Technische Universität Graz

10. Electrons in a Magnetic Field

Nov. 5, 2018

Welcome to phonopy

Phonopy is an open source package for phonon calculations at harmonic and quasi-harmonic levels.

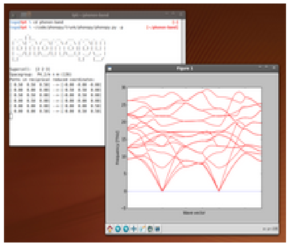
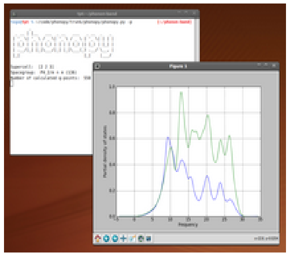
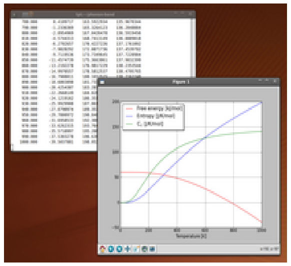
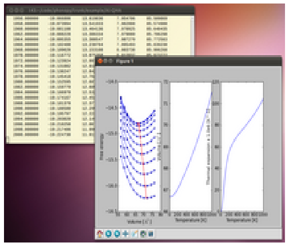
Phono3py is another open source package for phonon-phonon interaction and lattice thermal conductivity calculations. See the documentation at http://atztogo.github.io/phono3py/

Phonon database: A collection of first principles phonon calculations is available as open data at http://phonondb.mtl.kyoto-u.ac.jp/ , where the raw data of phonopy & VASP results are downloaded.

The following features of phonopy are highlighted:

- Phonon band structure, phonon DOS and partial-DOS
- Phonon thermal properties: Free energy, heat capacity (Cv), and entropy
- Phonon group velocity
- Thermal ellipsoids / Mean square displacements
- Irreducible representations of normal modes
- Dynamic structure factor for INS and IXS
- Non-analytical-term correction: LO-TO splitting (Born effective charges and dielectric constant are required.)
- Mode Grüneisen parameters
- Quasi-harmonic approximation: Thermal expansion, heat capacity at constant pressure (Cp)
- Interfaces to calculators: VASP, VASP DFPT, ABINIT, Quantu ESPRESSO, SIESTA, Elk, FHI-aims, WIEN2k, CRYSTAL, LAMMPS (external)
- Phonopy API for Python

A presentation in pdf for introduction to phonopy is downloaded ***here***.

Student projects

Calculate the phonon dispersion and/or phonon density of states for some crystal.

Explain how to use a band structure program like Quantum Espresso or VASP to calculate the phonon dispersion.

Explain how to use Phonopy to plot phonon dispersion, densities of states, and to animate phonon modes.

Charged particle in a magnetic field

$$\vec{F} = -e\vec{v} \times \vec{B} = ma$$

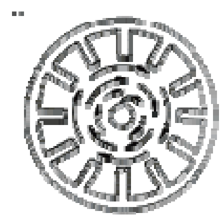
$$evB_z = \frac{mv^2}{R}$$

solve for velocity

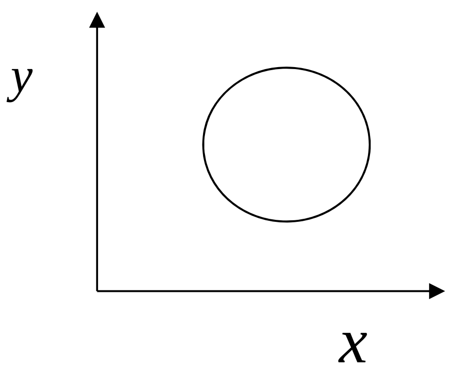
$$v = \frac{eB_z R}{m}$$

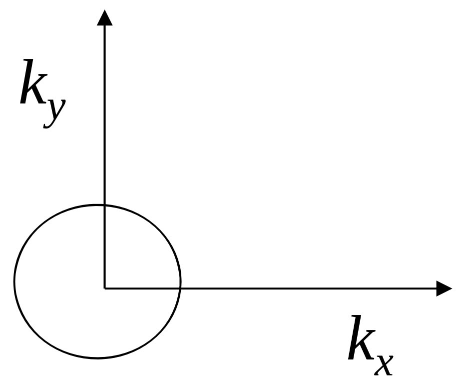
$$v = \omega_c R$$

$$\omega_c = \frac{eB_z}{m}$$



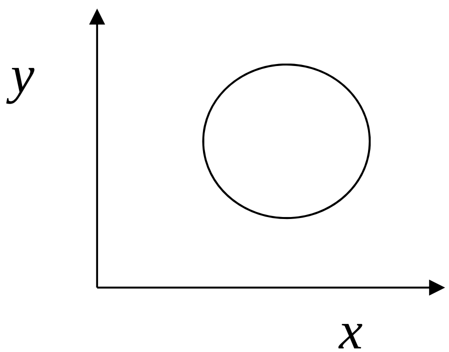
Magnetron



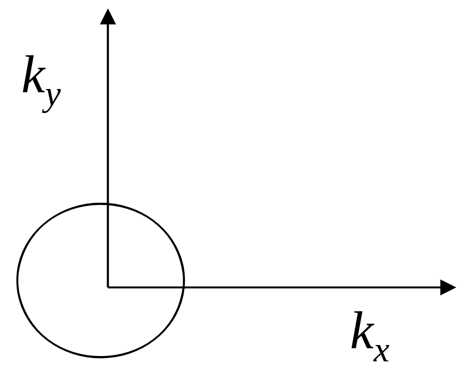


Why don't metals in a B field radiate?

Magnetron



$$\omega_c = \frac{eB_z}{m}$$



There are no lower lying states to fall into. We need a quantum description.

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

Magnetic force depends on the velocity, not on the position.

Electrons in a magnetic field

Lorentz force law $\vec{F} = q\left(\vec{E} + \vec{v} \times \vec{B}\right)$

Euler Lagrange equations $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) - \frac{\partial L}{\partial x_i} = 0$

Lagrangian: $L = \tfrac{1}{2} m v^2 - qV\left(\vec{r}, t\right) + q\vec{v} \cdot \vec{A}\left(\vec{r}, t\right)$

Kittel: Appendix G

http://lamp.tu-graz.ac.at/~hadley/ss2/IQHE/cpimf.php

Lagrangian

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right)-\frac{\partial L}{\partial x_i}=0$$

$$L=\tfrac{1}{2}mv^2-qV\left(\vec{r},t\right)+q\vec{v}\cdot\vec{A}\left(\vec{r},t\right)$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial v_x}\right)=\frac{d}{dt}\left(mv_x+qA_x\right)=m\frac{dv_x}{dt}+q\frac{dA_x}{dt}$$

$$=m\frac{dv_x}{dt}+q\left(\frac{dx}{dt}\frac{\partial A_x}{\partial x}+\frac{dy}{dt}\frac{\partial A_x}{\partial y}+\frac{dz}{dt}\frac{\partial A_x}{\partial z}+\frac{\partial A_x}{\partial t}\right)$$

$$=m\frac{dv_x}{dt}+q\left(v_x\frac{\partial A_x}{\partial x}+v_y\frac{\partial A_x}{\partial y}+v_z\frac{\partial A_x}{\partial z}+\frac{\partial A_x}{\partial t}\right),$$

$$\frac{\partial L}{\partial x}=-q\frac{\partial V}{\partial x}+q\left(v_x\frac{\partial A_x}{\partial x}+v_y\frac{\partial A_y}{\partial x}+v_z\frac{\partial A_z}{\partial x}\right)$$

$$m\frac{dv_x}{dt}=-q\left(\frac{\partial V}{\partial x}+\frac{\partial A_x}{\partial t}\right)+q\left(v_y\left(\frac{\partial A_y}{\partial x}-\frac{\partial A_x}{\partial y}\right)+v_z\left(\frac{\partial A_z}{\partial x}-\frac{\partial A_x}{\partial z}\right)\right)$$

Lagrangian

$$m\frac{dv_x}{dt} = -q\left(\frac{\partial V}{\partial x} + \frac{\partial A_x}{\partial t}\right) + q\left(v_y\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) + v_z\left(\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z}\right)\right)$$

$$\vec{E} = -\nabla V - \frac{\partial \vec{A}}{\partial t} \qquad \text{and} \qquad \vec{B} = \nabla \times \vec{A}$$

$$m\frac{dv_x}{dt} = q\left(E_x + \left(\vec{v}\times\vec{B}\right)_x\right)$$

$$L = \tfrac{1}{2}mv^2 - qV\left(\vec{r},t\right) + q\vec{v}\cdot\vec{A}\left(\vec{r},t\right)$$

conjugate variable: $$p_x = \frac{\partial L}{\partial v_x} = mv_x + qA_x$$

kinetic momentum (mv_x)

field momentum (inductance) (qA_x)

$$v_x = \frac{1}{m}\left(p_x - qA_x\right)$$

Hamiltonian

$$v_x = \frac{1}{m}\left(p_x - qA_x\right)$$

$$L = \tfrac{1}{2}mv^2 - qV\left(\vec{r},t\right) + q\vec{v}\cdot\vec{A}\left(\vec{r},t\right)$$

Legendre transformation $H = \vec{v}\cdot\vec{p} - L$

$$H = \frac{1}{2m}\left(\vec{p} - q\vec{A}\right)^2 + qV$$

Classical result

$$\vec{p} \rightarrow -i\hbar\nabla$$

Schrödinger equation $$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\nabla - q\vec{A}\right)^2\psi + qV\psi$$

Landau Levels

free particles in a magnetic field

$$\frac{1}{2m}\left(-i\hbar\nabla - q\vec{A}\right)^2 \psi(\vec{r}) = E\psi(\vec{r}). \qquad V = 0$$

Landau gauge $\vec{A} = B_z x\hat{y}.$

$$\vec{B} = \nabla \times \vec{A} = B_z x\hat{y} = \left(\frac{dA_z}{dy} - \frac{dA_y}{dz}\right)\hat{x} + \left(\frac{dA_x}{dz} - \frac{dA_z}{dx}\right)\hat{y} + \left(\frac{dA_y}{dx} - \frac{dA_x}{dy}\right)\hat{z}.$$

$$\vec{B} = B_z\hat{z}.$$

Landau Levels

free particles in a magnetic field

$$\frac{1}{2m}\left(-i\hbar\nabla - q\vec{A}\right)^2 \psi(\vec{r}) = E\psi(\vec{r}). \qquad V=0$$

Landau gauge $\quad \vec{A} = B_z x\hat{y}.$

$$\left(-i\hbar\nabla - q\vec{A}\right)^2 = \left(-i\hbar\nabla - qB_z x\hat{y}\right)\cdot\left(-i\hbar\nabla - qB_z x\hat{y}\right)$$

$$-i\hbar\nabla\cdot\left(-qB_z x\hat{y}\right) = -i\hbar\left(\frac{d}{dx}\hat{x} + \frac{d}{dy}\hat{y} + \frac{d}{dz}\hat{z}\right)\cdot\left(-qB_z x\hat{y}\right) = i\hbar qB_z x\frac{d}{dy}$$

$$\frac{1}{2m}\left(-\hbar^2\nabla^2 + i2\hbar qB_z x\frac{d}{dy} + q^2B_z^2x^2\right)\psi = E\psi.$$

The solution has the form

$$\psi = e^{ik_y y}e^{ik_z z}\phi(x).$$

Landau Levels

$$\frac{1}{2m}\left(-\hbar^2\nabla^2 + i2\hbar q B_z x\frac{d}{dy} + q^2B_z^2x^2\right)\psi = E\psi.$$

The solution has the form

$$\psi = e^{ik_y y}e^{ik_z z}\phi(x).$$

Substitute this into the equation

$$\frac{1}{2m}\left(-\hbar^2\frac{\partial^2}{\partial x^2} + \hbar^2k_z^2 + \hbar^2k_y^2 - 2\hbar q B_z k_y x + q^2B_z^2x^2\right)\phi(x) = E\phi(x).$$

Landau Levels

The equation for $\phi(x)$ is

$$\frac{1}{2m}\left(-\hbar^2\frac{\partial^2}{\partial x^2}+\hbar^2k_z^2+\underbrace{\hbar^2k_y^2-2\hbar qB_zk_yx+q^2B_z^2x^2}_{\left(\hbar k_y-qB_zx\right)^2}\right)\phi(x)=E\phi(x).$$

$$\frac{1}{2m}\left(-\hbar^2\frac{\partial^2}{\partial x^2}+q^2B_z^2\left(x-\frac{\hbar k_y}{qB_z}\right)^2\right)\phi(x)=\left(E-\frac{\hbar^2k_z^2}{2m}\right)\phi(x).$$

This is the equation for a harmonic oscillator

$$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{K}{2}\left(x-x_0\right)^2\right)\phi(x)=E'\phi(x).$$

Landau Levels

$$\frac{1}{2m}\left(-\hbar^2\frac{\partial^2}{\partial x^2}+q^2B_z^2\left(x-x_0\right)^2\right)\phi(x)=\left(E-\frac{\hbar^2k_z^2}{2m}\right)\phi(x). \quad x_0=\frac{\hbar k_y}{qB_z}$$

$$\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{K}{2}\left(x-x_0\right)^2\right)\phi(x)=E'\phi(x).$$

This is the equation for a harmonic oscillator

$$\frac{K}{2}\Leftrightarrow\frac{q^2B_z^2}{2m}$$

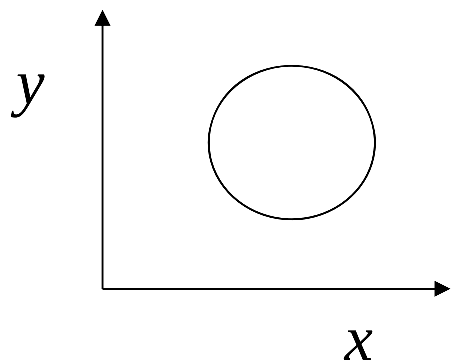
$$\omega_c=\sqrt{\frac{K}{m}}\Leftrightarrow\frac{qB_z}{m}$$

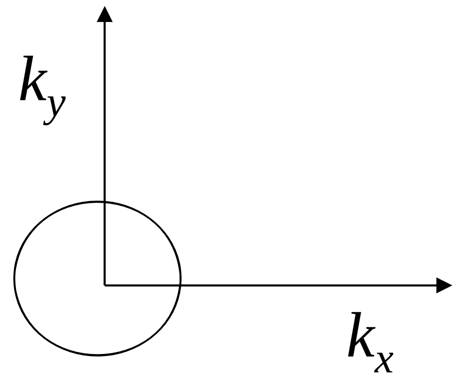
$$E_{k_z,v}=\frac{\hbar^2k_z^2}{2m}+\hbar\omega_c\left(v+\tfrac{1}{2}\right) \qquad \omega_c=\frac{qB_z}{m}$$

Charged particle in a magnetic field

Bohr - Sommerfeld quantization

$$2\pi R = v\lambda$$



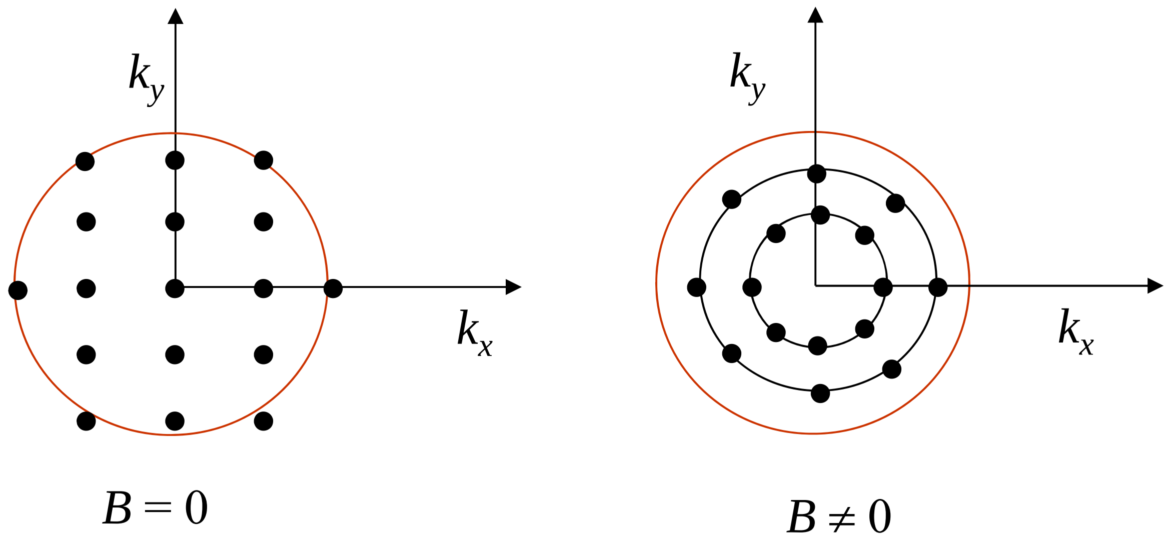


Circular motion is harmonic motion. Harmonic motion is quantized.

$$E_v = \hbar\omega_c\left(v + \tfrac{1}{2}\right) = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right)$$

v labels the Landau level

Landau levels



The number of solutions is conserved

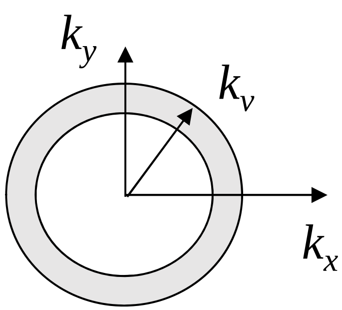
$$\psi = e^{ik_y y}\phi(x - x_0). \qquad x_0 = \frac{\hbar k_y}{qB_z}$$

In 2-D, the *k*-volume per *k* state is: $\left(\frac{2\pi}{L}\right)^2$

Density of states 2D

$$E_\nu = \hbar\omega_c\left(\nu + \tfrac{1}{2}\right)$$

The number of states between ring ν-1 and ring ν is



$$\frac{\pi\left(k_\nu^2 - k_{\nu-1}^2\right)}{\left(\frac{2\pi}{L}\right)^2} \qquad \frac{\hbar^2 k_\nu^2}{2m} = \hbar\omega_c\left(\nu + \tfrac{1}{2}\right)$$

$$k_\nu^2 - k_{\nu-1}^2 = \frac{2m\omega_c}{\hbar}\left[\left(\nu + \tfrac{1}{2}\right) - \left(\nu - 1 + \tfrac{1}{2}\right)\right] = \frac{2m\omega_c}{\hbar}$$

The number of states between ring ν-1 and ring ν is $\dfrac{m\omega_c}{2\pi\hbar}L^2$

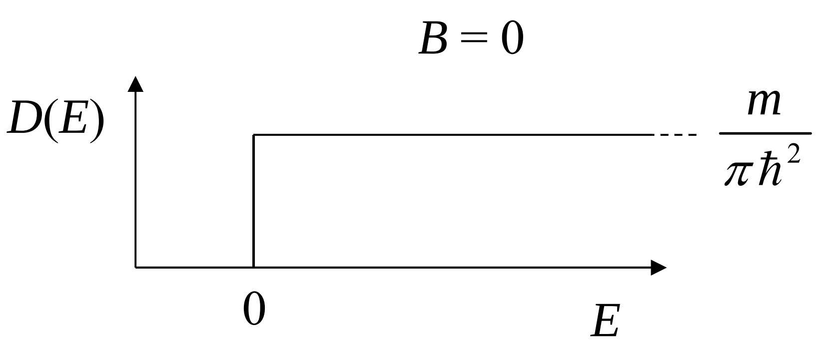
The density of states per spin is $\dfrac{m\omega_c}{2\pi\hbar}$

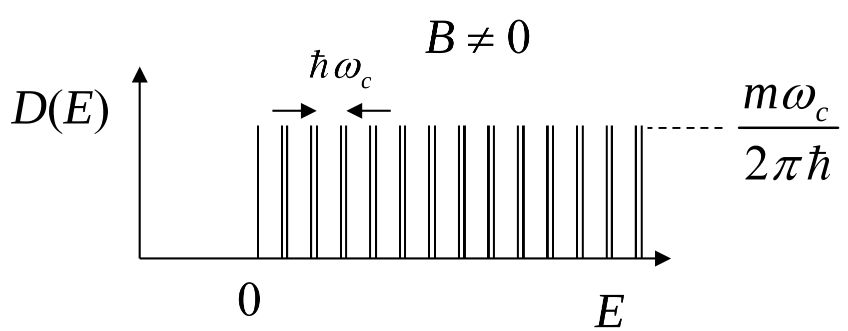
Spin

In a magnetic field, there is a shift of the energy of the electrons because of their spin.

$$E = -\vec{\mu}\cdot\vec{B} = \pm\frac{g}{2}\mu_B B$$

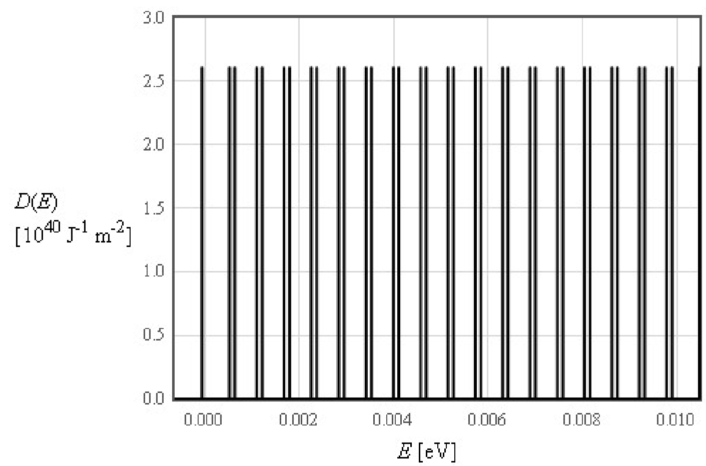
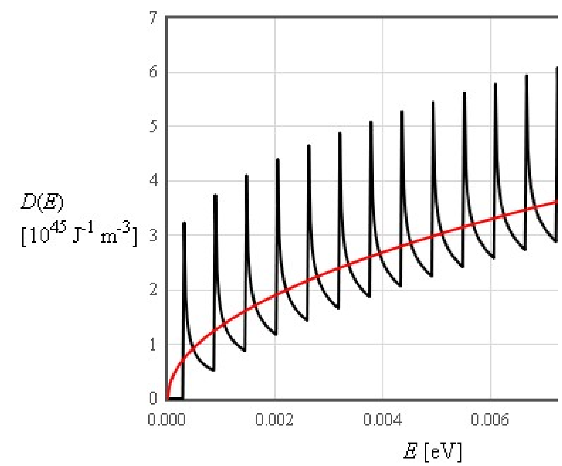
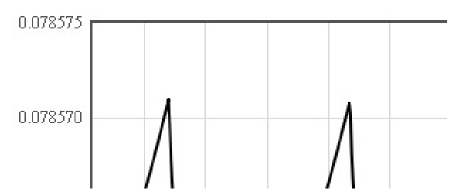
Bohr magneton $\mu_B = \dfrac{e\hbar}{2m_e}$ g-factor $g \approx 2$ $\hbar\omega_c = \dfrac{\hbar eB}{m} = 2\mu_B B$



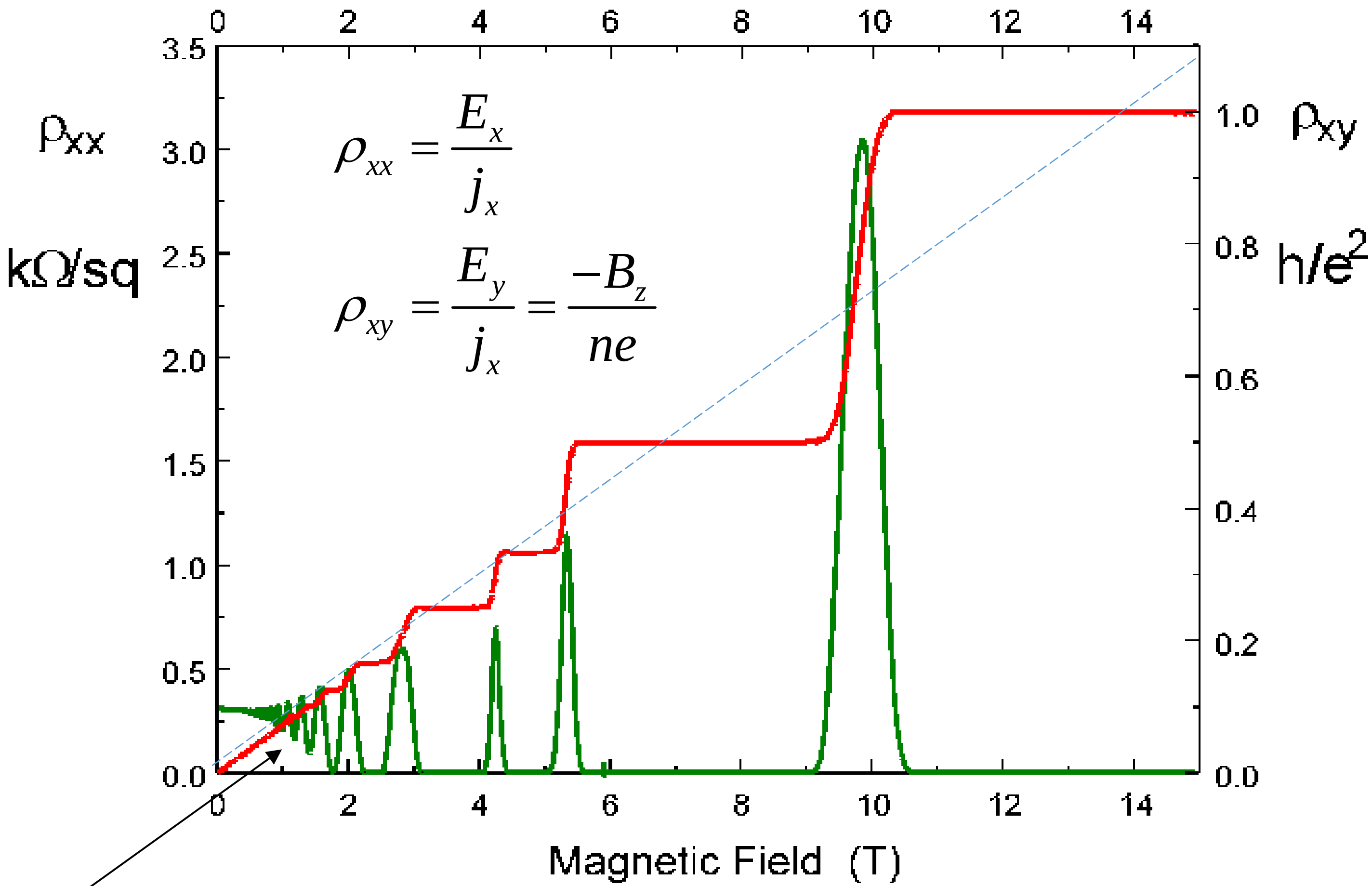


$$D(E) = \frac{m\omega_c}{2\pi\hbar}\sum_{\nu=0}^{\infty}\delta\left(E-\hbar\omega_c\left(\nu+\tfrac{1}{2}-\tfrac{g}{4}\right)\right)+\delta\left(E-\hbar\omega_c\left(\nu+\tfrac{1}{2}+\tfrac{g}{4}\right)\right)$$

ization of the Schrödinger equation for free electrons a magnetic field in 2 and 3 dimensions.

	2-D Schrödinger equation $i\hbar\frac{d\psi}{dt}=\frac{1}{2m}\left(-i\hbar\nabla-\lvert e\rvert\vec{A}\right)^2\psi$	3-D Schrödinger equation $i\hbar\frac{d\psi}{dt}=\frac{1}{2m}\left(-i\hbar\nabla-\lvert e\rvert\vec{A}\right)^2\psi$
Eigenfunction solutions	$\psi=g_v(x)\exp\left(ik_y y\right)$ $g_v(x)$ is a harmonic oscillator wavefunction	$\psi=g_v(x)\exp\left(ik_y y\right)\exp\left(ik_z z\right)$ $g_v(x)$ is a harmonic oscillator wavefun
Energy eigenvalues	$E=\hbar\omega_c\left(v+\frac{1}{2}\right)$ J $v=0,1,2,\cdots \qquad \omega_c=\frac{\lvert eB_z\rvert}{m}$	$E=\frac{\hbar^2k_z^2}{2m}+\hbar\omega_c\left(v+\frac{1}{2}\right)$ J $v=0,1,2,\cdots \qquad \omega_c=\frac{\lvert eB_z\rvert}{m}$
Density of states	$D(E)=\frac{m\omega_c}{2\pi\hbar}\sum_{v=0}^{\infty}\delta\left(E-\hbar\omega_c\left(v+\frac{1}{2}\right)-\frac{g\mu_B}{2}B\right)+\delta\left(E-\hbar\omega_c\left(v+\frac{1}{2}\right)+\frac{g\mu_B}{2}B\right)$ $\text{J}^{-1}\text{m}^{-2}$  Calculate DoS	$D(E)=\frac{(2m)^{3/2}\omega_c}{4\pi^2\hbar^2}\sum_{v=0}^{\infty}\frac{H\left(E-\hbar\omega_c\left(v+\frac{1}{2}\right)\right)}{\sqrt{E-\hbar\omega_c\left(v+\frac{1}{2}\right)}}$  Calculate DoS
	$E_F=\hbar\omega_c\left(\text{Int}\left(\frac{\pi\hbar n}{m\omega_c}\right)+\frac{1}{2}\right)$ 	

Quantum Hall Effect



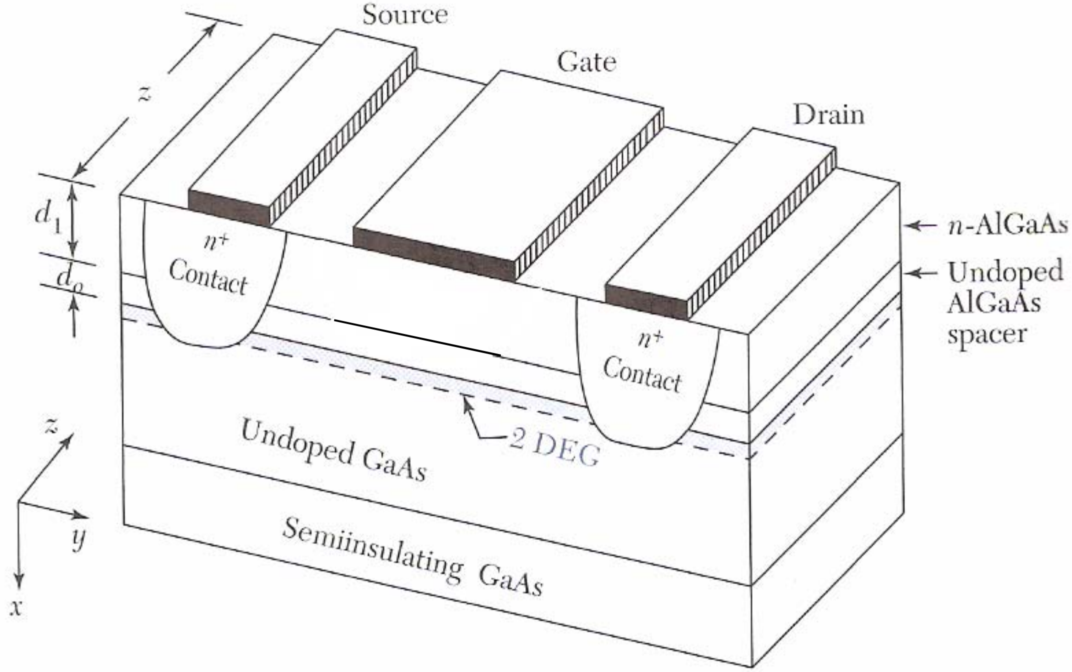
$$\rho_{xx} = \frac{E_x}{j_x}$$

$$\rho_{xy} = \frac{E_y}{j_x} = \frac{-B_z}{ne}$$

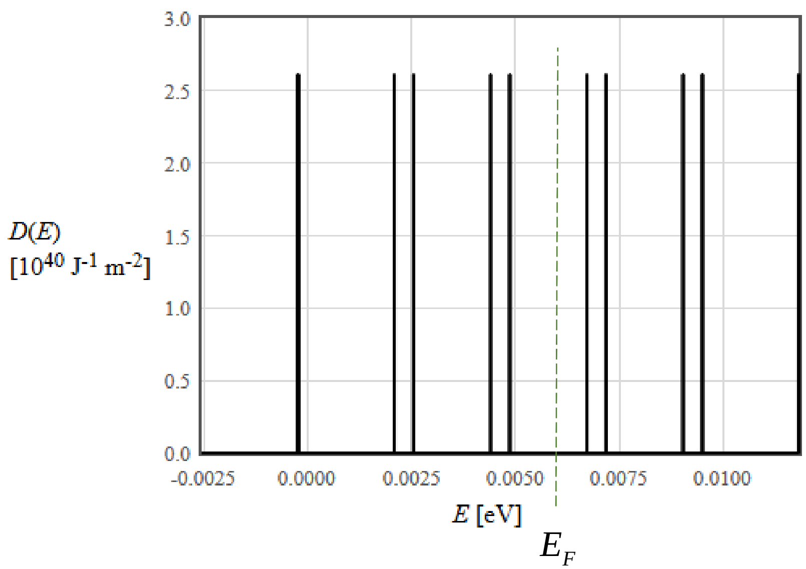
Shubnikov-De Haas oscillations

Resistance standard
25812.807557(18) Ω

HEMT High electron mobility transistor



Quantum hall effect



If the Fermi energy is between Landau levels, the electron density n is an integer v times the degeneracy of the Landau level $n = D_0 v$

$$\rho_{xy} = \frac{E_y}{j_x} = \frac{-B_z}{ne}$$

Each Landau level can hold the same number of electrons.

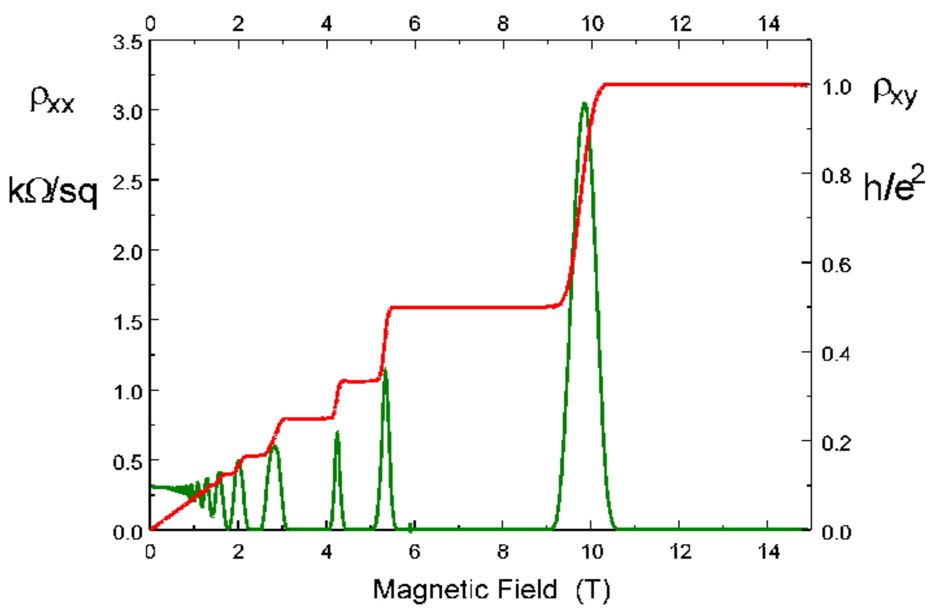
$$\rho_{xy} = \frac{-B_z}{ne} = \frac{-hD_0}{ve^2 D_0} = \frac{-h}{ve^2}$$

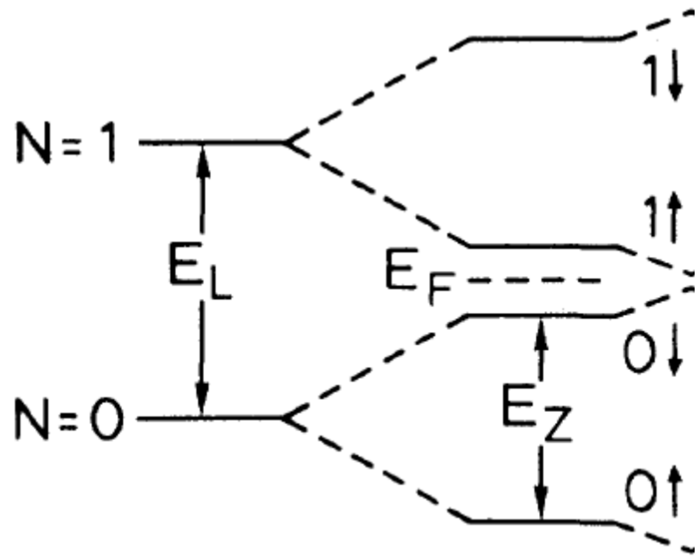
$$D_0 = \frac{m\omega_c}{2\pi\hbar} = \frac{eB_z}{h}$$

$$\omega_c = \frac{eB_z}{m} \qquad B_z = \frac{hD_0}{e}$$

Quantum hall effect

$$\rho_{xy} = \frac{h}{\nu e^2}$$





S. Koch, R. J. Haug, and K. v. Klitzing, Phys. Rev. B 47, 4048–4051 (1993)