

(Assignments ToC)

Lattice and beyond (a refreshment)

Tue 19.04.2005, Sheet 1

-
- Ex. 1.1.: Face centered cubic lattice and its Brillouin-zone
Ex. 1.2.: The δ sum rules for crystals
Ex. 1.3.: Fourier transform of the Yukawa and Coulomb potential
-

Normal modes of harmonic networks

Tue 26.04.2005, Sheet 2

-
- Ex. 2.1.: Lattice dynamics of a monoatomic linear chain with fixed boundary conditions
Ex. 2.2.: Square lattice
-

Second quantization I (bosonic gymnastic)

Tue 03.05.2005, Sheet 3

-
- Ex. 3.1.: Bosonic commutation relations
Ex. 3.2.: Calculating with bosonic operators I
Ex. 3.3.: Calculating with bosonic operators II (optional)
-

From Molecular Orbitals to Bloch states

Fri 20.05.2005, Sheet 4

-
- Ex. 4.1.: The electron-problem for the benzene molecule (tight binding model)
Ex. 4.2.: The Kronig-Penney model
-

Band structure I: the fcc lattice

Tue 24.05.2005, Sheet 5

-
- Ex. 5.1.: Electronic structure for free electrons in a fcc lattice
Ex. 5.2.: Tight binding s -bands in fcc crystals
-

Band structure II: graphene and carbon nanotubes

Tue 31.05.2005, Sheet 6

-
- Ex. 6.1.: Electronic structure of graphene
Ex. 6.2.: Electronic structure of single wall carbon nanotubes
-

Electronic Density of States

Tue 07.06.2005, Sheet 7

-
- Ex. 7.1.: Electrons in the continuum
Ex. 7.2.: Tight binding electrons
Ex. 7.3.: Infinite dimensional DOS (optional)
-

Second quantization II (fermionic gymnastic)

Tue 21.06.2005, Sheet 8

- Ex. 8.1.: Fermionic commutation relations
 - Ex. 8.2.: Yukawa-correlated fermions
 - Ex. 8.3.: Calculating with fermion operators
-

Screening and Peierls instability

Tue 28.06.2005, Sheet 9

- Ex. 9.1.: The dielectric function
 - Ex. 9.2.: Linear response of the one-dimensional electron gas
 - Ex. 9.3.: Coupled electronic bands (optional)
-

Density functional theory

Tue 11.07.2005, Sheet 10

- Ex. 10.1.: Functional derivatives
- Ex. 10.2.: Density functional theory in the Thomas Fermi approximation

Assignments to Solid State Theory I

G. Cuniberti
F. Pump(Phy 4.1.29)
(Phy 4.1.30)Room Phy 7.1.21, h 10.15
Tue 19.04.2005 (**Sheet 1**)sheet online: <http://www-MCG.uni-R.de/teaching/>**Problem set: Lattice and beyond (a refreshment)****1.1. Face centered cubic lattice and its Brillouin-zone**As known from the *Struktur der Materie II (Festkörperphysik)* course, the vectors

$$\mathbf{a}_1 = (0, 1, 1)a/2, \quad \mathbf{a}_2 = (1, 0, 1)a/2, \quad \mathbf{a}_3 = (1, 1, 0)a/2,$$

span the unit cell of the fcc lattice.

- Draw the fcc lattice together with the vectors \mathbf{a}_i .
- Calculate the volume of the unit cell.
- Determine the three vectors \mathbf{b}_i such that $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$, which span the unit cell of the reciprocal lattice.
- Show that for the vectors

$$\mathbf{G} = \frac{2\pi}{a}(H, K, L)$$

of the reciprocal lattice the value of the components H , K and L are either all even or odd! (*The reciprocal lattice of an fcc lattice is indeed a bcc lattice!*)

- Build the first Brillouin-zone (the Wigner Seitz cell of the bcc lattice)!

Hint: You might find useful to 3d-image the fcc lattice using a molecular visualization software.¹

1.2. The δ sum rules for crystals

Lattice-periodic functions or crystal functions are periodic functions,

$$f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R}) \quad \forall \mathbf{R},$$

where \mathbf{R} is a lattice vector.

¹As an example you can run `<molekel -xyz fcc.xyz>`. You can find for free the molekel software on the net and a fcc coordinate file, e.g., in the following clickable link <http://www-MCG.uni-R.de/downloads/fcc.pdf>.

(a) Show that

$$f(\mathbf{r}) = \sum_{\mathbf{k}} F(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\mathbf{G}} F(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}} ,$$

with

$$F(\mathbf{G}) = \frac{1}{\Omega} \int_{\Omega} d\mathbf{r} f(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} ,$$

where \mathbf{G} is a reciprocal lattice vector, $\Omega = V/N$ is the volume of the unit cell and N the number of cells in the Born-von-Kármán volume.

(b) Show that

$$\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} = N \delta_{\mathbf{k},\mathbf{0}} ,$$

where \mathbf{k} is a vector in the Brillouin-zone which agrees to the Born-von-Kármán boundary conditions. How could one modify this relation if \mathbf{k} -vector is not limited to the first Brillouin-zone ?

(c) Show that

$$\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} = N \delta_{\mathbf{R},\mathbf{0}} ,$$

where the sum has to be taken over all \mathbf{k} -vectors in the first Brillouin-zone consistently with the Born-von-Kármán boundary conditions.

1.3. Fourier transform of the Yukawa and Coulomb potential

The 3d Yukawa potential is given as

$$V_Y(\mathbf{r}) \equiv V_Y(r) = \frac{A}{r} \exp(-\alpha r) \quad (\alpha > 0) .$$

(a) Calculate the Fourier transform $F_Y(\mathbf{k})$ of the Yukawa potential

$$F_Y(\mathbf{k}) = \int d\mathbf{r} V_Y(\mathbf{r}) \exp(-i\mathbf{k}\cdot\mathbf{r}) .$$

(b) Calculate the Fourier transform $F_C(\mathbf{k})$ of the 3d Coulomb potential

$$V_C(\mathbf{r}) \equiv V_C(r) = \frac{A}{r} .$$

(c) Compare this result with what is obtained by Fourier transforming the Poisson equation for a point charge in 3d. Discuss the 2d and 1d case!

Note: The Yukawa potential -as it will be seen in coming lectures- is the Thomas-Fermi screening for a single point charge in 3d.

Assignments to Solid State Theory I

G. Cuniberti
F. Pump

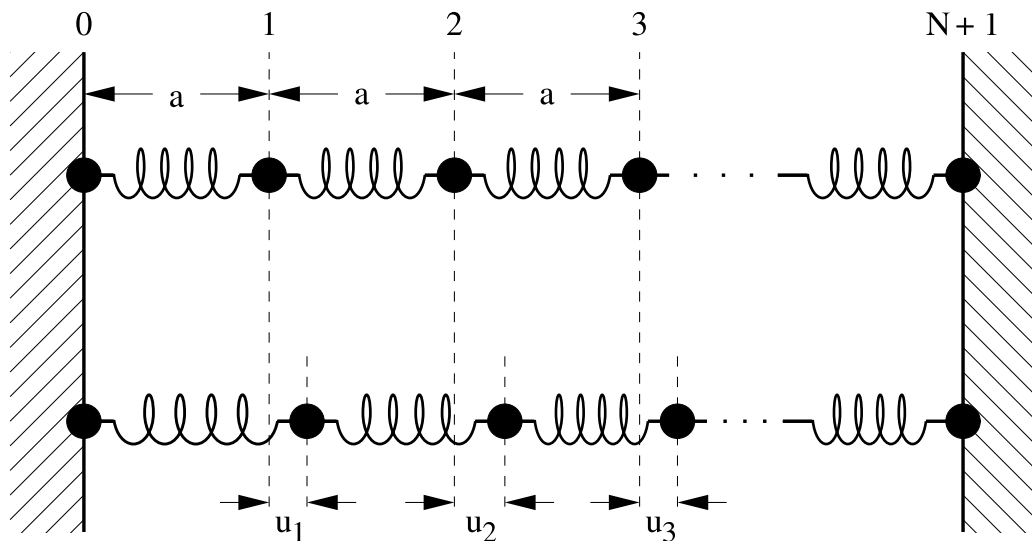
(Phy 4.1.29)
(Phy 4.1.30)

Room Phy 7.1.21, h 10.15
Tue 26.04.2005 (**Sheet 2**)

sheet online: <http://www-MCG.uni-R.de/teaching/>

Problem set: Normal modes of harmonic networks**2.1. Lattice dynamics of a monoatomic linear chain with fixed boundary conditions**

Consider a linear chain containing $N + 2$ “atoms” (please read “classical particles”!) of mass M . The chain atoms are interacting via nearest neighbor harmonic forces (spring constant k and equilibrium distance a). However *the first and the last atom are constrained to two rigid walls*.



Note that we have $N + 1$ springs, but N degrees of freedom. The equilibrium distance of the j th atom is thus $\mathbf{R}_j^0 = ja$. The instantaneous atomic positions are given by specifying the atomic displacements $\mathbf{u}_j(t)$ such that $\mathbf{R}_j(t) = \mathbf{R}_j^0 + \mathbf{u}_j(t)$. Since we are constrained to strictly 1d we can drop off the vector notation. The coordinates $u_0 = u_{N+1} = 0$ (the displacements of the rigid walls!), so they are *not* dynamical variables. The system Hamiltonian is thus

$$H = \frac{1}{2M} \sum_{j=1}^N P_j^2 + \frac{k}{2} \sum_{j=0}^N (u_{j+1} - u_j)^2.$$

The equations of motion read:

$$M\ddot{u}_j = k(u_{j+1} + u_{j-1} - 2u_j), \quad j = 1, \dots, N.$$

(a) Verify that the m th normal mode can be written as

$$u_j^{(m)}(t) \propto \sin\left(\frac{\pi m j}{N+1}\right) \exp(-i\omega_m t), \quad 1 \leq m \leq N,$$

and find the correspondent normal (eigen)frequencies ω_m .

Hint: Recall that $\sin(\alpha + \beta) + \sin(\alpha - \beta) = 2 \sin \alpha \cos \beta$, and $1 - \cos \gamma = 2 \sin^2 \gamma/2$.

(b) Are the normal modes degenerate or not? What is the value of the maximum frequency? What is the value of the minimum frequency? Does the zero-frequency mode exist in this system or not? Why?

(c) Calculate the mode density in frequencies, in the limit $N \gg 1$. Compare this result with the usual density of modes

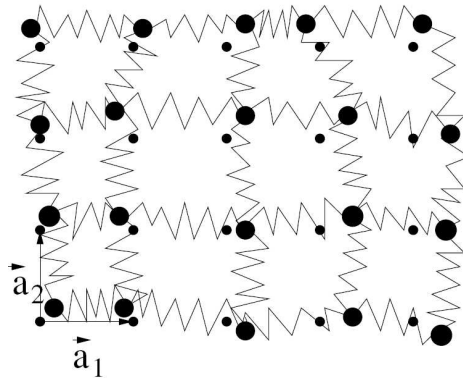
$$\mathcal{D}(\omega) = \frac{2N}{\pi} \frac{1}{\sqrt{\omega_{\max}^2 - \omega^2}}$$

calculated (in class²) for N masses and N springs with periodic boundary condition.

Note: In the case of the fixed boundary conditions it is *wrong* to speak about group velocity because all modes are stationary.

2.2. Square lattice

Consider a monoatomic, two-dimensional square lattice of N^2 atoms of mass M , as shown in the figure.



The basis vectors are $\mathbf{a}_1 = a\hat{x}$ and $\mathbf{a}_2 = a\hat{y}$. Consider periodic boundary conditions with $N \rightarrow \infty$.

Consider a potential energy with the form

$$V = \frac{k}{2} \sum_{\langle i,j \rangle} \|\mathbf{u}_i - \mathbf{u}_j\|^2,$$

where $\langle i, j \rangle$ denotes nearest neighbour lattice sites.

²C. Kittel, *Quantum Theory of Solids, Series in Modern Condensed Matter Physics*, 2nd revised ed. (John Wiley & Sons, Inc., 1987).

- (a) Show that the force constant matrices $\Phi(\mathbf{R}_j^0)$ are diagonal and nonzero up to $\mathbf{R}_j^0 = \mathbf{0}$ or $\mathbf{R}_j^0 = \pm \mathbf{a}_i$ with $(i = 1, 2)$.
 Hint: Remember the definition of the force constant matrices, where α, β indicate the x or y component:

$$\Phi_{\alpha\beta}(\mathbf{R}_j^0 = 0) = \sum_{\ell} \frac{\partial^2 V}{\partial u_{\ell}^{(\alpha)} \partial u_{\ell}^{(\beta)}} \Big|_{\mathbf{u}_{\ell} \equiv 0},$$

$$\Phi_{\alpha\beta}(\mathbf{R}_j^0 \neq 0) = - \frac{\partial^2 V}{\partial u_j^{(\alpha)} \partial u_j^{(\beta)}} \Big|_{\mathbf{u}_j \equiv 0}.$$

- (b) Write the equations of motion in terms of the force constant matrices by making use of the standard exponential Ansatz seen in class. The problem is transformed into the calculus of the 2×2 dynamical matrix

$$D_{\alpha\beta}(\mathbf{q}) = \frac{1}{M} \sum_j \Phi_{\alpha\beta}(\mathbf{R}_j^0) \exp(i\mathbf{q} \cdot \mathbf{R}_j^0).$$

- (c) The eigenvalues of $\mathbf{D}(\mathbf{q})$ are the squares of the two phonon frequencies $\omega(\mathbf{q})$ (in this case they are degenerate).
 Plot the dispersion relation ω vs. \mathbf{q} for the special directions of \mathbf{q} : $\Gamma \rightarrow \mathbf{X} \rightarrow \mathbf{M} \rightarrow \Gamma$.

Hint: The high symmetry points $\Gamma, \mathbf{X}, \mathbf{M}$ in the reciprocal space lattice are

$$\begin{aligned} \Gamma &= (0, 0), \\ \mathbf{X} &= \left(\frac{\pi}{a}, 0\right), \\ \mathbf{M} &= \left(\frac{\pi}{a}, \frac{\pi}{a}\right). \end{aligned}$$

- (d) (optional) Alternatively, consider the following bond-stretching potential:

$$V = \frac{k}{2} \sum_{\langle i,j \rangle} \left[\frac{\mathbf{R}_i - \mathbf{R}_j}{\|\mathbf{R}_i - \mathbf{R}_j\|} \cdot (\mathbf{u}_i - \mathbf{u}_j) \right]^2.$$

Is the 2d square lattice stable with this potential? And by extending the sum to second nearest neighbours (diagonals)?

Follow again steps (a)-(c) for this potential in the case of 1st nearest neighbour coupling and then for 1st + 2nd nearest neighbour coupling. Compare the three different results obtained.

Assignments to Solid State Theory I

G. Cuniberti (Phy 4.1.29)
F. Pump (Phy 4.1.30)

Room Phy 7.1.21, h 10.15
Tue 03.05.2005 (**Sheet 3**)

sheet online: <http://www-MCG.uni-R.de/teaching/>

Problem set: Second quantization I (bosonic gymnastic)**3.1. Bosonic commutation relations**

Refresh the physics of the simple harmonic oscillator

$$\hat{H} = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2},$$

which can be written in “second quantized” form, by expressing x and p in terms of *boson* creation and annihilation operators:

$$\hat{H} = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right), \quad a^\dagger = \frac{1}{\sqrt{2\hbar}} \left(\sqrt{m\omega} \hat{x} - i \frac{\hat{p}}{\sqrt{m\omega}} \right).$$

(a) Show that the following basis commutation relations hold

$$[a, a^\dagger] = 1, \quad [a, a] = 0, \quad a|0\rangle = 0$$

where $[A, B] = AB - BA$, $|0\rangle$ the vacuum, and \dagger indicates the Hilbert space adjoint. From these, determine all normalized eigenstates $|n\rangle$ ($\langle n, m | = \delta_{nm}$) of $a^\dagger a$, and show that they have the following properties,

$$\begin{aligned} a^\dagger a |n\rangle &= n |n\rangle, \quad n = 0, 1, 2, \dots \\ a |n\rangle &= \sqrt{n} |n-1\rangle, \\ a^\dagger |n\rangle &= \sqrt{n+1} |n+1\rangle. \end{aligned}$$

(b) Compute $F = -k_B T \log Z$ with

$$Z = \text{Tr} \left\{ \exp -\frac{\hbar\omega}{k_B T} \left(a^\dagger a + \frac{1}{2} \right) \right\} = \sum_n \left\langle n, \exp \left[-\frac{\hbar\omega}{k_B T} \left(a^\dagger a + \frac{1}{2} \right) \right] n \right\rangle$$

3.2. Calculating with bosonic operators I

(a) Show that for two non commuting bosonic operators A , and B it holds

$$[A, B^n] = \sum_{k=0}^{n-1} B^k [A, B] B^{n-1-k}.$$

(b) Prove —using (a)— that for bosonic operators b, b^\dagger

$$\begin{aligned} [b, (b^\dagger)^n] &= n(b^\dagger)^{n-1} = \frac{\partial (b^\dagger)^n}{\partial b^\dagger}, \\ [b^\dagger, b^n] &= -nb^{n-1} = -\frac{\partial b^n}{\partial b}, \\ [b, f(b^\dagger)] &= \frac{\partial f(b^\dagger)}{\partial b^\dagger}, \\ [b^\dagger, f(b)] &= -\frac{\partial f(b)}{\partial b}, \end{aligned}$$

where the functions $f(b^\dagger)$ and $f(b)$ are representable as a power series ($[b, b^\dagger] = 1$).

3.3. Calculating with bosonic operators II (optional)

(a) Using the previous arguments (Ex 3.3) show that the following relations hold

$$g_1(\alpha; b, b^\dagger) = e^{-\alpha b^\dagger} b e^{\alpha b^\dagger} = b + \alpha, \quad h_1(\alpha; b, b^\dagger) = e^{-\alpha b} b^\dagger e^{\alpha b} = b^\dagger - \alpha.$$

In a similar fashion, simplify the following expressions

$$\begin{aligned} g_2(\alpha; b, b^\dagger) &= e^{-(\alpha^* b^\dagger - \alpha b)} b e^{(\alpha^* b^\dagger - \alpha b)}, & h_2(\alpha; b, b^\dagger) &= e^{-(\alpha^* b^\dagger - \alpha b)} b^\dagger e^{(\alpha^* b^\dagger - \alpha b)}, \\ g_3(\alpha; b, b^\dagger) &= e^{-\alpha b^\dagger b} b e^{\alpha b^\dagger b}, & h_3(\alpha; b, b^\dagger) &= e^{-\alpha b^\dagger b} b^\dagger e^{\alpha b^\dagger b}. \end{aligned}$$

Hint: Introduce a dummy variable λ as in

$$g_i(\lambda, \alpha; b, b^\dagger) = e^{-\lambda f(\alpha; b, b^\dagger)} b e^{\lambda f(\alpha; b, b^\dagger)}$$

and calculate the derivative $\partial g_i(\lambda, \alpha; b, b^\dagger) / \partial \lambda$. Same thing for $h_i(\lambda, \alpha; b, b^\dagger)$.

(b) Deduce the results in (a) from the differential equations for g_i and h_i , obtained by differentiating g_i and h_i with respect to α .

(c) Prove the relation

$$e^{-\alpha b^\dagger} e^{\beta b} e^{\alpha b^\dagger} = e^{\beta \alpha} e^{\beta b}$$

(d) Prove the identity

$$e^{\alpha b^\dagger} e^{\beta b} = \exp\left(\alpha b^\dagger + \beta b - \frac{\alpha \beta}{2}\right)$$

Hint: Show first that the quantity

$$f(\lambda) = e^{\lambda \alpha b^\dagger} e^{\lambda \beta b} e^{\lambda^2 \frac{\alpha \beta}{2}}$$

satisfies the following relation

$$\frac{\partial f(\lambda)}{\partial \lambda} = (\alpha b^\dagger + \beta b) f(\lambda).$$

Assignments to Solid State Theory I

G. Cuniberti (Phy 4.1.29)
 F. Pump (Phy 4.1.30)

Room Phy H 33, h 13.15
 Fri 20.05.2005 (Sheet 4)

sheet online: <http://www-MCG.uni-R.de/teaching/>

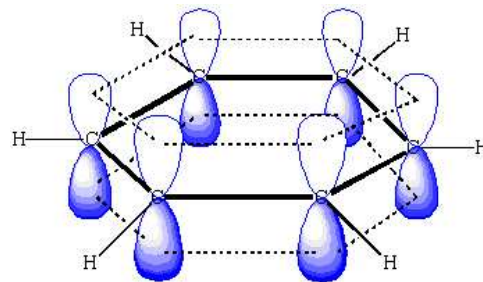
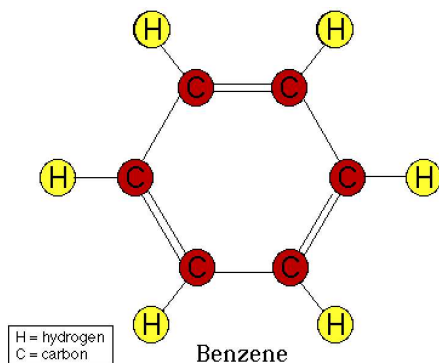
Problem set: From Molecular Orbitals to Bloch states

4.1. The electron-problem for the benzene molecule (tight binding model)

A benzene molecule consists of a ring of six carbon atoms each accompanied by one hydrogen atom, whereas all atoms are arranged in one plane (as depicted in the left figure below). We consider here only the electronic problem which is separated from the motion of the nuclei. Therefore we assume all the atoms to be in equilibrium position. The carbon atoms are in the corners of a regular hexagon, given by the coordinates \mathbf{R}_i ($i = 1, \dots, 6$).

Each C-atom is bonded to its two neighboring C-atoms via σ -bonds, which are built of hybridized $2s$, $2p_x$ and $2p_y$ orbitals from the two C-atoms. Furthermore each C-atom is bonded to an H-atom by the overlap of another hybridized C-orbital and an $1s$ orbital of the H-atom.

This means that per C-atom remains one $2p_z$ orbital, occupied with one electron. These orbitals are oriented perpendicular to the plane determined by the atoms (see the figure on the right).



The wave functions ϕ_i of these orbitals are localized at the positions of the carbon atom i ($i = 1, \dots, 6$) so that we can write

$$\phi_i(\mathbf{r}) = \phi(\mathbf{r} - \mathbf{R}_i),$$

where $\phi(\mathbf{r})$ is the π orbital wavefunction.

Assume that the wave function for the benzene molecular orbitals is given by a linear combination of these $2p_z$ -wave functions (this principle is called LCAO, Linear Combination of Atomic Orbitals):

$$\Psi = \sum_{i=1}^6 c_i \phi_i.$$

The single particle Hamiltonian in the π orbital base is determined by the on-site energy ε and the nearest neighbor interaction t , so that the Hamiltonian can be written as follows

$$H_{i,j} = \varepsilon\delta_{i,j} - t\delta_{i,j+1} - t\delta_{i,j-1}.$$

The Kronecker δ 's should be taken within the periodic boundary conditions: $\delta_{6,0} = \delta_{7,1} = 1$, this means that the ring is closed and the electrons can jump from C-atom 1 to C-atom 6 (and vice versa).

- Find the coefficients c_i in Ψ using the rotational symmetry of the molecule. First show that the Hamiltonian commutes with an operator C describing a rotation about $\frac{\pi}{3}$ and use the fact that the wave functions Ψ are also eigenfunctions of the rotation operator C .
- Solve the eigenvalue/eigenvector problem using the c_i from above and discuss the wave functions with respect to symmetry and nodes.

Hint: Write the Hamiltonian as a matrix and rewrite the Schrödinger equation in matrix representation.

Note: You can also view the problem as a tight binding linear chain of $N = 6$ atoms with periodic boundary conditions. Use Bloch theorem to diagonalize H analytically.

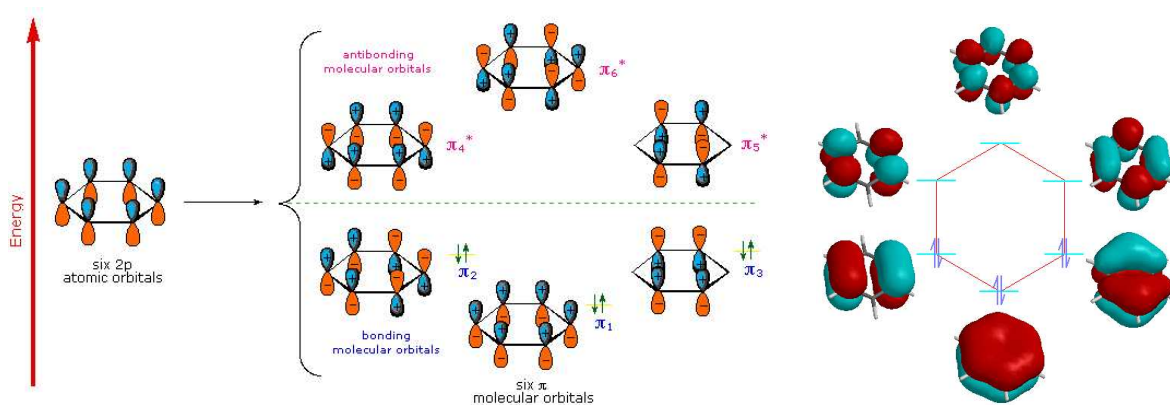
- Using a plotting program draw the molecular orbitals for the different eigenenergies knowing the formal expression of the π orbital (in polar coordinates):

$$\phi(\mathbf{r}) = \phi(r, \theta, \varphi) \propto r \cdot \exp(-\zeta r) \cos \theta,$$

where $\zeta = 16.18 \text{ nm}^{-1}$.

Note that the eigenvalues $\varepsilon \pm t$ are degenerate, how will you choose the eigenfunctions in that case?

You should finally be able to reproduce the plot in the figure below on the right.



4.2. The Kronig-Penney model

The Kronig-Penney model (the Dirac comb) is a simple one-dimensional model to understand the electronic band structure of a crystalline solid.

A periodic 1d crystal potential (with the lattice constant a) is approximated by a series of δ -functions:

$$V(x) = V_0 \sum_{n=-\infty}^{+\infty} \delta(x - na), \quad V_0 > 0. \quad (1)$$

As the Hamiltonian $H = p^2/(2m) + V(x)$ is periodic (i.e. H is invariant under translations of multiples of a) all physical properties have to be invariant under these translations, too. This is especially relevant for the electron density:

$$|\Psi(x + a)|^2 = |\Psi(x)|^2.$$

As a consequence,

$$\Psi(x + a) = \exp(iqa) \cdot \Psi(x).$$

The free parameter q denotes the possible eigenstates (Bloch theorem):

$$\Psi_q(x + a) = \exp(iqa) \cdot \Psi_q(x).$$

- (a) Show that the solutions of the Schrödinger equation satisfy the Kronig-Penney equation

$$\cos(qa) = \cos(\alpha_q) + P \frac{\sin(\alpha_q)}{\alpha_q}$$

with $P = \frac{V_0 m a}{\hbar}$ and $\alpha_q^2 = \frac{2mE_q}{\hbar^2} a^2$.

Hint: Solve the Schrödinger equation in regions with $V(x) = 0$ using the ansatz

$$\Psi_q(x) = A \exp(ikx) + B \exp(-ikx) \quad \text{with} \quad k^2 = \frac{2mE_q}{\hbar^2}.$$

Use the Bloch theorem, the continuity of $\Psi_q(x)$ and the discontinuity of $\partial_x \Psi_q(x)$ at $x = na$ to determine the coefficients A and B .

- (b) Plot $f(\alpha_q) = \cos(\alpha_q) + P \frac{\sin(\alpha_q)}{\alpha_q}$ as a function of α_q . Show that for $V_0 \neq 0$, the Kronig-Penney equation $\cos(qa) = f(\alpha_q)$ leads to forbidden energy regions (energy gaps).
- (c) The original version of the Kronig-Penney model was formulated for a periodic potential of rectangular scatterers. Repeat the previous calculations by replacing the delta distributions in (1) with the following step function

$$s(x; b) = \begin{cases} \frac{1}{b} & \text{if } |x| < \frac{b}{2} \\ 0 & \text{elsewhere} \end{cases}$$

so that the potential $V(x)$ now reads

$$V(x) = V_0 \sum_{n=-\infty}^{+\infty} s(x - na; b), \quad V_0 > 0, \quad b < a.$$

Assignments to Solid State Theory I

G. Cuniberti (Phy 4.1.29)
F. Pump (Phy 4.1.30)

Room Phy 7.1.21, h 10.15
Tue 24.05.2005 (**Sheet 5**)

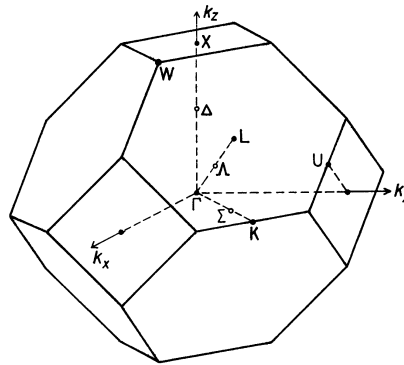
sheet online: <http://www-MCG.uni-R.de/teaching/>

Problem set: Band structure I: the fcc lattice**5.1. Electronic structure for free electrons in a fcc lattice**

Consider the general form for the energy bands of a free electron in a crystal

$$\varepsilon_n(\mathbf{k}) = \frac{\hbar^2(\mathbf{k} + \mathbf{G}_n)^2}{2m},$$

where n is the band index and \mathbf{G}_n a reciprocal lattice vector, and m the electron mass. The first Brillouin-zone of a fcc crystal is shown in the following figure.



- (a) Calculate, in the free electron approximation, the energy bands of an fcc crystal in the following cases: In the $[001]$ -direction, which is given by

$$\Gamma X := (k_x = k_y = 0, k_z = \xi \frac{2\pi}{a}, \text{ with } 0 \leq \xi \leq 1),$$

for the following \mathbf{G} -vectors

- i. $\mathbf{G} = 0$ (Γ point).
- ii. \mathbf{G} as Γ nearest neighbor.
- iii. \mathbf{G} as Γ second nearest neighbor.

Plot for the corresponding cases the energy bands.

- (b) Repeat the same calculation for the $[111]$ -direction given by

$$\Gamma L := (k_x = k_y = k_z = \xi \frac{2\pi}{a}, \text{ with } 0 \leq \xi \leq \frac{1}{2}).$$

- (c) Calculate the ratio of the bandwidth for the energetically smallest band along $[001]$ and $[111]$, which is defined by

$$\Theta_{\text{FE}} = \frac{E(X) - E(\Gamma)}{E(L) - E(\Gamma)}.$$

5.2. Tight binding s -bands in fcc crystals

The equation for determining the energy of a crystal band in the tight binding approximation can be represented by means of a development into single atomic orbitals

$$[\varepsilon_{\text{AT}} - \varepsilon(\mathbf{k})] S(\mathbf{k}) + A(\mathbf{k}) = 0 . \quad (2)$$

Where ε_{AT} is the energy level of the considered atomic orbital and $\varepsilon(\mathbf{k})$ the energy band of the same atomic orbital. In the special case of an atomic s -state (defined via the quantum number j) the Fourier transformed overlap integral is defined via

$$S(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} S(0, \mathbf{R}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \int d^3r \chi_s^*(\mathbf{r}) \chi_s(\mathbf{r} - \mathbf{R}),$$

where $\chi_s(\mathbf{r})$ is the atomic s -wavefunction. Furthermore, the Fourier transformed potential matrix element writes

$$A(\mathbf{k}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} A(0, \mathbf{R}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \int d^3r \chi_s^*(\mathbf{r}) \Delta v(\mathbf{r}) \chi_s(\mathbf{r} - \mathbf{R}),$$

where $\Delta v(\mathbf{r}) = v(\mathbf{r}) - v_{\text{AT}}(\mathbf{r})$, and $v_{\text{AT}}(\mathbf{r})$ is the atomic potential with $\mathbf{R} = 0$ and $v(\mathbf{r})$ is the crystal potential.

- (a) Calculate the general expression for the crystal band energies in Eq. (2) and find the explicit dependence on the *on-site* term ($\mathbf{R} = 0$).
- (b) Determine the band energy of the fcc crystal, by making use of the following two approximations
 - Only the *on-site* contribution of the overlap integral is non vanishing.
 - Only potential matrix elements up to the nearest neighbor are non vanishing.

Hint: Use the symmetry of the lattice and of the s -wavefunction.

- (c) Within the previous two approximations, calculate the explicit form of the energy dispersion for fcc lattices in the following cases:
 - i. Along ΓX .
 - ii. Along ΓL .
 - iii. Along $\Gamma K := (k_z = 0, k_x = k_y = \xi \frac{2\pi}{a}, \text{ with } 0 \leq \xi \leq \frac{3}{4})$.
 - iv. Along $\Gamma W := (k_z = 0, k_x = \xi \frac{2\pi}{a}, k_y = \xi \frac{\pi}{a}, \text{ with } 0 \leq \xi \leq 1)$.
- (d) Show that at the square planar areas of the BZ the orthogonal component of the derivative of $\varepsilon(\mathbf{k})$ vanishes.
- (e) Calculate Θ_{TB} (see question 1.c in the previous exercise) and compare the results with the case for free electrons.

Assignments to Solid State Theory I

G. Cuniberti (Phy 4.1.29)
 F. Pump (Phy 4.1.30)

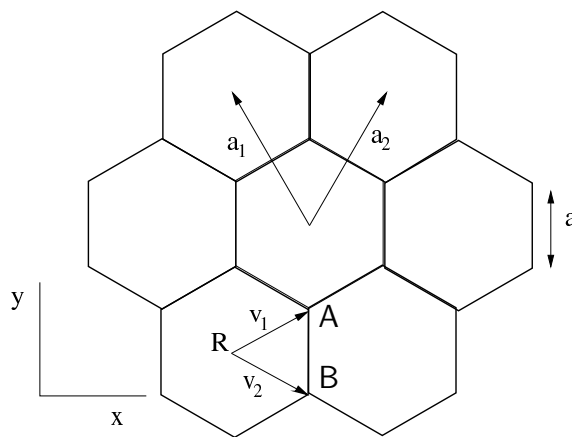
Room Phy 7.1.21, h 10.15
 Tue 31.05.2005 (**Sheet 6**)

sheet online: <http://www-MCG.uni-R.de/teaching/>

Problem set: Band structure II: graphene and carbon nanotubes

6.1. Electronic structure of graphene

A graphene sheet is a honeycomb lattice of carbon atoms (see figure). Let the distance



between carbon atoms be a . A good model for graphene is to consider a single plane in which there is one valence electron per carbon atom. We will use the tight-binding approximation, in which this electron can occupy a single p_z orbital at each carbon site. Let \mathbf{R} denote the centers of the hexagons in the honeycomb: these form the underlying hexagonal Bravais lattice. Please notice that the latter is indeed a Bravais lattice differently from the graphene honeycomb lattice. The unit cell spanned by \mathbf{a}_1 and \mathbf{a}_2 contains two carbon atoms conventionally labelled as A and B atom, located at $\mathbf{R} + \mathbf{v}_A$, $\mathbf{R} + \mathbf{v}_B$, as shown in the figure. Denote the tight-binding hopping amplitude connecting these sites by t . Choose the zero of energy so that the energy of an isolated atomic orbital is zero. The entire Hamiltonian consists of the nearest-neighbor hopping.

- Find the reciprocal lattice, and construct the first Brillouin zone.
- Write down the tight-binding equations governing the system. How many bands do you find? What are the energy-wavevector relations?

Hint: You will need to solve a two-by-two matrix eigenvalue problem. This exercise was first attacked by Wallace in 1947.³

³You might want to read the original paper “P. R. Wallace, Phys. Rev. **71**, 622 (1947)”. It is available online (when logged in the [uni-r.de](http://www.uni-r.de) domain) under <http://link.aps.org/abstract/PR/v71/p622> . Alternatively you can refer to some more recent formulation as, e.g., in Section 2.4 “Band structure of graphene” of Dr. Hauptmann’s PhD thesis (<http://www.nbi.dk/~nygard/JonasSpeciale2003.pdf>).

- (c) Show that the Fermi energy is equal to zero, by verifying that this gives the correct electron density. Find the set of \mathbf{k} points for which $\varepsilon(\mathbf{k}) = 0$. Show that these correspond to the corners of the first Brillouin zone.
- (d) Show that, near to a (first) Brillouin zone corner with wavevector \mathbf{K} (note that \mathbf{K} is the location of a BZ corner, not a reciprocal lattice vector), the spectrum is approximately

$$\varepsilon(\mathbf{k}) \approx \pm v \sqrt{(k_x - K_x)^2 + (k_y - K_y)^2}.$$

Determine the velocity v in terms of t and a . This behavior is intermediate between a metal (with a Fermi surface instead of points \mathbf{K}) and an insulator (with a band gap). Indeed, graphite behaves as a semi-metal, with poor conductivity significantly higher than in an insulator.

- (e) **optional**: Graphite is composed of a stack of graphene layers identically atop one another in the z direction (a distance d apart), and there is some small residual hopping t_{\perp} between orbitals in neighboring layers at the same (x, y) position. Sketch the Fermi surface, assuming $t_{\perp} \ll t$.

6.2. Electronic structure of single wall carbon nanotubes

Carbon nanotubes Carbon nanotubes are made up of a section of the graphene lattice that has been wrapped up into a cylinder. You can specify the way the lattice is wound up by identifying the winding vector \mathbf{W} . The winding vector must be a Bravais lattice vector, and so can be specified by two integers:

$$\mathbf{W} = n \mathbf{a}_1 + m \mathbf{a}_2,$$

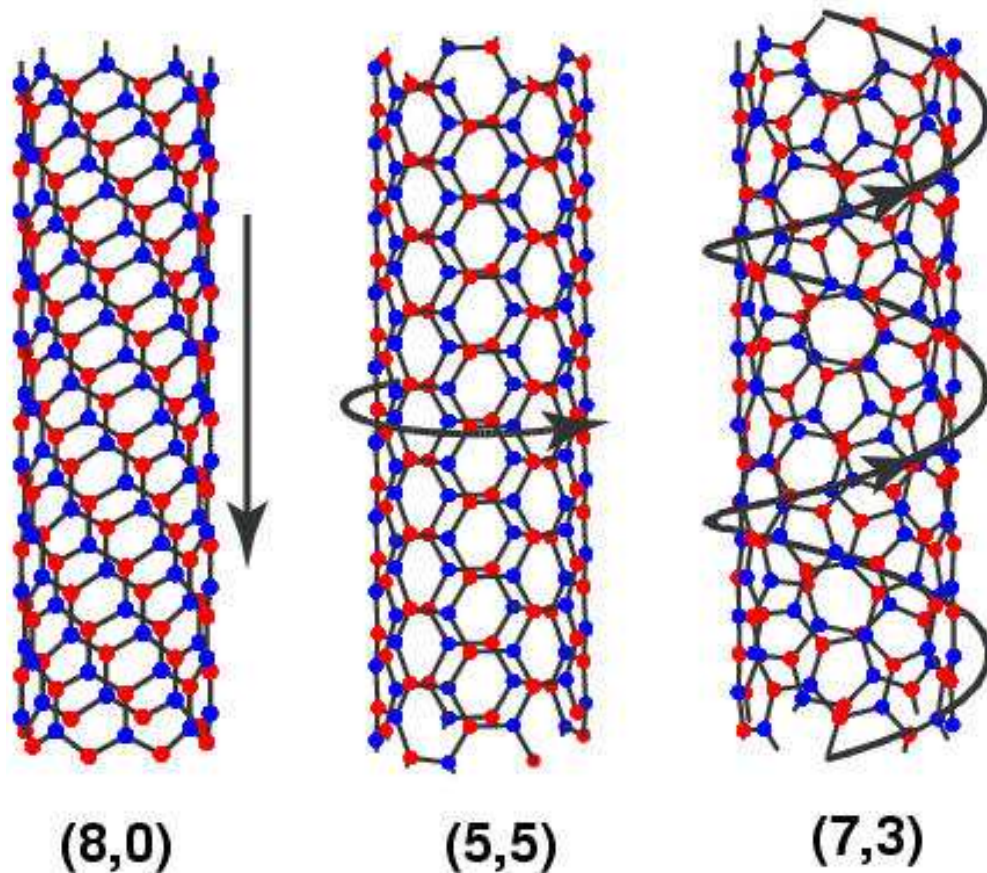
where n and m are integers. To construct a nanotube, take a graphene lattice and mark one atom (either A type or B type) as the origin. Shift the origin of the vector \mathbf{W} on the chosen atom. The new vector $\tilde{\mathbf{W}}$ will point to another atom of the same type. Roll up the sheet perpendicular to $\tilde{\mathbf{W}}$ so that the second atom sits exactly on top of the first. You have constructed a (n, m) nanotube!

A bit of nomenclature. We can specify some special tubes said *achiral*: they are (n, n) tubes which are called *armchair* tubes, and $(n, 0)$ *zig-zag* tubes (Bruckmandl would be probably more appropriate, but there is no mention of this in the literature yet...). All other tubes are said *chiral*.

- (a) Build a $(5, 5)$ armchair tube (*i.e.* with scissors and adhesive tape!) by making use of the provided transparencies.⁴
- (b) Construct a $(8, 0)$ zig-zag tube.
- (c) Build a chiral $(7, 3)$ tube.

⁴A pdf is also available under the following (clickable) link <http://www-MCG.uni-R.de/downloads/graphene.pdf>.

- (d) Let's determine the band structure of a nanotube. To do so, impose periodic boundary conditions on the wavefunction in the direction around the cylinder. Show that this means that $\mathbf{k} \cdot \mathbf{W} = 2\pi\ell$, where ℓ is an integer.
- (e) Draw the graphene first Brillouin zone from the previous problem, indicating (a) the points \mathbf{K} (where the energy of the graphene layer is zero, $E = E_F$) and (b) the lines given by the quantization conditions –introduced in the previous point– for $(n, m) = (3, 3)$ and $(n, m) = (2, 0)$.
- (f) Plot the energy versus k_x for the allowed values of k_y in the (3,3) tube above. Then plot the energy versus versus k_y for the allowed values of k_x in the (2, 0) tube.
- For each case, is the nanotube metallic or insulating according to band theory?
- (g) For which n and m are the Brillouin zone corners allowed wavevectors for a nanotube? Show that the tubes satisfying this condition are metallic!
- (h) **optional:** In reality, one expects that the curvature of the nanotube cylinder affects the tight-binding matrix elements slightly. Consider this effect for the special cases of armchair, and zig-zag tubes. In these cases, the curvature effect can be modeled by making the hopping matrix element slightly different ($= t'$) on transversal bonds (parallel to the winding vector in the case of the armchair tubes) than the other ones ($= t$). How does this affect the metallicity of the armchair and zig-zag tubes?



Assignments to Solid State Theory I

G. Cuniberti (Phy 4.1.29)
 N. Nemeč (Phy 4.1.30)

Room Phy 7.1.21, h 10.15
 Tue 07.06.2005 (**Sheet 7**)

sheet online: <http://www-MCG.uni-R.de/teaching/>

Problem set: Electronic Density of States

Consider the general definition of d -dimensional density of states (DOS) for one band $E(\mathbf{k})$

$$\begin{aligned}
 g(E_0) &= \frac{1}{N} \sum_{\mathbf{k}\sigma} \delta(E - E(\mathbf{k})) = \frac{2}{N} \sum_{\mathbf{k}} \delta(E - E(\mathbf{k})) \\
 &= \frac{2V}{N} \int_{\text{1.BZ}} \frac{d^d \mathbf{k}}{(2\pi)^d} \delta(E_0 - E(\mathbf{k})) = \frac{2V}{N} \int_{S(E_0)} \frac{dS}{(2\pi)^d} \frac{1}{|\partial E(\mathbf{k})/\partial \mathbf{k}|} \quad (3)
 \end{aligned}$$

where the prefactor two indicates the spin-degeneracy and $S(E_0)$ is the isosurface the reciprocal space defined by $E(\mathbf{k}) = E_0$.

7.1. Electrons in the continuum

Calculate the DOS for different analytically-known energy dispersions.

(a) *Massive and massless free particles in d dimensions*

Calculate the density of states $g(E)$ for massless and massive particles in $d = 1, 2$ and 3 dimensions, and prove the the following results.

	$d = 1$	$d = 2$	$d = 3$
massless ($E \sim k$)	$g(E) = \text{const}$	$g(E) \sim E$	$g(E) \sim E^2$
massive ($E \sim k^2$)	$g(E) \sim 1/\sqrt{E}$	$g(E) = \text{const}$	$g(E) \sim \sqrt{E}$

(b) *DOS in superconductors*

In the BCS-theory of superconductivity⁵ the excitation spectrum of single-electron states is given by:

$$E(\mathbf{k}) = E_F + \text{sign}(\varepsilon(\mathbf{k}) - E_F) \sqrt{(\varepsilon(\mathbf{k}) - E_F)^2 + \Delta(\mathbf{k})^2}$$

where $\varepsilon(\mathbf{k})$ is the electron energy in absence of superconductivity and E_F is the Fermi energy. A simplified interaction leads to constant $\Delta(\mathbf{k}) = \Delta$. Starting from the DOS of the system without superconductance $g(\varepsilon)$, calculate the DOS of the full system $g'(E)$, assuming that E_F is not close to a band-edge.

Hint: Consider the integral-definition of the DOS: For constant Δ , the problem boils down to a change of variables...

⁵J. Bardeen and L. N. Cooper and J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957); *ibid.* **106**, 162 (1957).

(c) *Hybridized states*

If electrons can jump between a broad band (described by $E_c(\mathbf{k})$) and a narrow energy level at E_0 , then the band structure exhibits signs of *hybridization*: A mixing of electronic states when the $E_c(\mathbf{k})$ and the E_0 energies are close. In a simple model, the hybridized energy levels can be calculated as

$$E'(\mathbf{k}) = (E_c(\mathbf{k}) + E_0)/2 \pm \sqrt{(E_c(\mathbf{k}) - E_0)^2/4 + \Delta^2}$$

where Δ is the coupling parameter, proportional to the probability of hopping events per time.

Assume that the broad band has the constant DOS $g_c(E) = g_0$ for $E_1 < E < E_2$ (with the *bandwidth* $W = E_2 - E_1$) and $g_c(E) = 0$ otherwise. The DOS of the narrow band is sharply peaked with the same total number of states: $g = g_0 W \delta(E - E_0)$. Calculate the DOS for the hybridized system.

(d) *Two dimensional electron gas (2DEG)*

The dimensionality of a real electron system can be reduced by confining potentials in certain directions. Consider an electron gas in the potential

$$V(x, y, z) = V_0 \Theta(|z| - \ell/2).$$

- Plot the DOS in the limit $V_0 \rightarrow \infty$?
- Assume $\ell = 10$ nm. Up to which temperature T can we consider the electrons to be two-dimensional?
- If we can produce a potential with $V_0 = 100$ meV and reach $T = 20$ mK, for which range of thicknesses ℓ can we consider the system a 2DEG?

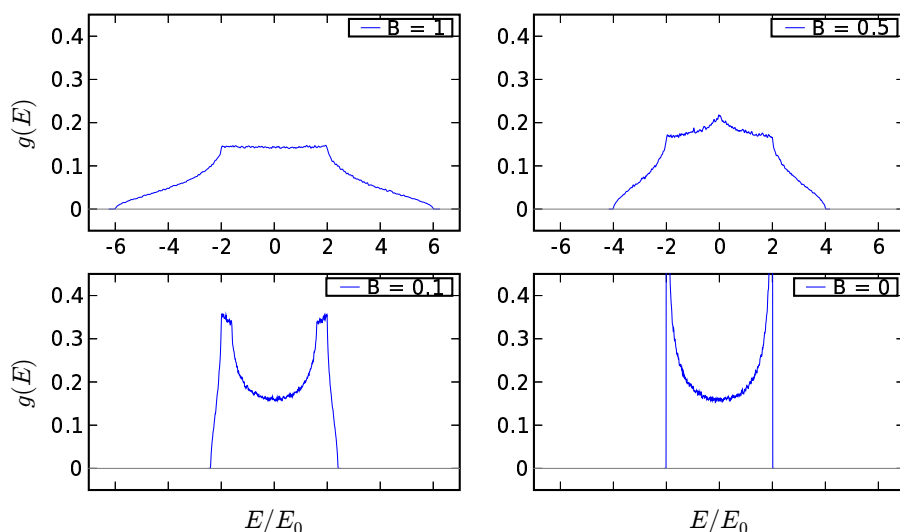
7.2. Tight binding electrons

The energy band of an anisotropic orthorhombic lattice in the s-orbital tight-binding approximation leads to the following dispersion relation

$$E(\mathbf{k}) = -\frac{E_0}{2} [A_x \cos(k_x a_x) + A_y \cos(k_y a_y) + A_z \cos(k_z a_z)],$$

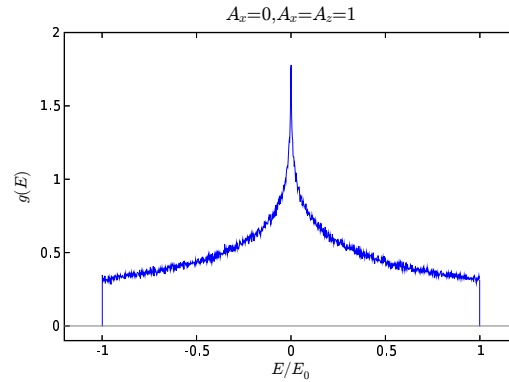
($E_0 = 1$ eV defines the energy scale). We want to investigate the crossover between $d = 1$ and $d = 3$ electron systems, so we assume $A_x = 1, A_y = A_z = B \in [0, 1]$.

The figure below shows the DOS calculated numerically for different values of B by statistical integration of Eq. (3).



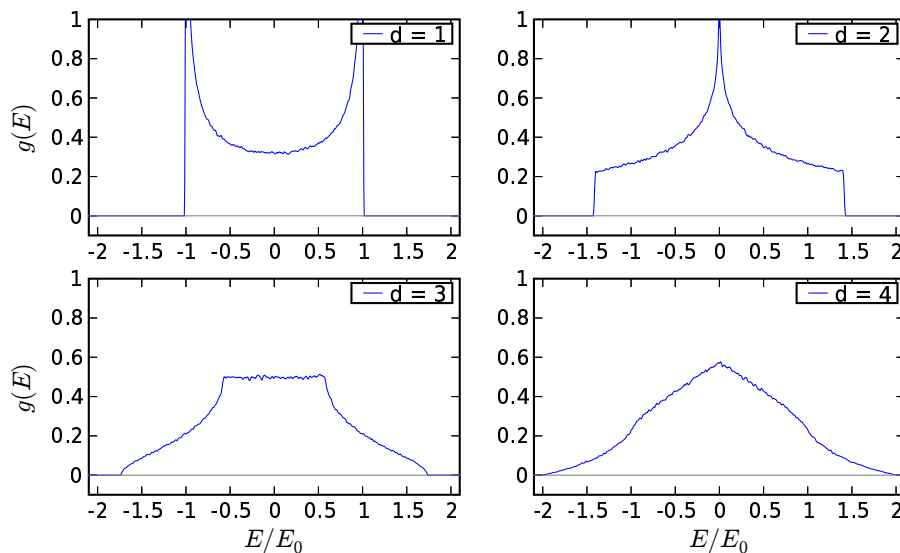
- Consider $B \ll 1$: What is the shape of the energy isolines cuts in the k_x - k_y -plane?
- Show that for a half-filled band the DOS (and therefore thermodynamic properties like total energy, total number of electrons and specific heat) of this system are similar to a truly one-dimensional electron gas.
Hint: A simple approximation of the isolines at $E = 0$ allows direct integration.
- For low electron densities, the system differs considerably from a truly 1D system even at low B . Estimate the electron density, at which the crossover happens.
- Compare the behavior at the band edge between $d = 1$ and $d = 3$ system.

- (e) Consider now the case $A_x = 0$ and $A_y = A_z = 1$ as shown below and explain the behavior of the DOS around $E = 0$!



7.3. Infinite dimensional DOS (optional)

The figure below shows the DOS for an isotropic tight-binding lattice in $d = 1, 2, 3, 4$ dimensions. The bandwidth is set to \sqrt{d} . What is the DOS for $d \rightarrow \infty$? Why has the bandwidth to be scaled like \sqrt{d} ? What is its physical meaning? ⁶



Hint: Consider calculating the problem via Monte Carlo integration: The integration variables $\mathbf{k} = (k_1, k_2, \dots, k_d)$ are turned into independent uniformly distributed random variables in the interval $[0, 2\pi/a]$. The DOS $g(k)$ is the distribution of the sum $E(\mathbf{k}) = \frac{E_0}{2\sqrt{d}} \sum_1^d (-\cos k_i a)$ which, for $d \rightarrow \infty$, follows the *central limit theorem*.

⁶W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62**, 324 (1989).

Assignments to Solid State Theory I

G. Cuniberti (Phy 4.1.29)
 N. Nemeč (Phy 4.1.30)

Room Phy 7.1.21, h 10.15
 Tue 21.06.2005 (**Sheet 8**)

sheet online: <http://www-MCG.uni-R.de/teaching/>

Problem set: Second quantization II (fermionic gymnastic)**8.1. Fermionic commutation relations**

The basis commutation relations for fermion creation and annihilation operators

$$[a, a^\dagger]_+ = 1, \quad [a, a]_+ = 0, \quad a|0\rangle = 0$$

where $[A, B]_+ = AB + BA$, $|0\rangle$ the vacuum, and \dagger indicates the Hilbert space adjoint.

- (a) From these, determine all normalized eigenstates $|n\rangle$ of $a^\dagger a$, and show that they have the following properties,

$$\begin{aligned} a^\dagger a |n\rangle &= n |n\rangle, \quad n = 0, 1 \\ a |1\rangle &= |0\rangle, \\ a^\dagger |0\rangle &= |1\rangle, \\ \langle n, m \rangle &= \delta_{nm} \end{aligned}$$

- (b) Compute $F = -k_B T \log Z$ with

$$Z = \text{Tr} \left\{ \exp \left(-\frac{\hbar\omega}{k_B T} a^\dagger a \right) \right\} = \sum_n \left\langle n, \exp \left(-\frac{\hbar\omega}{k_B T} a^\dagger a \right) n \right\rangle$$

8.2. Yukawa-correlated fermions

Consider a system of fermions created by the field $\psi^\dagger(\mathbf{r})$ interacting under the Yukawa potential

$$V_Y(\mathbf{r}) \equiv V_Y(r) = \frac{A}{r} \exp(-\alpha r) \quad (\alpha > 0)$$

- (a) Write the Hamiltonian in second quantized form, using the position basis.
 (b) Write the Hamiltonian in second quantized notation in the momentum basis, where

$$c_{\mathbf{k}}^\dagger = \int d^3r \psi^\dagger(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}.$$

Hint: You will find it helpful to derive the Fourier representation

$$V_Y(\mathbf{r}) = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi A}{(q^2 + \alpha^2)}.$$

8.3. Calculating with fermion operators

- (a) Similarly to exercise 3.3, simplify the following expressions involving the fermionic operators a , and a^\dagger

$$\begin{aligned} g_1(\alpha; a, a^\dagger) &= e^{-\alpha a^\dagger} a e^{\alpha a^\dagger}, & h_1(\alpha; a, a^\dagger) &= e^{-\alpha a} a^\dagger e^{\alpha a}, \\ g_2(\alpha; a, a^\dagger) &= e^{-(\alpha^* a^\dagger - \alpha a)} a e^{(\alpha^* a^\dagger - \alpha a)}, & h_2(\alpha; a, a^\dagger) &= e^{-(\alpha^* a^\dagger - \alpha a)} a^\dagger e^{(\alpha^* a^\dagger - \alpha a)}, \\ g_3(\alpha; a, a^\dagger) &= e^{-\alpha a^\dagger a} a e^{\alpha a^\dagger a}, & h_3(\alpha; a, a^\dagger) &= e^{-\alpha a^\dagger a} a^\dagger e^{\alpha a^\dagger a}. \end{aligned}$$

- (b) Show that the operators s^+ , s^- , and s^z , defined in terms of the fermionic operators $a_{\uparrow,\downarrow}^\dagger$ and $a_{\uparrow,\downarrow}$ (the indices \uparrow, \downarrow characterize the electron possible spin states)

$$\begin{aligned} s^+ &= \hbar a_{\uparrow}^\dagger a_{\downarrow} \\ s^- &= \hbar a_{\downarrow}^\dagger a_{\uparrow} \\ s^z &= \frac{\hbar}{2} (a_{\uparrow}^\dagger a_{\uparrow} - a_{\downarrow}^\dagger a_{\downarrow}) \end{aligned}$$

satisfy the commutation relations for spin components, that is

$$\begin{aligned} [s^+, s^-] &= 2\hbar s^z \\ [s^\pm, s^z] &= \mp \hbar s^\pm \end{aligned}$$

Hint: Use the fact that

$$\begin{aligned} [A, BC] &= [A, B]C + B[A, C] \\ [AB, C] &= A[B, C] + [A, C]B \end{aligned}$$

Assignments to Solid State Theory I

G. Cuniberti (Phy 4.1.29)

Room Phy 7.1.21, h 10.15

R. Heid, R. Gutierrez (Phy 4.1.38)

Tue 28.06.2005 (**Sheet 9**)sheet online: <http://www-MCG.uni-R.de/teaching/>**Problem set: Screening and Peierls instability****9.1. The dielectric function**

Consider an electron system which is subject to a small external potential $\Phi^{\text{ext}}(\mathbf{r})$ generated by an external charge density $\rho^{\text{ext}}(\mathbf{r})$. This perturbation induces an electronic charge density $\rho^{\text{ind}}(\mathbf{r})$ and a corresponding potential $\Phi^{\text{ind}}(\mathbf{r})$. Recall from electrodynamics, that when using Fourier-transformed quantities like $\rho^{\text{ind}}(\mathbf{q}) = \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \rho^{\text{ind}}(\mathbf{r})$, a potential is related to the generating charge density by the Poisson equation as $q^2\Phi(\mathbf{q}) = 4\pi\rho(\mathbf{q})$. For small external potentials the following approximate relation holds (linear response):

$$\begin{aligned}\Phi^{\text{ext}}(\mathbf{q}) &= \epsilon(\mathbf{q})\Phi^{\text{tot}}(\mathbf{q}) \\ \rho^{\text{ind}}(\mathbf{q}) &= \chi(\mathbf{q})\Phi^{\text{tot}}(\mathbf{q}),\end{aligned}\quad (4)$$

where $\Phi^{\text{tot}} = \Phi^{\text{ext}} + \Phi^{\text{ind}}$ is the total potential felt by the electrons. Eqs. (4) define the static dielectric function $\epsilon(\mathbf{q})$ and the static susceptibility $\chi(\mathbf{q})$.

- Derive a relationship between $\epsilon(\mathbf{q})$ and $\chi(\mathbf{q})$.
- Obtain an expression for the static susceptibility in terms of the electronic properties for a free electron gas. Start with the expression for the charge density

$$\rho(\mathbf{r}) = -2e \sum_{\mathbf{k}} f_{\mathbf{k}} \left| \tilde{\psi}_{\mathbf{k}}(\mathbf{r}) \right|^2, \quad (5)$$

where $f_{\mathbf{k}} = f(E_{\mathbf{k}}) = 1/(1+e^{(E_{\mathbf{k}}-E_{\text{F}})/(k_{\text{B}}T)})$ is the Fermi function. The electronic wave function in the presence of the perturbation $H_1 = -e\Phi^{\text{tot}}(\mathbf{r})$ is given in first-order perturbation theory by

$$\tilde{\psi}_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r}) + \sum_{\mathbf{k}' \neq \mathbf{k}} \psi_{\mathbf{k}'}(\mathbf{r}) \frac{\langle \psi_{\mathbf{k}'} | H_1 | \psi_{\mathbf{k}} \rangle}{E_{\mathbf{k}} - E_{\mathbf{k}'}} \quad (6)$$

Evaluate the matrix elements for a free electron gas, and show that the static susceptibility can be expressed as

$$\chi(\mathbf{q}, T) = 2e^2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}}} \quad (7)$$

(c) Show that for $|\mathbf{q}| \rightarrow 0$ and $T \rightarrow 0$, the susceptibility approaches the limit

$$\chi \rightarrow -e^2 g(E_F) \quad (8)$$

where $g(E_F)$ is the electronic density of states at the Fermi energy.

Hint: Calculate first the limit $|\mathbf{q}| \rightarrow 0$ and then use the relation $\partial f / \partial E \approx -\delta(E - E_F)$ for $T \rightarrow 0$.

9.2. Linear response of the one-dimensional electron gas

Consider free electrons in one dimension with dispersion relation $E_k = \frac{\hbar^2 k^2}{2m}$. Similarly to Eq. (7), the static susceptibility in one dimension is given by

$$\chi(q, T) = 2e^2 \int \frac{dk}{2\pi} \frac{f_k - f_{k+q}}{E_k - E_{k+q}} \quad (9)$$

- Calculate $\chi(q, T)$ for $T = 0$, where the Fermi function is just a step function. Verify explicitly that for $q \rightarrow 0$, $\chi(q) \rightarrow -e^2 g(E_F)$.
- Plot the ratio $\chi(q, T) / \chi(0)$ for $T = 0$ as function of the reduced variable $x = q / (2k_F)$ with k_F the Fermi wavevector ($E_F = \frac{\hbar^2 k_F^2}{2m}$). What is the behavior at $x = 1$?
- Replace the quadratic dispersion relation $E_k = \frac{\hbar^2 k^2}{2m}$ by a linearized one of the form

$$\tilde{E}_k - E_F = c(|k| - k_F) \quad (10)$$

Determine c by the requirement that both dispersion relations should have the same derivative at k_F .

With this linearized dispersion relation, calculate $\chi(q, T)$ for $q = 2k_F$ for temperatures $T \ll E_F / k_B$ and show that it diverges logarithmically for $T \rightarrow 0^+$.

Hint: Use the relations $\tilde{E}_{k+2k_F} - E_F = -(\tilde{E}_k - E_F)$ and the asymptotic behavior $\int_0^y dx \frac{\tanh x}{x} \approx \ln y + C$ for $y \gg 1$, with $C \approx \ln(2.268)$

- Calculate and plot $\chi(q, T)$ for arbitrary q for the set of temperatures given by $E_F / (k_B T) = 4, 16, 64, 256$ by numerically integrating Eq. (9).

9.3. Coupled electronic bands (optional)

Consider the following model Hamiltonian of two electronic coupled bands in one dimension

$$H = \sum_k \left\{ \epsilon_k (c_{1k}^\dagger c_{1k} - c_{2k}^\dagger c_{2k}) + \Delta (c_{1k}^\dagger c_{2k} + c_{2k}^\dagger c_{1k}) \right\} \quad (11)$$

where the (positive real) quantity Δ describes a k -independent coupling energy. Consider new fermionic operators defined by

$$\gamma_{1k} = u_k c_{1k} - v_k c_{2k}; \quad \gamma_{2k} = v_k c_{1k} + u_k c_{2k} \quad (12)$$

with real numbers u_k and v_k .

- (a) Derive a relation between u_k and v_k , for which the new operators obey the standard fermionic anticommutation relations $[\gamma_{ik}, \gamma_{jl}^\dagger]_+ = \delta_{ij} \delta_{kl}$ and $[\gamma_{ik}, \gamma_{jl}]_+ = [\gamma_{ik}^\dagger, \gamma_{jl}^\dagger]_+ = 0$.
- (b) Diagonalize the Hamiltonian by expressing H in terms of the new fermionic operators. Under which condition do the off-diagonal couplings vanish? Derive an expression for the effective band energies of the new operators.
- (c) For a linear dispersion $\epsilon_k = \hbar v_F k$, show that the energy spectrum shows a gap of size 2Δ .

Note: The model Hamiltonian appears in the mean-field description of the low-temperature Peierls-distorted linear chain.

Assignments to Solid State Theory I

G. Cuniberti (Phy 4.1.29)
 F. Pump (Phy 4.1.30)

Room Phy 7.1.21, h 10.15
 Tue 11.07.2005 (**Sheet 10**)

sheet online: <http://www-MCG.uni-R.de/teaching/>

Problem set: Density functional theory**10.1. Functional derivatives**

Consider the definition of functional derivative $\delta F[n]/\delta n(\mathbf{r})$ as

$$\lim_{\epsilon \rightarrow 0} \left[\frac{F[n + \epsilon \delta n] - F[n]}{\epsilon} \right] = \int \frac{\delta F[n]}{\delta n(\mathbf{r})} \delta n(\mathbf{r}) \, d\mathbf{r} \quad .$$

Calculate the functional derivative for the following functionals.

- (a) The kinetic energy in the Thomas Fermi approximation

$$T_{\text{TF}}[n] = C \int n^{5/3}(\mathbf{r}) \, d\mathbf{r} \quad .$$

- (b) The Hartree energy

$$E_{\text{H}}[n] = \frac{e^2}{2} \iint \frac{n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, d\mathbf{r} \, d\mathbf{r}' \quad .$$

- (c) The gradient correction of the kinetic energy in the Thomas Fermi approximation introduced by von Weizsäcker

$$T_{\text{W}}[n] = \frac{1}{8} \int \frac{\nabla n(\mathbf{r}) \cdot \nabla n(\mathbf{r})}{n(\mathbf{r})} \, d\mathbf{r} \quad .$$

Hint: Use the Green's theorem and take vanishing boundary conditions on a suitable surface.

10.2. Density functional theory in the Thomas Fermi approximation

Consider the total energy of an N electron system in the Thomas Fermi approximation

$$E_{\text{TF}}[n] = T_{\text{TF}}[n] + E_{\text{H}}[n] + V[n] \quad ,$$

where $T_{\text{TF}}[n]$ and $E_{\text{H}}[n]$ are given in the previous exercise and

$$V[n] = \int v(\mathbf{r}) n(\mathbf{r}) \, d\mathbf{r} \quad .$$

- (a) By minimizing the total energy, formulate the corresponding density functional theory equations

$$\frac{5}{3}[n(\mathbf{r})]^{2/3} + v_{\text{H}}(\mathbf{r}) + v(\mathbf{r}) = \mu \quad .$$

v_{H} is the functional derivative of the Hartree energy.

- (b) Repeat the same calculation for the case in which the electron density is described via

$$n(\mathbf{r}) = \begin{cases} A_{\lambda} e^{-\lambda r} & \text{when } r < a \\ 0 & \text{when } r > a \end{cases} ,$$

where $r = |\mathbf{r}|$, $a > 0$ and $\lambda > 0$.