Advanced Solid State Physics

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1 Introduction

Solid state physics is the study of how atoms arrange themselves into solids and what properties these solids have. From the microscopic structure of solids it is possible to calculate many macroscopic properties.

2 Quantization

2.1 Schrödinger Equation

The framework of most solid state physics theory is the **Schrödinger equation** of non relativistic quantum mechanics:

$$\frac{-\hbar^2}{2m}\nabla^2\Psi + V(\mathbf{r})\Psi = E\Psi \tag{1}$$

If we want to quantize the motion of some particle, different problems arise due to its properties. For photons, which have no mass, we don't know what to put into the mass term of the Schrödinger equation.
Phonons are related to the vibration of the atoms in the lattice. If we imagine the whole crystal as a mass-spring system, the normal mode solutions (all components oscillate with the same frequency) which propagate through it are called Phonons. So if we quantize a Phonon, we don't know which mass to take again. Because a phonon represents the vibration of all atoms in the crystal with same frequency.
Another problem for the Schrödinger Equation in this form is the formulation of the magnetic field. The potential works fine if the particle moves in a coulomb potential which depends on the position r . The magnetic field however depends on the velocity, which is not contained in the potential term $V(r)$.

2.2 Recipe for Quantisation

1. Start with classical equations of motion (EOM) and find the Lagrangian $L(q_i, \dot{q}_i)$ by inspection. q_i is called the generized coordinate, and $\dot{q}_i$ is the generized velocity.
   It is often convenient to look out for the normal mode solutions of the system, because the normal modes move independently from each other. So the quantum equations can be solved individually.
   The **Lagrangian**:
   $$L = E_{kin} - E_{pot} \tag{2}$$
   For complicated systems (e.g. the mass is not known) the Lagrangian needs to be constructed by inspection, so it fulfills the **Euler-Lagrange equations**:
   $$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \tag{3}$$

2. **Conjugated variable**:
   $$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{4}$$

3. **Legendre-transformation** to find the Hamiltonian of the system:
   $$H = \sum_i p_i \dot{q}_i - L \tag{5}$$
   Remember from Theoretical mechanics:
   $$H = p \cdot v - L = 2\ E_{kin} - (E_{kin} - E_{pot}) = E_{kin} + E_{pot} \tag{6}$$

4. Quantize the Conjugated variable and formulate Schrödinger Equation

$$p \to -i\hbar\nabla.$$

$$H\Psi(q) = E\Psi(q) \tag{7}$$

2.3 Example: Harmonic Oszillator

The first example how a given system can be quantized is a one dimensional harmonic oscillator. It's assumed that just the equation of motion

$$m\ddot{x} = -kx$$

with m the mass and the spring constant k is known from this system. Now the Lagrangian L must be constructed by inspection:

$$L(x, \dot{x}) = \frac{m\dot{x}^2}{2} - \frac{kx^2}{2}$$

It is the right one if the given equation of motion can be derived by the Euler-Lagrange eqn. (3), like in this example. The next step is to get the conjugate variable, the generalized momentum p:

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x}$$

Then the Hamiltonian has to be constructed with the Legendre transformation:

$$H = \sum_i p_i \dot{q}_i - L = \frac{p^2}{2m} + \frac{kx^2}{2}.$$

With replacing the conjugate variable p with

$$p \to -i\hbar\frac{\partial}{\partial x}$$

because of position space[1] and inserting in eqn. (48) the Schrödinger equation for the one dimensional harmonic oscillator is derived:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2} + \frac{kx^2}{2}\Psi(x) = E\Psi(x)$$

2.4 Example: LC - circuit

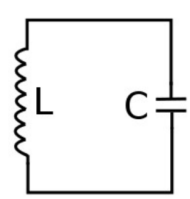


Abbildung 1: LC-Circuit [1]

The classical equation descriping the LC-circuit are:

$$V = L\frac{dI}{dt} \qquad I = -C\frac{dV}{dt} \tag{8}$$

[1] position space: Ortsraum

The charge Q on the capacitor is : $Q = C \cdot V$

$$Q/C = -L\frac{d^2Q}{dt^2} \qquad compare\ harmonic\ oszillator : -Kx = m \cdot a \tag{9}$$

The form of the equation is quite similar to the one of the harmonic oszillator, so we can construct the Lagrangian straight forward:

- Lagrangian

$$\mathcal{L}(Q, \dot{Q}) = \frac{L\dot{Q}^2}{2} - \frac{Q^2}{2C} \tag{10}$$

- Conjugated Variable:

$$p = \frac{\partial \mathcal{L}}{\partial \dot{Q}} = L\dot{Q} \tag{11}$$

- Hamiltonian

$$\mathcal{H}(Q, \dot{Q}) = L\dot{Q}^2 - \mathcal{L} = \frac{L\dot{Q}^2}{2} + \frac{Q^2}{2C} \tag{12}$$

- Quantize and formulate Schrödinger Equation

$$p \to i\hbar\frac{\partial}{\partial Q} \tag{13}$$

$$-\frac{\hbar^2}{2L}\frac{\partial^2\Psi(Q)}{\partial Q^2} + \frac{Q^2}{2C}\Psi(Q) = E\Psi(Q)$$

This recipe of quantization works for every system. Notice the similarity between the LC-circuit and the Harmonic Oszillator. An experiment could be done where light is shined on the LC-circuit. It would be absorbed only in units of $\hbar\omega$, where ω is the oszillation frequency.

2.5 Example: Transmission Line

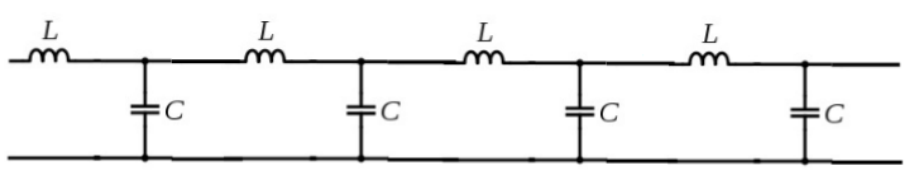


Abbildung 2: Transmission-line [1]

If you want to understand Dissipation(=loss of energy to by conversion to heat) quantummechanically, the transmission line is good model. The transmission line is basically a chain of LC-circuits, where waves are carried away.
A resistor is dissipating energy like a transmission line: The current is converted to heat and the heat flows away by phonons flowing down the transmissionn line.

Additionally to the time dependence on the voltage and current in the simple LC-circuit, there is a dependence on the space r of the capacitor or inductor.
The voltage of a particular capacitor changes proportional to the spacial change of current (flowing to the left / to the right)

$$-\frac{dI}{dx} = C\frac{dV}{dt} \tag{14}$$

The current in a particular inductor changes proportional to the difference of voltage of the capacitors.

$$-\frac{dV}{dx} = L\frac{dI}{dt} \tag{15}$$

Compining these two equation (e.g. time derivative of first one & spacial derivative of second one) yields the wave equation:

$$\frac{dV^2}{dx^2} = LC\frac{d^2V}{dt^2} \tag{16}$$

Solve the wave equation for this system with the **normal mode** solution:

$$V_k = V_0 \exp i(kx - \omega t) \qquad ...normal\ mode\ solution\ of\ voltage \tag{17}$$

Plugging this into the wave equation delivers the dispersion relation:

$$k^2 = LC\omega^2 \quad \rightarrow \quad \omega = \frac{1}{LC}k \quad \rightarrow \quad \omega = ck \tag{18}$$

The transmission line has wavelike solutions, where the frequency is linear proportional to the wavevector and the proportional constant is the speed of light $c = \frac{1}{\sqrt{LC}}$

We can find the relationship between current and voltage and define an impedance:

$$Z = \frac{V}{I} = \sqrt{\frac{L}{C}} \tag{19}$$

The impedance of the transmission line is not oszillating and is practically equal to the impedance of a comparable resistor. Transmission lines are quantummechanical models for resistors and dissipating elements.

2.5.1 Quantization of the wave equation

As already mentioned at the beginning the Schrödinger equation can not be used to quantize the transmission line, because we don't know which mass to put into the formula. One has to use the recipe given in chapter: 2.2

- Lagrangian:
  If you plug a normal mode solution into the wave equation and take the derivative only with respect to space you get something like the EOM for the harmonic oszillator. The equivalent for the mass turns out to be 1 and the equivalent for the spring constant is c^2k^2. The Lagrangian has to fulfill the Euler Lagrange Equations and can be found similarly as for the harmonic oszillator.

$$V_k = V_0 \exp i(kx - \omega t) \qquad c\frac{dV^2}{dx^2} = \frac{d^2V}{dt^2} \tag{20}$$

$$\rightarrow -c^2k^2V_k = \frac{d^2V_k}{dt^2}V_k \qquad\qquad -c^2k^2x = 1 \cdot a \tag{21}$$

$$\mathcal{L}(V_k, \dot{V_k}) = \frac{\dot{V_k}^2}{2} - \frac{c^2k^2}{2}V_k^2 \tag{22}$$

- **Conjugated variable**:

$$p_i = \frac{\partial L}{\partial \dot{V_k}} = \dot{V_k} \tag{23}$$

- **Legendre-transformation** to find the Hamiltonian of the system:

$$H = \dot{V_k}\dot{V_k} - L = \frac{\dot{V_k}^2}{2} + \frac{c^2k^2}{2}V_k^2 \tag{24}$$

- Quantize the Conjugated variable and formulate **Schrödinger Equation**

$$p \to -i\hbar\nabla \qquad \dot{V}_k \to -i\hbar\frac{\partial}{\partial V_k}$$

$$\frac{-\hbar^2}{2}\frac{d^2\Psi}{dV_k^2} + \frac{c^2k^2}{2}V_k^2\Psi = E\Psi \tag{25}$$

The result is quite similar to the form of the harmonic oscillator and the two system have the same solution. j is the number of photons in the mode of frequency ω

$$E = \hbar\omega(j + \frac{1}{2}) \qquad j = 0, 1, 2, ... \tag{26}$$

$$\omega = c|k| \to \ f = \frac{c}{\lambda} \quad \text{...dispersion relation for wave equation} \tag{27}$$

2.5.2 Ammonia

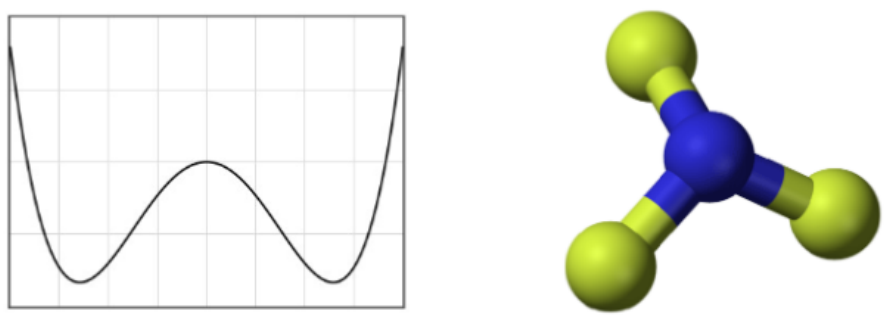


Abbildung 3: Model of Ammonia [1]

Ammonia is a molecular system which oszillates like a LC-circuit. The Nitrogen sticks out of the Hydrogen plane either on the one site or the other. These two positions are equivalent in energy and represent a double well potential. The idea is to apply an electric field and force all Nitrogen atoms to one site. This corresponds to the overlap of the ground and 1st excited state(The ground state is symmetric, the first excited antisymmetric so the combination of the two states yields a spatial probability distribution which peaks only at one site of the ammonia) Due to the different frequency of the ground- and first excited states, the overlap of these two changes in time, so that after a while all the nitrogen atoms are at the other site. If one would measure where the nitrogen atoms are after the electric field was turned of, oscillations like the ones of the LC-circuit would appear.

This behavior was the reason for the famous discussion about whether Schrödingers cat is alive or dead. A cat is put in a box with a radio active decaying substance. If there is an decay, the cat is poisoned and dies. To do an appropriate experiment, you would have to put 1000 cats into 1000 boxes and measure how many die in time. So first you wait 1 second - you open the box and no cat died. So you wait 10 seconds - a view cats die, you replace them and wait 20 seconds - more cats die and so on. You would expect a time where you open the box and all cats are alive - this would be the quantum mechanical oscillation. With cats it doesn't - they just die. It has to do with how the dissipation is coupled with the variable being dead or alive.

2.5.3 Dissipation

Dissipation in solids states physics is important to describe the current flowing e.g. through a metal. If there is no electric field, all electrons are in the ground state and there are as many left moving k states as right moving, so they cancel each other out.
If an electric field was applied there are more right moving waves than left moving, a current flows. The electrons scatter, generate phonons(heat) which is carried away by the transmission line.

2.6 Quantisation of the EM-field

2.6.1 A brief summary of Electrodynamics

A summary of Electrodynamic & FQM, For more detail check out the Advanced Solid State-homepage Maxwell equations:

$$\nabla E = \frac{\rho}{\epsilon_0} = 0 \quad \text{Gauses law in vacuum} \tag{28}$$

$$\nabla B = 0 \tag{29}$$

$$\nabla \text{ x } E = \frac{-\partial B}{\partial t} \quad \text{Faradays law} \tag{30}$$

$$\nabla \text{ x } B = \mu_0 \epsilon_0 \frac{\partial E}{\partial t} \quad \text{Amperes law} \tag{31}$$

A vectorpotential is defined as:

$$B = \nabla \text{ x } A \tag{32}$$

$$E = -\nabla V - \frac{\partial A}{\partial t} \tag{33}$$

Where the electrostatical potential for vacuum = 0. There are more possible vector potential for one quantity, so an additional demand can be made, in our case the Coulomb Gauge:

$$\nabla A = 0 \tag{34}$$

Within this Gauge the first 3 equations are self consistent. In Coulomb Gauge all information is contained in Amperes law.

$$\nabla \text{ x } B = \mu_0 \epsilon_0 \frac{\partial B}{\partial t} \rightarrow \quad \nabla \text{ x } \nabla \text{ x } A = -\mu_0 \epsilon_0 \frac{\partial^2 A}{\partial t^2} \tag{35}$$

Use a vector identity ($\nabla A = 0$ in Coulomb Gauge):

$$\nabla \text{ x } \nabla \text{ x } A = \nabla(\nabla A) - \nabla^2 A \tag{36}$$

Finally results in the wave equation for EM-radiation in vacuum:

$$c^2 \nabla^2 A = \frac{\partial^2 A}{\partial t^2} \qquad c = \frac{1}{\sqrt{\mu_0 \epsilon_0}} \tag{37}$$

If we look for normal mode solutions we get the same answers as for the transmission line (formally in 3D)

$$A(r,t) = A \cdot \exp i(kr - \omega t) \tag{38}$$

Dispersion relation:

$$\omega = c|k| \leftrightarrow f = \frac{c}{\lambda} \tag{39}$$

If we evaluate the wave equations for the electrostatic field and the magnetic field, it can be noticed that they propaged in the same direction, but oscillate in normal planes:

$$E = -\frac{\partial A}{\partial t} = -\omega A_0 sin(k_x x - \omega t) e_z \tag{40}$$

$$B = \nabla \text{ x } A = k_x A_0 sin(k_x x - \omega t) e_y \tag{41}$$

2.6.2 Quantize

We follow the same procedure to quantize the 3D wave equation as for the transmission line. First we look for normal mode solutions and take the spacial derivative. The normal mode solutions carry an index s indicating that there are 2 possible polarization for every direction.
Start out with the **wave equation** for the EM-field:

$$c^2\nabla^2 A = \frac{\partial^2 A}{\partial t^2} \tag{42}$$

Normal mode solution for the wave vector k:

$$A_k = A_s \exp i(kr - \omega t) \tag{43}$$

$$-c^2k^2A_s = \frac{\partial^2 A}{\partial t^2} \qquad \text{vgl. harm. oszi. } -Kx = m \cdot a \tag{44}$$

- Find the **Lagrangian** by comparison with harmonic oscillator:

$$\mathcal{L}(A_s, \dot{A}_s) = \frac{\dot{A_s}^2}{2} - \frac{c^2k^2}{2}A_s^2 \tag{45}$$

- **Conjugated variable**:

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{A}_k} = \dot{A}_k \tag{46}$$

- **Legendre-transformation** to find the Hamiltonian of the system:

$$\mathcal{H} = \dot{A}_s\dot{A}_s - \mathcal{L} = \frac{\dot{A_s}^2}{2} + \frac{c^2k^2}{2}A_s^2 \tag{47}$$

- Quantize the Conjugated variable and formulate **Schrödinger Equation**

$$p_i \to -i\hbar\nabla \qquad \dot{A}_s \to -i\hbar\frac{\partial}{\partial A_s}$$

$$\frac{-\hbar^2}{2}\frac{d^2\Psi}{dA_s^2} + \frac{c^2k^2}{2}A_s^2\Psi = E\Psi \tag{48}$$

- **Quantum solutions** The eigen vectors for this problem will also be the hermite polynomials and the corresponding eigenenergys are given in the solution of the harmonic oscillator. j_s indicates the number of photons in mode s.

$$E_s = \hbar\omega(j_s + \frac{1}{2}) \qquad j_s = 0, 1, 2, ... \tag{49}$$

  Dispersion relation

$$w_s = c|k_s| \tag{50}$$

3 Photons

3.1 Thermodynamic properties of non-interacting bosons

For detailed derivation of the grand canonical partition function $\mathcal{Z}_{gr}$ see Script: Statistische Physik (Von der Linden) or homepage: Fortgeschrittene Festkörperphysik/outline/photons/Thermodynamic properties of non-interacting bosons

We start out with the grand canonical potential for non-interacting bosons. The difference in between non interacting bosons and fermions is the occupation of a particular state. For bosons

we can but from $i = 0, 1, 2...\infty$ particles in a state with energy ϵ_i. For non interacting fermions a state can either be occupied or not ($i = 0, 1$). With some mathematical clues the **grand canonical partition function** can be found:

$$\mathcal{Z}_{gr} = \prod_i \left[\frac{1}{1 - \exp\left(-\frac{\epsilon_i - \mu}{k_B T}\right)} \right] \tag{51}$$

Fundamental theorem of statistical physics:

$$\Phi = -k_b T \ln(\mathcal{Z}_{gr}) = k_B T \sum_i \ln\left[1 - \exp\left(\frac{\mu - \epsilon_i}{k_B T}\right)\right] \tag{52}$$

The sum can be converted in an integral over the density of states (For mathematical completeness check script: Statistische Physik (VdL):

$$\phi = \frac{\Phi}{V} = k_B T \int_{-\infty}^{\infty} D(E) \ln\left[1 - \exp\left(\frac{\mu - E}{k_B T}\right)\right] dE \tag{53}$$

The grand canonical potential is defined as:

$$\Phi = -p \cdot dV - S \cdot dT - N \cdot d\mu \tag{54}$$

so the particle density can be calculated:

$$n = -\frac{\partial \phi}{\partial \mu} = k_B T \int_{-\infty}^{\infty} D(E) \frac{1}{1 - \exp\left(\frac{\mu - E}{k_B T}\right)} \exp\left(\frac{\mu - E}{k_B T}\right) \cdot \frac{1}{k_B T} dE = \int_{-\infty}^{\infty} D(E) \underbrace{\frac{1}{\exp\left(\frac{E - \mu}{k_B T}\right) - 1}}_{F_{BE}(E)} dE \tag{55}$$

In this expression we recognize the Bose Einstein function: F_{BE}. All of this calculation is based on the assumption of **non interacting** bosons. If there were any interaction the Bose Einstein function would not describe this accurately. Photons do not interact very much, so the Bose Einstein function is a valid assumption.

From the grand canonical potential many other thermodynamic properties can be derived:

$$u = f + Ts = \int_{-\infty}^{\infty} E D(E) F_{BE} dE \tag{56}$$

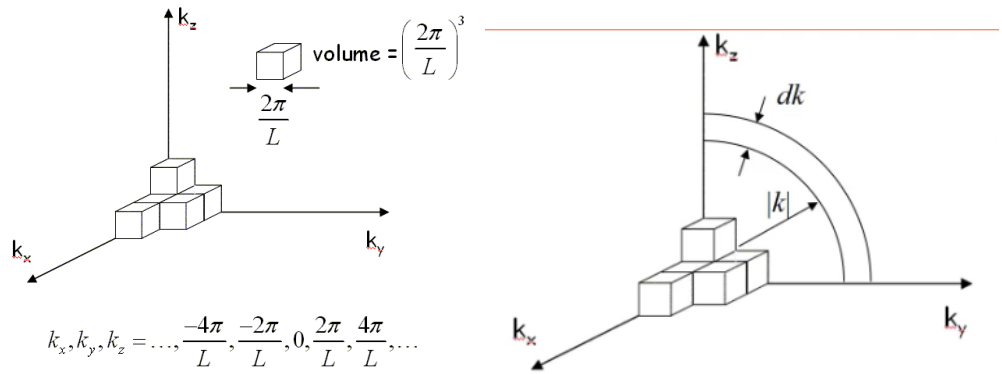
$$c_v = \frac{\partial u}{\partial T} \tag{57}$$

$$s = -\frac{\partial \phi}{\partial T} \tag{58}$$

For photons the chemical potential is zero. This is derived from the fact that the number of photons is not conserved. (As long as energy and momentum are conserved, photons can be absorbed and emitted)

$$\left.\frac{\partial F}{\partial N}\right|_{T,V} = 0 = \mu. \tag{59}$$

3.2 Density of states



(a) (b)

Abbildung 4: Density of states for photons in vacuum

We start out with the density of states for photons in vacuum. You look at the EM-field in a cubic box of length L and apply periodic boundary conditions. An integer number of wavelengths must fit in the cube, $\lambda = L/n$, where n is an integer. This restricts the allowed wavevectors to k_x, k_y, $k_z = \frac{2\pi}{L}$. These allowed values of k form a cubic lattice in k space. The k space volume associated with each point is $(2\pi/L)^3$. There are p = 2 as many linearly independent normal modes as there are points in k-space because the electric field has two independent components that are perpendicular to the propagation direction.
The waves which have the same energy, have all the same frequency and absolute value of k. We look for the density of states in k-space. So we have to count the allowed points with k values between k and k + dk in a shell:

$$D(k)dk = p\frac{4\pi k^2 dk}{(2\pi/L)^3} = \frac{k^2 L^3}{\pi^2}dk \tag{60}$$

Using the relationship $\omega = c|k|$, the density of modes per unit volume in terms of frequency is,

$$D(\omega)d\omega = \frac{\omega^2}{c^3\pi^2}d\omega \tag{61}$$

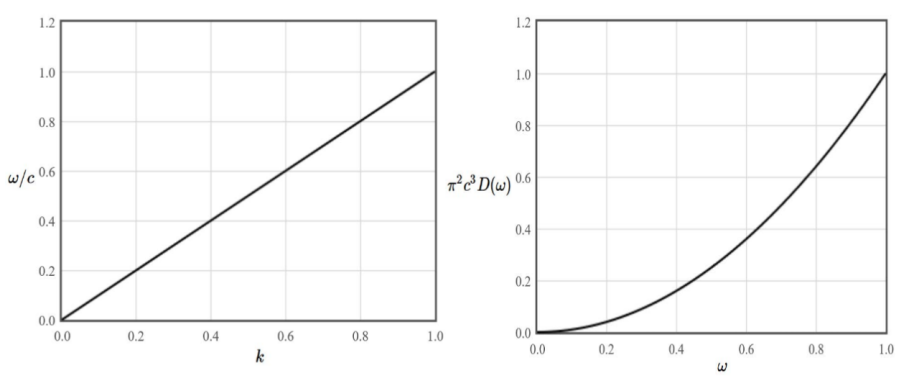


Abbildung 5: Dispersionrelation and Density of states for free photons in vacuum [1]

Using the relationship $E = \hbar\omega$, the density of modes per unit volume in terms of Energy is

$$D(E) = \frac{E^2}{\pi^2 c^3 \hbar^3} \tag{62}$$

3.3 Thermodynamic properties of light

With the density of states and the thermodynamic coherences the **energy spectral density**(=plank radiation curves) can be calculated. As a convention this is done in terms of wavelength for the 3D case:

$$u(\lambda) = E(\lambda)D(\lambda)F_{BE}(\lambda) = \frac{8\pi hc}{\lambda^5(\exp\frac{hc}{\lambda k_B T} - 1)} \tag{63}$$

The maximum of the plank radiation curves depends on the temperature. This is known as the Wiens displacement law: $\lambda_{max} = \frac{const.}{T}$
The **internal energy** is the integral over the energy spectral density. From the internal energy many thermodynamic properties can be derived.

$$u = \int_0^\infty u(\lambda)d\lambda = \frac{4\sigma T^4}{c} \tag{64}$$

3.4 Photonic crystals

In this section we look at light moving through a periodic structure. A photonic crystal is a structure with different dielectric functions in different (repeating) regions. To produce such a crystal, polystyrene spheres can be settled to an fcc structure in water. The empty parts in between them can be filled with Titaniumdioxid and the polystyrene spheres can be burned out. The structure you get is called an inverse opal. Light moves through the empty wholes with c_{vac} and through the TiO_2 it propagates slower. Long wavelength light will move through with some average (of the two materials) speed of light. However, when the wavelength of the light approaches the periodicity of the crystal, it gets diffracted. The diffraction condition is $\Delta k = G$.

Reminder: Reciprocal lattice vectors:

$$\vec{b_1} = \frac{2\pi\ \vec{a_2}\ \text{x}\ \vec{a_3}}{\vec{a_1}\ (\vec{a_2}\ \text{x}\ \vec{a_3})} \tag{65}$$

$$\vec{G} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3} \tag{66}$$

Any periodic function can be represented as a Fourier series:

$$f(\vec{r}) = \sum_G f_{\vec{G}} e^{i\vec{G}\vec{r}} \tag{67}$$

1D: The simplest example for a photonic crystal would be in one dimension. When light strikes the interface between two materials with different indices of refraction, part of the light is transmitted and part is reflected. In layered materials, there are reflections from each layer. Most of the time, the reflections from the different layers add incoherently, but under certain conditions the reflections add constructively. When this happens, the layered material acts like a mirror for a particular range of frequencies. It completely reflects certain frequencies while letting others pass through. The lowest k value with diffrection in this example corresponds to 1 sin-wave per period a in Abb. 6. $k = \frac{2\pi}{\lambda}$, the second: 2 sin-waves per period a: $k = \frac{4\pi}{\lambda}$ and so on.

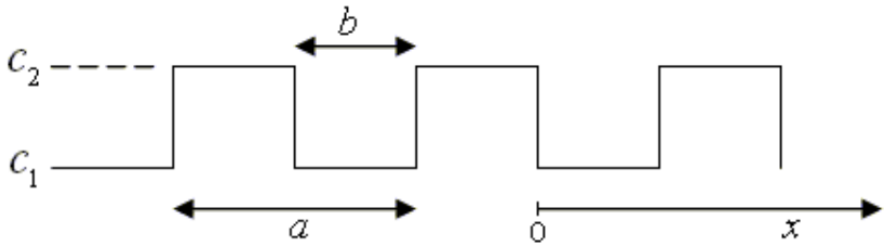
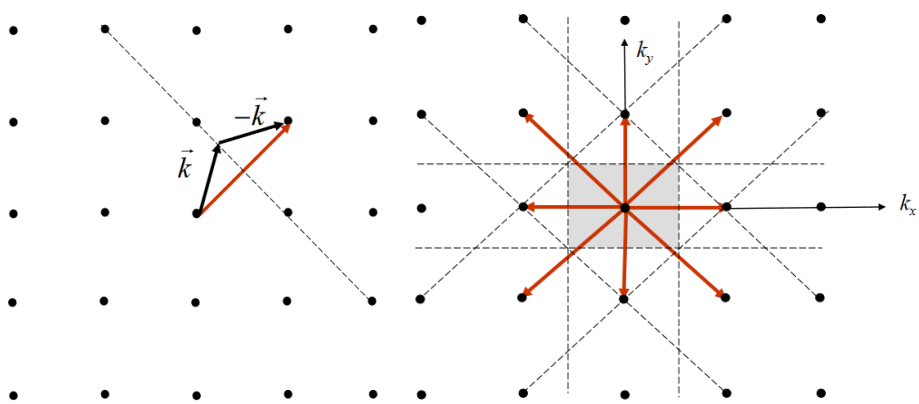


Abbildung 6: Speed of light in a layered material in 1D [1]

2D: For 2 Dimensions the diffraction condition ($\vec{k} - \vec{k'} = \vec{G}$) is shown in Im. 7a. Most of the scattering is elastic, so $|k| = |k'|$. For every couple of k & k' vectors which satisfy these conditions we expect diffraction to occur.



(a) Diffractoin in reciprocal space [1]

(b) Brillouinzone in 2D

Abbildung 7

In Im. 7b the brillouinzone construction is showen. At the Brillouinzonebounderies we expect diffraction to occur.
The first brillouinzone is very important for further calculations, because due to the bloch theorem, any k vector can be shifted back into the first brillouin zone.

3.4.1 Bloch theorem

Start out with an arbitrary function which satisfies periodic boundary conditions:

$$f(\vec{r}) = \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k}\vec{r}} \tag{68}$$

Now we can reorder the sum into k inside the first Brillouinzone and shift any k outside the first Brillouinzone back into with the periodicity of the crystal.

$$f(\vec{r}) = \sum_{\vec{k} \in 1Bz} \sum_{\vec{G}} c_{\vec{k}+\vec{G}} e^{i(\vec{k}+\vec{G})\vec{r}} \tag{69}$$

Look at just one particular k: We can pull out the factor of e^k and recognize that the remaining term is just a periodic function.

$$f_k(\vec{r}) = e^{i\vec{k}\vec{r}} \sum_{\vec{G}} c_{\vec{k}+\vec{G}} e^{i\vec{G}\vec{r}} = e^{i\vec{k}\vec{r}} u_k(\vec{r}) \tag{70}$$

This result is called Bloch form and is important because it is an eigenvector of the Translation operator. If we can find the Bloch form of a system, it represents the normal mode solution. And the bloch theorem states that any normal mode solution of the crystal can be shifted back into the first brillouin zone.

3.4.2 Empty lattice approximation

A good first guess how the bandstructure of a photonic crystal will look like is given by the empty lattice approximation. You let the light move through a periodic structure, but the speed of light is everywhere the same = c_{vac}. We already discussed light in vacuum in Im. 5. The difference of the empty lattice approximation to the case of photons in vacuum is, that there are brillouinzones. Due to the Bloch theorem we can shift all bands back into the first brillouinzone and reflect them at the boundaries. This assumption can be seen in Im. 8.

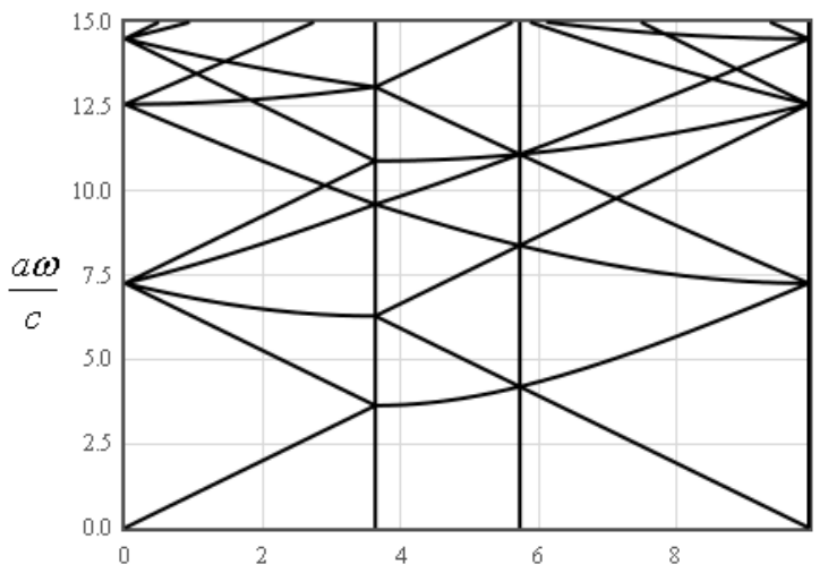


Abbildung 8: Empty lattice approximation for photonic crystal [1]

If there were different speed of lights, the bands would band over, hit the brillouinzone at 90 ° and little gaps would appear.

3.4.3 Plane wave methode

We start out with a crystal where the speed of light is a periodic function of position (like in the case of photonic crystals).

$$c(\vec{r})^2 \nabla^2 A = \frac{\partial^2 A}{\partial t^2} \tag{71}$$

The speed of light is can be written as a fourier series in terms of the periodicity of the crystal.

$$c(\vec{r}) = \sum_{\vec{G}} b_{\vec{G}} e^{i\vec{G}\vec{r}} \tag{72}$$

The vector potential can be written as a fourier series (plane waves). We assume a box which is bigger than the periodicity of the crystal. Therefor there are much more allowed k values than G values.

$$A_j = \sum_{\vec{k}} A_{\vec{k}} e^{i(\vec{k}\vec{r} - \omega t)} \tag{73}$$

Put c and A in the differential equation:

$$\sum_{\vec{G}} b_{\vec{G}} e^{i\vec{G}\vec{r}} \sum_{\vec{\kappa}} (-\kappa^2) A_{\vec{\kappa}} e^{i(\vec{\kappa}\vec{r}-\omega t)} = -\omega^2 \sum_{\vec{k}} A_{\vec{k}} e^{i(\vec{k}\vec{r}-\omega t)} \tag{74}$$

$$\sum_{\vec{\kappa}} \sum_{\vec{G}} (-\kappa^2) b_{\vec{G}} A_{\vec{\kappa}} e^{i(\vec{G}\vec{r}-\vec{\kappa}\vec{r}-\omega t)} = -\omega^2 \sum_{\vec{k}} A_{\vec{k}} e^{i(\vec{k}\vec{r}-\omega t)} \tag{75}$$

The right hand side can only be equivalent to the left hand side if the two exponential terms are equal:

$$\vec{G} + \vec{\kappa} = \vec{k} \quad \rightarrow \quad \vec{G} = \vec{k} - \vec{\kappa} \tag{76}$$

And the result are algebraic equations called central equations:

$$\sum_{\vec{G}} (\vec{k} - \vec{G})^2 b_{\vec{G}} A_{\vec{k}-vecG} = \omega^2 A_{\vec{k}} \tag{77}$$

The b values are known as they define the periodicity of the speed of light in different regions. The G are the reciprocal lattice vectors of the crystal. You choose a k in the first brillouinzone and calculate the frequency ω and the amplitudes A. Move to the next k and repeat ec.
To check the result of the plane wave methode you can set the speed of light everywhere the same. You expect the result of the empty lattice approximation.

Literatur

[1] Peter Hadley. Vorlesungsfolien. Accessed: 08.07.2017.

[2] Autor. title, 2008. Accessed: 25.3.2016.
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