi^4}{5} Nk_B \left(\frac{T}{T_D}\right)^3.$$



Contribution from the electron gas is linear in T , but tiny, and usually negligible.

9. Fermion systems

9.1. Electron gas

The ideal Fermi gas is a good approximation for example for the conducting electrons in a metal.

When the single particle energies are $\epsilon_k = \frac{\hbar^2 k^2}{2m}$ the density of 1-particle states is (g_s : spin degeneracy)

$$\begin{aligned} \omega_1(\epsilon) &= V \frac{g_s}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{\epsilon} \\ &= V 2\pi g_s \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{\epsilon}. \end{aligned}$$

The density of particles is

$$\rho = \frac{\bar{N}}{V} = \frac{g_s}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty d\epsilon \frac{\sqrt{\epsilon}}{e^{\beta(\epsilon-\mu)} + 1}.$$

The energy per particle will be

$$\bar{\epsilon} = \frac{E}{\bar{N}} = \frac{\int_0^\infty d\epsilon \frac{\epsilon^{3/2}}{e^{\beta(\epsilon-\mu)} + 1}}{\int_0^\infty d\epsilon \frac{\epsilon^{1/2}}{e^{\beta(\epsilon-\mu)} + 1}}.$$

Degenerate Fermi gas

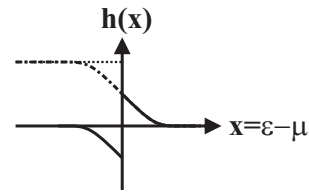
Assume that $k_B T \ll \mu$. Let us write the average occupation \bar{n} as a step function + correction:

$$\frac{1}{e^{\beta(\epsilon-\mu)} + 1} = \theta(\mu - \epsilon) + h(\epsilon - \mu),$$

where

$$h(x) = \text{sign}(x) \frac{1}{e^{\beta|x|} + 1}.$$

The function $h(x)$ deviates from zero only at the narrow domain $|x| \lesssim k_B T \ll \mu$.



Let's evaluate the integral

$$\begin{aligned} &\int_0^\infty d\epsilon \frac{\phi(\epsilon)}{e^{\beta(\epsilon-\mu)} + 1} \\ &= \int_0^\infty d\epsilon \phi(\epsilon) [\theta(\mu - \epsilon) + h(\epsilon - \mu)] \\ &= \int_0^\mu d\epsilon \phi(\epsilon) + \int_0^\infty d\epsilon h(\epsilon) [\phi(\mu + \epsilon) - \phi(\mu - \epsilon)] \\ &\quad + \int_\mu^\infty d\epsilon h(\epsilon) \phi(\mu - \epsilon). \end{aligned}$$

The last term is of the order

$$h(\mu) = \frac{1}{e^{\mu/k_B T} + 1} \approx e^{-\mu/k_B T}$$

and can be discarded.

If $\phi(\epsilon)$ regular enough in the vicinity of $\epsilon \approx \mu$ we can expand

$$\phi(\mu + \epsilon) - \phi(\mu - \epsilon) \approx 2\phi'(\mu)\epsilon + 2\frac{1}{3!}\phi'''(\mu)\epsilon^3 + \dots$$

Now

$$\begin{aligned} \int_0^\infty d\epsilon \frac{\phi(\epsilon)}{e^{\beta(\epsilon-\mu)} + 1} \\ \approx \int_0^\mu d\epsilon \phi(\epsilon) \\ + 2\phi'(\mu)(k_B T)^2 \int_0^\infty dz \frac{z}{e^z + 1} \\ + 2\phi'''(\mu) \frac{1}{3!} (k_B T)^4 \int_0^\infty dz \frac{z^3}{e^z + 1} \\ + \dots \end{aligned}$$

and we end up with *Sommerfeld's expansion*

$$\begin{aligned} \int_0^\infty d\epsilon \frac{\phi(\epsilon)}{e^{\beta(\epsilon-\mu)} + 1} \approx \int_0^\mu d\epsilon \phi(\epsilon) + \frac{\pi^2}{6} (k_B T)^2 \phi'(\mu) \\ + \frac{7\pi^4}{360} (k_B T)^4 \phi'''(\mu) + \dots \end{aligned}$$

This was obtained again using Riemann ζ -function:

$$\zeta(x) = \frac{1}{\Gamma(x)} \int_0^\infty \frac{u^{x-1}}{e^u - 1} du = \sum_{k=1}^\infty \frac{1}{k^x}$$

(Check <http://mathworld.wolfram.com/RiemannZetaFunction.html>)
Now

$$\frac{1}{e^u + 1} = \frac{1}{e^u - 1} - \frac{2}{e^{2u} - 1},$$

and thus

$$\frac{1}{\Gamma(x)} \int_0^\infty \frac{u^{x-1}}{e^u + 1} du = \zeta(x) - 2^{1-x} \zeta(x).$$

Now

$$\begin{aligned} \zeta(1) &= \infty \\ \zeta(2) &= \frac{\pi^2}{6} \\ \zeta(3) &= 1.2020\dots \\ \zeta(4) &= \frac{\pi^4}{90} \\ \zeta(5) &= 1.0369\dots \\ \zeta(6) &= \frac{\pi^6}{945} \end{aligned}$$

Temperature $T = 0$

Now

$$\bar{n}(\epsilon) = \theta(\mu - \epsilon)$$

and $h(x) = 0$.

The *Fermi energy* is

$$\epsilon_F = \mu = \frac{\hbar^2 k_F^2}{2m}.$$

The *Fermi momentum* is

$$p_F = \hbar k_F.$$

The density is

$$\begin{aligned} \rho &= \frac{g_s}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^\mu d\epsilon \sqrt{\epsilon} \\ &= \frac{g_s}{6\pi^2} \left(\frac{2m\epsilon_F}{\hbar^2} \right)^{3/2} \end{aligned}$$

or

$$\rho = \frac{g_s}{6\pi^2} k_F^3.$$

The spin degeneracy factor of electrons is $g_s = 2 \cdot \frac{1}{2} + 1 = 2$, so

$$\rho = \frac{k_F^3}{3\pi^2}.$$

For the average energy per particle we get

$$\begin{aligned} \bar{\epsilon} &= \epsilon_F \frac{\int_0^1 dx x^{3/2}}{\int_0^1 dx x^{1/2}} = \epsilon_F \frac{2/5}{2/3} \\ &= \frac{3}{5} \epsilon_F. \end{aligned}$$

The total energy is

$$E = \frac{3}{5} \epsilon_F N = \frac{3}{5} N \frac{\hbar^2}{2m} \left(\frac{6\pi^2 \rho}{g_s} \right)^{2/3}.$$

Since

$$E = \text{constant} \times N^{5/3} V^{-2/3},$$

we have

$$-p = \left(\frac{\partial E}{\partial V} \right)_N = -\frac{2}{3} \frac{E}{V}$$

or

$$pV = \frac{2}{3} E,$$

which is actually valid at all temperatures (homework).

Metallic electron gas

When we write the density as

$$\rho = \frac{\bar{N}}{V} = \frac{1}{\frac{4}{3} \pi r_i^3}$$

and define the dimensionless number

$$r_s = \frac{r_i}{a_0},$$

where a_0 is the Bohr radius

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2} = 0.529 \text{ \AA},$$

we can see that

$$\rho = \frac{1.613 \cdot 10^{30}}{r_s^3} \frac{1}{\text{m}^3}.$$

For metals we have

$$1.9 \lesssim r_s \lesssim 5.6.$$

The Fermi wave number will become

$$k_F = \frac{1}{a_0 r_s} \sqrt[3]{\frac{9\pi}{4}} = \frac{1.92}{a_0 r_s}.$$

The Fermi velocity is

$$\begin{aligned} v_F &= \frac{p_F}{m} = \frac{\hbar k_F}{m} = \frac{1.92 \hbar}{m a_0 r_s} \\ &= \frac{4.2 \cdot 10^6 \text{ m}}{r_s} \frac{\text{m}}{\text{s}}. \end{aligned}$$

For example in aluminium

$$v_F = 2029 \frac{\text{km}}{\text{s}} = \frac{c}{148}.$$

The Fermi temperature or the degeneracy temperature T_F is defined so that

$$k_B T_F = \epsilon_F.$$

Now

$$\epsilon_F = \underbrace{\frac{\hbar^2}{2m a_0^2}}_{\text{binding energy of hydrogen}} \left(\frac{1.92}{r_s} \right)^2 = \frac{3.69}{r_s^2} 13.6 \text{ eV}.$$

Because

$$\boxed{1 \text{ eV} = 11604 k_B \text{ K}},$$

we have

$$T_F = \left(\frac{1.92}{r_s} \right)^2 13.6 \cdot 11604 \text{ K}.$$

For aluminium the Fermi temperature is $T_F = 136\,000 \text{ K}$. In general, the metals satisfy

$$T \ll T_F,$$

so the metallic electron gas is highly degenerate.

Specific heat

Let now $T > 0$, but $T \ll T_F$. We can now solve $\mu = \mu(T)$ by requiring that $\frac{N}{V} = \rho$ remains constant when we vary the temperature. With the help of the Sommerfeld expansion we get

$$\begin{aligned} \frac{2}{3} \epsilon_F^{3/2} &= \frac{4\pi^2}{g_s} \left(\frac{\hbar^2}{2m} \right)^{3/2} \rho = \int_0^\infty d\epsilon \frac{\epsilon^{1/2}}{e^{\beta(\epsilon-\mu)} + 1} \\ &= \frac{2}{3} \mu^{3/2} + \frac{\pi^2}{12} (k_B T)^2 \frac{1}{\sqrt{\mu}} + \dots \end{aligned}$$

so that we can write

$$\frac{2}{3} \mu^{3/2} \left[1 + \frac{\pi^2}{8} (k_B T)^2 \frac{1}{\epsilon_F^2} + \dots \right] = \frac{2}{3} \epsilon_F^{3/2}.$$

From this we get for the chemical potential the expression

$$\mu(T) = \epsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\epsilon_F} \right)^2 + \dots \right].$$

In order to obtain the energy, we use

$$\begin{aligned} &\int_0^\infty d\epsilon \frac{\epsilon^{3/2}}{e^{\beta(\epsilon-\mu)} + 1} \\ &\approx \frac{2}{5} \mu^{5/2} + \frac{\pi^2}{4} (k_B T)^2 \sqrt{\mu} + \dots \\ &= \frac{2}{5} \epsilon_F^{5/2} \left[1 + \frac{5}{12} \pi^2 \left(\frac{k_B T}{\epsilon_F} \right)^2 \right] + \dots \end{aligned}$$

Now the energy/particle is

$$\begin{aligned} \bar{\epsilon}(T) &= \frac{\int_0^\infty d\epsilon \frac{\epsilon^{3/2}}{e^{\beta(\epsilon-\mu)} + 1}}{\int_0^\infty d\epsilon \frac{\epsilon^{1/2}}{e^{\beta(\epsilon-\mu)} + 1}} \\ &= \frac{3}{5} \epsilon_F \left[1 + \frac{5}{12} \pi^2 \left(\frac{k_B T}{\epsilon_F} \right)^2 \right] \\ &= \frac{3}{5} \epsilon_F + \frac{\pi^2}{4} \frac{k_B^2 T^2}{\epsilon_F}. \end{aligned}$$

The heat capacity can now be written as

$$\boxed{C_V = \frac{\partial N \bar{\epsilon}}{\partial T} = N \frac{\pi^2}{2} \frac{k_B^2}{\epsilon_F} T = N k_B \frac{\pi^2}{2} \frac{T}{T_F}}.$$

This is small when compared e.g. with the specific heat of the Maxwell-Boltzmann gas ($C_V = N k_B \frac{3}{2}$), or the Debye heat capacity, because $T_D \ll T_F$. This is understandable because the number of those particles that can be excited with the thermal energy $\sim k_B T$ is \ll MB or BE gases due to the Pauli exclusion principle. At $T \sim$ few K the electronic C_V dominates.

Why $C_V^{\text{el}} \propto T$ but $C_V^{\text{Debye}} \propto T^3$?

This is due to the Fermi surface: consider the number of states in \mathbf{k} -phase space around the $T = 0$ state, where $\Delta k \sim k_B T$. For phonons the fluctuations are around $k = 0$, with number of states

$$\Delta N \sim (\Delta k)^3 \propto T^3.$$

For electrons the $T = 0$ state is a Fermi sphere, with

$$\Delta N \sim k_F^2 \Delta k \propto T.$$

Pauli's paramagnetism

The magnetic moment of the electron is

$$\boldsymbol{\mu} = -\frac{e}{m} \mathbf{s}$$

or

$$\mu_z = -\mu_B \sigma_z,$$

where

$$\mu_B = \frac{e \hbar}{2m} = 5.66 \cdot 10^{-5} \frac{\text{eV}}{\text{T}}$$

and

$$\sigma_z = \frac{2}{\hbar} s_z = \pm 1.$$

In an external magnetic field the energy of an electron is

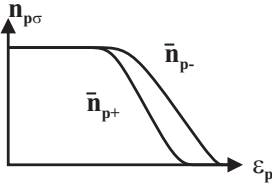
$$\epsilon_{\mathbf{p}\sigma_z} = \epsilon_{p\pm} = \frac{\mathbf{p}^2}{2m} - \mu_z B = \epsilon_{\mathbf{p}} + \mu_B B \sigma_z$$

when the kinetic energy is

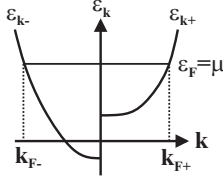
$$\epsilon_{\mathbf{p}} = \frac{\mathbf{p}^2}{2m}.$$

We treat electrons as non-interacting so that the grand canonical partition function is as before, provided that we replace $\epsilon_{\mathbf{p}} \rightarrow \epsilon_{\mathbf{p}} + \mu_B B \sigma_z$. The occupation numbers of the states are now

$$\bar{n}_{\mathbf{p}\sigma_z} = \bar{n}_{p\pm} = \frac{1}{e^{\beta(\epsilon_p + \mu_B B \sigma_z - \mu)} + 1}.$$



Because the metallic electron gas is strongly degenerate ($T \ll T_F$), we can restrict the temperature $T = 0$.



The Fermi wave vectors can be determined from the conditions

$$\begin{aligned} \frac{\hbar^2 k_{F+}^2}{2m} + \mu_B B &= \mu \\ \frac{\hbar^2 k_{F-}^2}{2m} - \mu_B B &= \mu. \end{aligned}$$

Because the number density is

$$\rho = \frac{g_s}{6\pi^2} k_F^3,$$

the spin population densities are

$$\begin{aligned} \rho_+ &= \frac{k_{F+}^3}{6\pi^2} \\ \rho_- &= \frac{k_{F-}^3}{6\pi^2}. \end{aligned}$$

If the strength of the magnetic field is

$$B_0 = \frac{\epsilon_F}{\mu_B},$$

the magnetic energy is of the same order as the Fermi energy. For metals $\epsilon_F \approx 5\text{eV}$, so $B_0 \approx 10^5\text{T}$. Thus the realistic magnetic fields are $\ll B_0$ and we can work at the small B limit. Denoting

$$k_{F\pm} = k_F \pm \delta k_F,$$

so

$$\begin{aligned} \frac{\hbar^2 k_{F\pm}^2}{2m} \pm \mu_B B &= \frac{\hbar^2 k_F^2}{2m} \pm \frac{\hbar^2 k_F}{m} \delta k_F \pm \mu_B B \\ &= \mu = \frac{\hbar^2 k_F^2}{2m}. \end{aligned}$$

From this we get

$$\delta k_F = -\frac{m\mu_B}{\hbar^2 k_F} B$$

and

$$\begin{aligned} \rho_{\pm} &= \frac{k_F^3}{6\pi^2} \pm \frac{k_F^2}{2\pi^2} \delta k_F \\ &= \frac{k_F^3}{6\pi^2} \mp \frac{k_F m \mu_B}{2\pi^2 \hbar^2} B. \end{aligned}$$

The *relative polarization* is

$$\begin{aligned} r &\equiv \frac{\rho_+ - \rho_-}{\rho_+ + \rho_-} = -\frac{3m\mu_B}{\hbar^2 k_F^2} B \\ &= -\frac{3\mu_B}{2\epsilon_F} B. \end{aligned}$$

The magnetization per volume element is

$$M = \frac{N}{V} \langle \mu_z \rangle = -\rho \mu_B \langle \sigma_z \rangle = -\rho \mu_B r$$

or

$$M = \frac{3}{2} \rho \frac{\mu_B^2}{\epsilon_F} B.$$

The susceptibility is, according to its definition,

$$\chi = \frac{\partial M}{\partial H} = \mu_0 \frac{\partial M}{\partial B}.$$

Pauli's paramagnetic susceptibility is then

$$\chi = \frac{3}{2} \mu_0 \rho \frac{\mu_B^2}{\epsilon_F}$$

provided that $T \ll T_F$ and $\mu_B B \ll \epsilon_F$. In aluminium the electron density is

$$\rho = 1.82 \cdot 10^{29} \text{m}^{-3}$$

and the Fermi energy

$$\epsilon_F = \left(\frac{1.92}{2.07} \right)^2 13.6\text{eV} = 11.7\text{eV}.$$

The susceptibility

$$\begin{aligned} \chi &= \frac{3}{2} \cdot 4\pi \cdot 10^{-7} \cdot 1.82 \cdot 10^{29} \cdot \frac{(5.66 \cdot 10^{-5})^2}{11.7} \\ &= \frac{\text{Vs}}{\text{Am}} \frac{1}{\text{m}^3} \frac{(\text{eV})^2}{\text{T}^2 \text{eV}} \\ &= 9.4 \cdot 10^{13} \frac{\text{eV Vs}}{\text{Am}^4} \left(\frac{\text{m}^2}{\text{Vs}} \right)^2 \\ &= 9.4 \cdot 10^{13} \cdot 1.6 \cdot 10^{-19} \\ &= 1.5 \cdot 10^{-5} \end{aligned}$$

is small because only the electrons very close to the Fermi surface can be polarized magnetically.

9.2. Two dimensional electron gas

The Hamiltonian for a free electron in the magnetic field

$$\mathbf{B} = \nabla \times \mathbf{A}$$

is given by

$$\mathcal{H}_0 = \frac{1}{2m^*} \left(-i\hbar\nabla + \frac{e}{c} \mathbf{A} \right)^2.$$

In a magnetic field electrons move in circular (or more generally spiralling) motion, with angular frequency, *cyclotron frequency*

$$\omega_c = eB/m^*c.$$

The size of the cycles is

$$\ell_0 = (\hbar c/eB)^{\frac{1}{2}},$$

the magnetic length.

Consider electrons

- confined to xy -plane.
- subjected to a perpendicular magnetic field $\mathbf{B} \parallel \hat{z}$.

We can choose the gauge

$$\mathbf{A} = (0, xB, 0)$$

and the single particle Hamiltonian is

$$\mathcal{H}_0 = \frac{1}{2m^*} \left[p_x^2 + \left(p_y + \frac{eB}{c} x \right)^2 \right].$$

Making the ansatz $\phi = e^{ik_y y} \psi(x)$, we see that the equation for ψ becomes that of a harmonic oscillator:

$$\frac{1}{2m^*} \left[p_x^2 + \frac{e^2 B^2}{c^2} (x - X)^2 \right] \psi(x) = E\psi(x),$$

where

$$X = -k_y \frac{\hbar c}{eB} = -k_y \ell_0^2.$$

Thus, the eigenenergies are the discrete *Landau levels*

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega_c, \quad n = 0, 1, 2, \dots$$

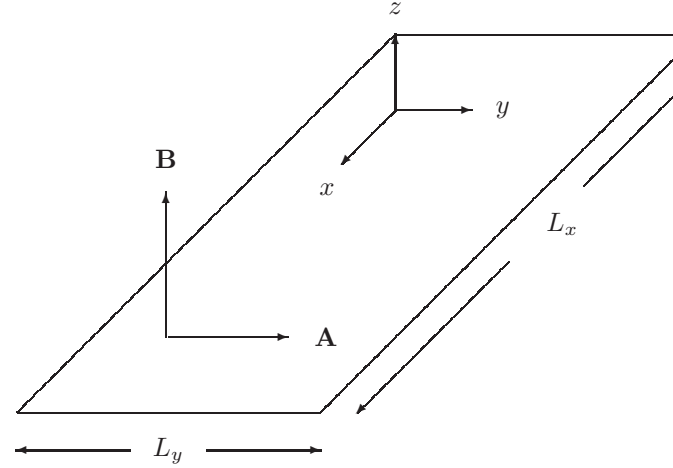
with $\omega_c = eB/m^*c$.

The full eigenfunctions are

$$\phi_{nX} = e^{ik_y y} e^{-(x-X)^2/2\ell_0^2} H_n \left(\frac{x-X}{\ell_0} \right),$$

where X gives the center for the oscillatory motion.

Confine the system in a rectangular cell



Using periodic boundary conditions we have

$$k_y = \frac{2\pi n_y}{L_y}, \quad n_y = 0, \pm 1, \pm 2, \dots$$

and

$$X = -\frac{2\pi n_y}{L_y} \ell_0^2, \quad 0 \leq X < L_x.$$

The number of allowed values of n_y , i.e. the degeneracy of each Landau level, is

$$N_s = \frac{L_x L_y}{2\pi \ell_0^2} = \frac{e}{\hbar c} \Phi = \frac{\Phi}{\Phi_0},$$

where $\Phi_0 = \hbar c/e$ is the flux quantum. Each electron within Landau level takes up area $2\pi \ell_0^2$. Thus, *on each Landau level there is exactly one state for each flux quantum and for each spin polarization.*

When N_e is the number of electrons in an area and N_s the number of flux quanta we define *the filling fraction* as

$$\nu = \frac{N_e}{N_s} \quad \left(= 4.136 \frac{n_0}{10^{15} \text{m}^{-2}} \frac{\text{T}}{B} \right).$$

To treat the spin we note that

- there should be the Zeeman coupling term

$$\mathcal{H}_{\text{Zeeman}} = \boldsymbol{\mu} \cdot \mathbf{B} = -g\mu_B B s_z$$

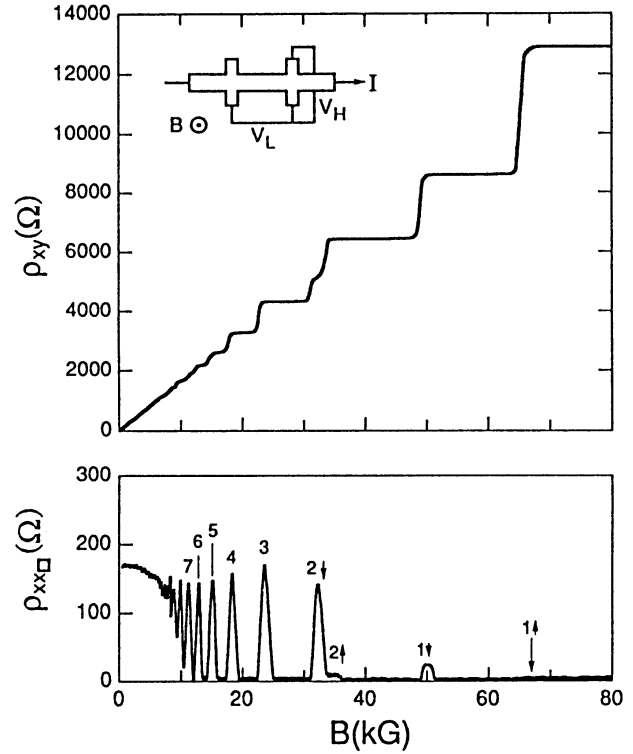
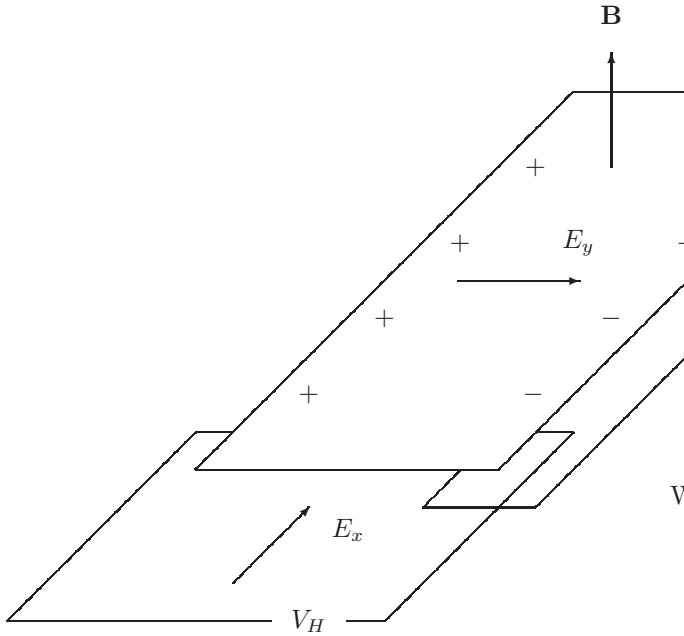
in the Hamiltonian. Here g is the Lande factor and μ_B the Bohr magneton.

- in addition to the Zeeman term there are no spin dependent terms in the Hamiltonian, not even in the interacting many body system.
- the problem can be solved disregarding the spin. At later stages we can add the total Zeeman energy

$$E_{\text{Zeeman}} = g\mu_B B s_z.$$

Quantum Hall states

Consider an experiment like



We observe that

- the Hall resistivity develops plateaus with

$$\rho_{xy} = \frac{E_y}{j_x} = \frac{h}{ne^2}, \quad n = 1, 2, 3, \dots$$

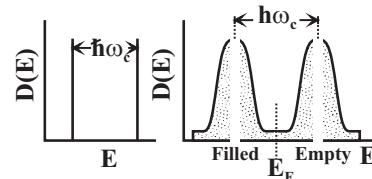
This quantization condition is obeyed with extreme accuracy. In fact, the current ISO standard for resistivity defines

$$\rho_{xy} = \frac{25812.807}{n} \Omega.$$

- at the same time the diagonal resistivity practically vanishes.

For the moment we assume that the electrons are polarized. If the current carrying electrons fill up exactly n Landau levels, it can be shown that $\rho_{xy} = h/ne^2$ and $\rho_{xx} = 0$. The plateaus can be explained by noting that

- in an ideal pure 2DEG the density of states is a series of δ -peaks separated by $\hbar\omega_c$.
- In real systems there are impurities and the δ -peaks are spread and between the Landau levels there are localized states, which do not contribute to conductivity.



The conductivity σ and the resistivity ρ are defined by $\mathbf{j} = \sigma \mathbf{E}$, $\mathbf{E} = \rho \mathbf{j}$. Classically the diagonal and Hall conductivities are

$$\sigma_{xx} \equiv \frac{j_x}{E_x} = \frac{n_0 e^2 \tau}{m} \frac{1}{1 + (\omega_c \tau)^2}$$

$$\sigma_{xy} \equiv \frac{j_x}{E_y} = -\frac{n_0 e c}{B} + \frac{\sigma_{xx}}{\omega_c \tau},$$

where τ is the relaxation time. In particular $\rho_{xy} = -B/n_0 e c$. Experimentally the resistivities behave like

- When B is changed, Landau levels shift: when a (smeared) level crosses ϵ_F , number of delocalized

(Hall conducting) electrons changes rapidly: jump in conductivity.

- When ϵ_F is between the Landau levels, little change in number of conducting electrons: Hall resistivity is constant.

The Hall conductivity can be written in the form

$$\sigma_{xy} = -\frac{n_0 e c}{B} + \Delta\sigma_{xy},$$

where, according to the Kubo formula, the contribution from a localized state $|\alpha\rangle$ to $\Delta\sigma_{xy}$ is

$$\Delta\sigma_{xy}^\alpha = \frac{f(E_\alpha) e c}{B}.$$

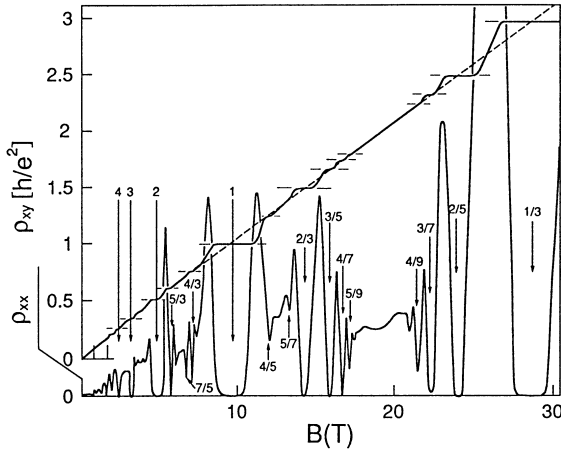
Here $f(E)$ is the Fermi distribution function.

When the number of electrons changes we observe (at $T = 0$) that

- as long as the Fermi level lies within the localized states, σ_{xy} remains constant.
- if all states below the Fermi level are localized, the terms in σ_{xy} cancel exactly and $\sigma_{xy} = 0$.
- for QHE to exist there must be extended states in Landau levels.

Fractional quantum Hall effect

Increasing the magnetic field (i.e. reducing the electron density) furthermore one finds resistivities to behave like



The plateaus in the Hall resistivity and the minima in the longitudinal resistivity correspond to filling fractions

$$\nu = \frac{p}{q},$$

where

- p and q are small integers ($\lesssim 11$).
- q is an *odd* integer.

This behaviour is called as the *Fractional Quantum Hall Effect* (FQHE) as opposed to the previous *Integer Quantum Hall Effect* (IQHE). Regarding the IQHE we note that

- the plateaus correspond to full Landau levels,
- the Landau levels are energetically far from each other as compared to typical electron-electron interaction energies (at least when $\nu \lesssim 5$).
- the mutual electronic interactions play practically no role.

While this single particle picture is sufficient in the IQHE it cannot explain the FQHE where

- the Landau levels are only partially filled, so that
- there is room for the Coulomb intra level interaction.

It turns out that the correlations due to the electron interaction are essential in the FQHE.

9.3. Relativistic electron gas

The rest energy of an electron is

$$mc^2 = 0.511 \text{keV}$$

and the relativistic total energy

$$\begin{aligned} \epsilon_p &= \sqrt{(mc^2)^2 + (cp)^2} \\ &= mc^2 + \frac{p^2}{2m} + \dots \end{aligned}$$

Denote by

$$k_c = \frac{mc}{\hbar} = 2.59 \cdot 10^{12} \text{m}^{-1}$$

the Compton wave number of an electron and by

$$\lambda_c = \frac{2\pi}{k_c} = 2.43 \cdot 10^{-12} \text{m}$$

its Compton wavelength.

Since $p = \hbar k$, we have

$$\epsilon_k = c\hbar \sqrt{k^2 + k_c^2}.$$

Using again the periodic boundary conditions in volume $V = L^3$, we obtain

$$\mathbf{k} = \frac{2\pi}{L} (n_x, n_y, n_z),$$

and we have the density at $T = 0$

$$\rho = \frac{k_F^3}{3\pi^2}.$$

When $k_F = (3\pi^2\rho)^{1/3}$ is of the order k_c , the relativistic corrections must be taken into account. The corresponding density is

$$\begin{aligned} \rho_c &= \frac{k_c^3}{3\pi^2} = 5.87 \cdot 10^{35} \frac{1}{\text{m}^3} \\ &\approx 10^6 \times \text{density of metallic electron gas} \end{aligned}$$

We have an *ultrarelativistic electron gas* when $k_F \gg k_c$ or correspondingly $\rho \gg \rho_c$.

Let us consider *cold* relativistic material, i.e. let us assume $T \ll T_F$.

The total energy is

$$E = N\bar{\epsilon} = N \frac{\int_0^{k_F} dk k^2 c\hbar \sqrt{k^2 + k_c^2}}{\int_0^{k_F} dk k^2},$$

where

$$\begin{aligned} \bar{\epsilon} &= mc^2 \frac{\int_0^{k_F/k_c} dx x^2 \sqrt{1+x^2}}{\int_0^{k_F/k_c} dx x^2} \\ &= mc^2 + mc^2 \frac{\int_0^{k_F/k_c} dx x^2 [\sqrt{1+x^2} - 1]}{\int_0^{k_F/k_c} dx x^2} \end{aligned}$$

is the average electronic energy. At the non relativistic limit we have

$$\begin{aligned} \bar{\epsilon} &\approx mc^2 \left[1 + \frac{\int_0^{k_F/k_c} dx x^2 [\frac{1}{2}x^2 + \dots]}{\int_0^{k_F/k_c} dx x^2} \right] \\ &= mc^2 \left[1 + \frac{3}{10} \left(\frac{k_F}{k_c} \right)^2 + \dots \right], \end{aligned}$$

from which our earlier results can be derived, provided that the rest energy of electrons is taken into account.

At the ultrarelativistic limit $k_F \gg k_c$ we get

$$\bar{\epsilon} \approx mc^2 \frac{\int_0^{k_F/k_c} dx x^3}{\int_0^{k_F/k_c} dx x^2} = \frac{3}{4} c\hbar k_F.$$

Thus the energy density is

$$\frac{E}{V} = \frac{3}{4} (3\pi^2)^{1/3} c\hbar \rho^{4/3}$$

and the pressure

$$p = - \left(\frac{\partial E}{\partial V} \right)_N$$

at the *ultrarelativistic limit* (compare photon gas!)

$$p = \frac{1}{3} \frac{E}{V} = \frac{1}{4} (3\pi^2)^{1/3} c\hbar \rho^{4/3}.$$

White dwarf

In a properly functioning star the pressure due to high temperature (caused by nuclear reactions, mainly $2\text{H} \rightarrow \text{He}$) and the gravitational force are in balance. When the nuclear fuel is consumed the star shrinks and pressure increases. If the mass of the star is large enough all material will become ionized. Depending on the mass of the star the final state can be

- *white dwarf*, if the Fermi pressure of the degenerate electron plasma prevents further compression.
- *neutron star* if the electron pressure is not enough to compensate the gravitational force. The matter compresses further, and electrons + protons \rightarrow neutrons. The degeneracy pressure of neutrons may stop further collapse.

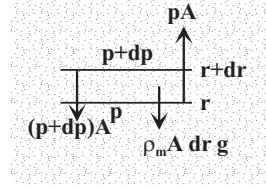
- If neutron pressure is not sufficient \rightarrow black hole.

Typical properties of a white dwarf:

- the diameter of the star $2R \approx 10^4 \text{ km}$.
- the total number of nuclei $N_N \approx 10^{57}$.
- the mass $M \approx 10^{30} \text{ kg} \approx M_\odot$, where $M_\odot = 1.989 \cdot 10^{30} \text{ kg}$ is the mass of the sun.
- the mass density $\rho_m \approx 10^{10} \text{ kg m}^{-3}$ is about $10^6 \times$ the density of the sun or of the earth.
- the number density of electrons $\rho \approx 10^{36} \text{ m}^{-3}$. Then $k_F \approx k_c$, so the electron gas is only moderately relativistic. In inner parts the gas can be much denser and thus ultrarelativistic.
- the pressure $p \approx 10^{22} \text{ Pa} \approx 10^{17} \text{ atm}$.
- the temperature in inner parts $T \approx 10^7 \text{ K} \approx T_\odot$. Since the Fermi temperature is $T_F \approx 10^{10} \text{ K} \gg T$ we, however, have a cold electron gas.

We can estimate the size of the star as follows:

Let $p(r)$ be the pressure at the distance r from the center of the star, $g(r)$ the corresponding gravitational acceleration and $\rho_m(r)$ the density.



The condition for the balance of hydrostatic mechanical forces is

$$\frac{dp}{dr} = -g(r)\rho_m(r).$$

Now

$$g(r) = \frac{GM(r)}{r^2},$$

where $M(r)$ is the mass inside of the radius r and

$$G = 6.673 \cdot 10^{-11} \frac{\text{Nm}^2}{\text{kg}^2}$$

is the gravitational constant. We get the pair of equations

$$\begin{aligned} \frac{dp(r)}{dr} &= -G \frac{M(r)\rho_m(r)}{r^2} \\ \frac{dM(r)}{dr} &= 4\pi r^2 \rho_m(r). \end{aligned}$$

Because in nuclei there are roughly as many neutrons as protons, and, on the other hand, there are as many protons as electrons, we have

$$\rho_m(r) \approx 2m_p \rho(r).$$

Here

$$m_p = 1.673 \cdot 10^{-27} \text{ kg}$$

is the proton mass and $\rho(r)$ the number density of the electrons.

As a first approximation the electron density of a star can be taken to be a constant ρ . Then

$$M(r) = \frac{8}{3} \pi m_p \rho r^3$$

and the total mass

$$M = \frac{8}{3} \pi m_p \rho R^3,$$

when R is the radius of the star. The pressure must now satisfy the differential equation

$$\frac{dp}{dr} = -\frac{16}{3} \pi m_p^2 \rho^2 Gr$$

with the boundary condition that the pressure vanishes at the surface, i.e.

$$p(R) = 0.$$

Integrating the differential equation we get for the pressure at the center

$$p = \frac{8\pi}{3} G m_p^2 \rho^2 R^2.$$

Since the electron gas is not quite ultrarelativistic we calculate more accurately than before. The average electronic energy is

$$\begin{aligned} \bar{\epsilon} &= mc^2 \frac{\int_0^{k_F/k_c} dx x^2 \sqrt{x^2 + 1}}{\int_0^{k_F/k_c} dx x^2} \\ &= mc^2 \frac{\int_0^{k_F/k_c} dx x^3 \left[1 + \frac{1}{2} \frac{1}{x^2} + \dots\right]}{\int_0^{k_F/k_c} dx x^2} \\ &= mc^2 \left[\frac{3}{4} \frac{k_F}{k_c} + \frac{3}{4} \frac{k_c}{k_F} + \dots \right]. \end{aligned}$$

From this we can get for the pressure

$$\begin{aligned} p &= \frac{\hbar c}{12\pi^2} (k_F^4 - k_c^2 k_F^2 + \dots) \\ &= \frac{1}{4} (3\pi^2)^{1/3} \hbar c \rho^{4/3} \left[1 - \frac{m^2 c^2}{\hbar^2 (3\pi^2 \rho)^{2/3}} + \dots \right]. \end{aligned}$$

This the equation of state of the relativistic electron gas. We require that the pressures obtained from the equation of state and from the hydrodynamic balance conditions are equal in the center, i.e.

$$\begin{aligned} \frac{8\pi}{3} G m_p \rho^2 R^2 &= \\ \frac{1}{4} (3\pi^2)^{1/3} \hbar c \rho^{4/3} &\left[1 - \frac{m^2 c^2}{\hbar^2 (3\pi^2 \rho)^{2/3}} + \dots \right]. \end{aligned}$$

When we substitute the electron density (as a function of the mass and radius)

$$\rho = \frac{3M}{8\pi m_p R^3}$$

we get the condition

$$\left(\frac{M}{M_c}\right)^{2/3} = 1 - \left(\frac{R}{R_c}\right)^2 \left(\frac{M_c}{M}\right)^{2/3},$$

where

$$\begin{aligned} M_c &= m_p \left(\frac{9\pi}{512}\right)^{1/2} \left(\frac{\hbar c}{G m_p^2}\right)^{3/2} \approx 0.52 \cdot 10^{57} m_p \\ R_c &= \frac{\hbar}{mc} \left(\frac{9\pi}{8}\right)^{1/3} \left(\frac{M_c}{m_p}\right)^{1/3} \approx 4700 \text{ km}. \end{aligned}$$

For the radius of the star we get

$$R = R_c \left(\frac{M}{M_c}\right)^{1/3} \left[1 - \left(\frac{M}{M_c}\right)^{1/3} \right].$$

We see that the white dwarf has the maximum mass $M = M_c$. A more careful calculation shows that the mass of a white dwarf cannot exceed *Chandrasekhar's limit*, about $1.4M_\odot$, without collapsing to a neutron star or a black hole.

9.4. Other Fermionic systems

Nuclear matter

The mass density of heavy nuclei is

$$\rho_m \approx 2.8 \cdot 10^{17} \text{ kg m}^{-3}.$$

When we assume that the proton and neutron densities are equal the Fermi wave numbers of both gases are

$$k_F \approx 1.36 \cdot 10^{15} \text{ m}^{-1}$$

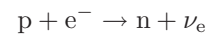
and the Fermi energies

$$\epsilon_F \approx 38 \text{ MeV}.$$

Since $m_n c^2 = 938 \text{ MeV}$, the nuclear matter is non relativistic. The attractive nucleon interactions cancel the pressure due to the kinetic energy.

Neutron star

When the mass of a star exceeds the Chandrasekhar limit the Fermi pressure of the electrons is not enough to cancel the gravitational force. The star continues its collapse. The star forms a giant nucleus where most electrons and protons have transformed via the reaction



to neutrons. The radius of the star is

$$R \approx 10 \text{ km},$$

the nucleon count

$$N_N \approx 10^{57}$$

and the mass density

$$\rho_m \approx 10^{18} \text{ kg m}^{-3}.$$

The pressure acting against the gravitation is mostly due to the pressure of the degenerate Fermi gas and to the strong, at short distances very repulsive nuclear forces. (Crude 1st approximation: substitute $m = m_e \rightarrow m_n$ in white dwarf result.)

Quark matter

When nuclear matter is compressed 2–10 times denser than in atomic nuclei, the nucleons start to "overlap" and their constituent quarks form a quark plasma.

Liquid ^3He

The nucleus is p+p+n and the nuclear spin $\frac{1}{2}$.

At low temperatures the nuclear spin determines the statistics, i.e. ^3He atoms are Fermions.

The Fermi temperature corresponding to the normal density is

$$T_F = \frac{\epsilon_F}{k_B} \approx 5\text{K}.$$

Since the mutual interactions between ^3He atoms are considerable the ^3He matter forms an interacting *Fermi liquid*. The ^3He liquid has two super phases (A and B). These are in balance with the normal phase at the critical point

$$T_c \approx 2.7\text{mK} < \frac{T_F}{1000}.$$