Formelsammlung

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January 10, 2025

Contents

Part I
Mathematics

1 Linear algebra

1.1 Matrix basics

Matrix-matrix product as sum	$$C_{ij} = \sum_k A_{ik} B_{kj} \quad (1)$$
Matrix-vector product as sum	$$\vec{c}_i = \sum_j A_{ij} \vec{b}_j \quad (2)$$
Symmetric matrix	$$A^{\mathrm{T}} = A \quad (3)$$ A $n \times n$ matrix
Unitary matrix	$$U^\dagger U = \mathbb{1} \quad (4)$$

1.1.1 Transposed matrix

Sum	$$(A + B)^{\mathrm{T}} = A^{\mathrm{T}} + B^{\mathrm{T}} \quad (5)$$
Product	$$(AB)^{\mathrm{T}} = B^{\mathrm{T}} A^{\mathrm{T}} \quad (6)$$
Inverse	$$(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1} \quad (7)$$
Exponential	$$\exp(A^{\mathrm{T}}) = (\exp A)^{\mathrm{T}} \quad (8)$$ $$\ln(A^{\mathrm{T}}) = (\ln A)^{\mathrm{T}} \quad (9)$$

1.2 Determinant

2x2 matrix	$$\det \begin{pmatrix} a & b \\ c & d \end{pmatrix} = a\,d - c\,b \quad (10)$$
3x3 matrix (Rule of Sarrus)	$$\det \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = a\,e\,i + b\,f\,g + c\,d\,h - g\,e\,c - h\,f\,a - i\,d\,b \quad (11)$$
Leibniz formla	$$\det(A) = \sum_{\sigma \in S_n} \left(\mathrm{sgn}(\sigma) \prod_{i=1}^{n} a_{i,\sigma(i)} \right) \quad (12)$$
Product	$$\det(A\,B) = \det(A)\det(B) \quad (13)$$

Inverse	$$\det(A^{-1}) = \det(A)^{-1} \tag{14}$$
Transposed	$$\det(A^{\mathrm{T}}) = \det(A) \tag{15}$$

1.3 math:linalg:misc

Normal equation Solves a linear regression problem	$$\underline{\theta} = (\underline{X}^{\mathrm{T}}\underline{X})^{-1}\underline{X}^{\mathrm{T}}\vec{y} \tag{16}$$ $\underline{\theta}$ hypothesis / weight matrix, $\underline{X}$ design matrix, $\vec{y}$ output vector
Inverse 2×2 matrix	$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad - bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \tag{17}$$
Singular value decomposition Factorization of complex matrices through rotating →rescaling →rotation.	$$A = U\Lambda V \tag{18}$$ A: $m \times n$ matrix, U: $m \times m$ unitary matrix, Λ: $m \times n$ rectangular diagonal matrix with non-negative numbers on the diagonal, V: $n \times n$ unitary matrix
2D rotation matrix	$$R = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \tag{19}$$
3D rotation matrices	$$R_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} \tag{20}$$ $$R_y = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \tag{21}$$ $$R_z = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{22}$$
Properites of rotation matrices	$$R^{\mathrm{T}} = R^{-1} \tag{23}$$ $$\det R = 1 \tag{24}$$ $$R \in \mathrm{SO}(n) \tag{25}$$ n dimension, $\mathrm{SO}(n)$ special othogonal group

1.4 Eigenvalues

Eigenvalue equation	$$Av = \lambda v \tag{26}$$ λ eigenvalue, v eigenvector

Characteristic polynomial Zeros are the eigenvalues of A	$$\chi_A = \det(A - \lambda \mathbb{1}) \overset{!}{=} 0 \quad (27)$$
Kramer's theorem If H is invariant under T and $\|\psi\rangle$ is an eigenstate of H, then $T\|\psi\rangle$ is also am eigenstate of H	$$THT^\dagger = H \quad \wedge \quad H\|\psi\rangle = E\|\psi\rangle \quad \Rightarrow \quad HT\|\psi\rangle = ET\|\psi\rangle \quad (28)$$
Eigendecomposition	$$A = V\Lambda V^{-1} \quad (29)$$ A diagonalizable, columns of V are eigenvectors v_i, Λ diagonal matrix with eigenvalues λ_i on the diagonal

TODO:Jordan stuff, blockdiagonal matrices, permutations, skalar product lapacescher entwicklungssatz maybe, cramers rule

2 Geometry

2.1 Trigonometry

Exponential function	$$\exp(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} \quad (30)$$
Sine	$$\sin(x) = \sum_{n=0}^{\infty} (-1)^n \frac{x^{(2n+1)}}{(2n+1)!} \quad (31)$$ $$= \frac{e^{ix} - e^{-ix}}{2i} \quad (32)$$
Cosine	$$\cos(x) = \sum_{n=0}^{\infty} (-1)^n \frac{x^{(2n)}}{(2n)!} \quad (33)$$ $$= \frac{e^{ix} + e^{-ix}}{2} \quad (34)$$
Hyperbolic sine	$$\sinh(x) = -i \sin ix \quad (35)$$ $$= \frac{e^x - e^{-x}}{2} \quad (36)$$
Hyperbolic cosine	$$\cosh(x) = \cos ix \quad (37)$$ $$= \frac{e^x + e^{-x}}{2} \quad (38)$$

2.2 Various theorems

Hypthenuse in the unit circle	$$1 = \sin^2 x + \cos^2 x \quad (39)$$

Addition theorems	$$\sin(x \pm y) = \sin x \cos y \pm \cos x \sin y \quad (40)$$ $$\cos(x \pm y) = \cos x \cos y \mp \sin x \sin y \quad (41)$$ $$\tan(x \pm y) = \frac{\sin(x \pm y)}{\cos(x \pm y)} = \frac{\tan x \pm \tan y}{1 \mp \tan x \tan y} \quad (42)$$
Double angle	$$\sin 2x = 2 \sin x \cos x \quad (43)$$ $$\cos 2x = \cos^2 x - \sin^2 x = 1 - 2\sin^2 x \quad (44)$$ $$\tan 2x = \frac{2 \tan x}{1 - \tan^2 x} \quad (45)$$
Other	$$\cos x + b \sin x = \sqrt{1 + b^2} \cos(x - \theta) \quad (46)$$ $\tan \theta = b$

2.2.1 Table of values

Degree	0°	30°	45°	60°	90°	120°	180°	270°
Radian	0	$\frac{\pi}{6}$	$\frac{\pi}{4}$	$\frac{\sqrt{\pi}}{3}$	$\frac{\pi}{2}$	$\frac{2\pi}{3}$	π	$\frac{3\pi}{2}$
$\sin(x)$	0	$\frac{1}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{3}}{2}$	1	$\frac{\sqrt{3}}{2}$	0	-1
$\cos(x)$	1	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{1}{2}$	0	$\frac{-1}{2}$	-1	0
$\tan(x)$	0	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	∞	$-\sqrt{3}$	0	∞

3 Calculus

3.1 Convolution

Convolution is **commutative**, **associative** and **distributive**.

Definition	$$(f * g)(t) = f(t) * g(t) = \int_{-\infty}^{\infty} f(\tau) g(t - \tau) \, \mathrm{d}\tau \quad (47)$$
Notation	$$f(t) * g(t - t_0) = (f * g)(t - t_0) \quad (48)$$ $$f(t - t_0) * g(t - t_0) = (f * g)(t - 2t_0) \quad (49)$$
Commutativity	$$f * g = g * f \quad (50)$$
Associativity	$$(f * g) * h = f * (g * h) \quad (51)$$
Distributivity	$$f * (g + h) = f * g + f * h \quad (52)$$

Complex conjugate	$$(f * g)^* = f^* * g^* \tag{53}$$

3.2 Fourier analysis

3.2.1 Fourier series

Fourier series Complex representation	$$f(t) = \sum_{k=-\infty}^{\infty} c_k \exp\left(\frac{2\pi i k t}{T}\right) \tag{54}$$ $f \in \mathcal{L}^2(\mathbb{R}, \mathbb{C})$ T-periodic
Fourier coefficients Complex representation	$$c_k = \frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} f(t) \exp\left(-\frac{2\pi i}{T} k t\right) \mathrm{d}t \quad \text{for } k \geq 0 \tag{55}$$ $$c_{-k} = \overline{c_k} \quad \text{if } f \text{ real} \tag{56}$$
Fourier series Sine and cosine representation	$$f(t) = \frac{a_0}{2} + \sum_{k=1}^{\infty} \left(a_k \cos\left(\frac{2\pi}{T} k t\right) + b_k \sin\left(\frac{2\pi}{T} k t\right)\right) \tag{57}$$ $f \in \mathcal{L}^2(\mathbb{R}, \mathbb{C})$ T-periodic
Fourier coefficients Sine and cosine representation If f has point symmetry: $a_{k>0} = 0$, if f has axial symmetry: $b_k = 0$	$$a_k = \frac{2}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} f(t) \cos\left(-\frac{2\pi}{T} k t\right) \mathrm{d}t \quad \text{for } k \geq 0 \tag{58}$$ $$b_k = \frac{2}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} f(t) \sin\left(-\frac{2\pi}{T} k t\right) \mathrm{d}t \quad \text{for } k \geq 1 \tag{59}$$ $$a_k = c_k + c_{-k} \quad \text{for } k \geq 0 \tag{60}$$ $$b_k = i(c_k - c_{-k}) \quad \text{for } k \geq 1 \tag{61}$$

TODO:cleanup

3.2.2 Fourier transformation

Fourier transform	$$\hat{f}(k) := \frac{1}{\sqrt{2\pi}^n} \int_{\mathbb{R}^n} \mathrm{e}^{-ikx} f(x) \, \mathrm{d}x \tag{62}$$ $\hat{f} : \mathbb{R}^n \mapsto \mathbb{C}, \; \forall f \in L^1(\mathbb{R}^n)$

for $f \in L^1(\mathbb{R}^n)$:

i) $f \mapsto \hat{f}$ linear in f

ii) $g(x) = f(x - h) \quad \Rightarrow \quad \hat{g}(k) = \mathrm{e}^{-ikn} \hat{f}(k)$

iii) $g(x) = \mathrm{e}^{ih \cdot x} f(x) \quad \Rightarrow \quad \hat{g}(k) = \hat{f}(k - h)$

iv) $g(\lambda) = f\left(\frac{x}{\lambda}\right) \quad \Rightarrow \quad \hat{g}(k) \lambda^n \hat{f}(\lambda k)$

3.3 Misc

Stirling approximation	$$\ln(N!) \approx N \ln(N) - N + \mathcal{O}(() \ln(N)) \tag{63}$$

Error function $\mathrm{erf}: \mathbb{C} \to \mathbb{C}$ and complementary error function erfc	$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\,\mathrm{d}t \quad (64)$$ $$\mathrm{erfc}(x) = 1 - \mathrm{erf}(x) \quad (65)$$ $$= \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2}\,\mathrm{d}t \quad (66)$$
Dirac-Delta of a function	$$\delta(f(x)) = \frac{\delta(x-x_0)}{\lvert g'(x_0)\rvert} \quad (67)$$ $g(x_0) = 0$

3.4 Logarithm

Logarithm identities	$$\log(xy) = \log(x) + \log(y) \quad (68)$$ $$\log\left(\frac{x}{y}\right) = \log(x) - \log(y) \quad (69)$$ $$\log\left(x^d\right) = d\log(x) \quad (70)$$ $$\log\left(\sqrt[y]{x}\right) = \frac{\log(x)}{y} \quad (71)$$ $$x^{\log(y)} = y^{\log(x)} \quad (72)$$
Integral of natural logarithm	$$\int \ln(x)\,\mathrm{d}x = x\left(\ln(x) - 1\right) \quad (73)$$ $$\int \ln(ax+b)\,\mathrm{d}x = \frac{ax+b}{a}\left(\ln(ax+b) - 1\right) \quad (74)$$

3.5 Integrals

Partial integration	$$\int_a^b f'(x)\cdot g(x)\,\mathrm{d}x = \left[f(x)\cdot g(x)\right]_a^b - \int_a^b f(x)\cdot g'(x)\,\mathrm{d}x \quad (75)$$
Integration by substitution	$$\int_a^b f(g(x))\,g'(x)\,\mathrm{d}x = \int_{g(a)}^{g(b)} f(z)\,\mathrm{d}z \quad (76)$$
Gauss's theorem / Divergence theorem Divergence in a volume equals the flux through the surface	$$\iiint_V (\vec{\nabla}\cdot\vec{F})\,\mathrm{d}V = \oiint_A \vec{F}\cdot\mathrm{d}\vec{A} \quad (77)$$ $A = \partial V$
Stokes's theorem	$$\int_A (\vec{\nabla}\times\vec{F})\cdot\mathrm{d}\vec{S} = \oint_S \vec{F}\cdot\mathrm{d}\vec{r} \quad (78)$$ $S = \partial A$

3.5.1 List of common integrals

cal:log:integral

Arcsine, arccosine, arctangent

$$\int \frac{1}{\sqrt{1-x^2}}\,\mathrm{d}x = \arcsin x \tag{79}$$
$$\int -\frac{1}{\sqrt{1-x^2}}\,\mathrm{d}x = \arccos x \tag{80}$$
$$\int \frac{1}{x^2+1}\,\mathrm{d}x = \arctan x \tag{81}$$

Arcsinh, arccosh, arctanh

$$\int \frac{1}{\sqrt{x^2+1}}\,\mathrm{d}x = \operatorname{arsinh} x \tag{82}$$
$$\int \frac{1}{\sqrt{x^2-1}}\,\mathrm{d}x = \operatorname{arcosh} x \quad \text{for } (x>1) \tag{83}$$
$$\int \frac{1}{1-x^2}\,\mathrm{d}x = \operatorname{artanh} x \quad \text{for } (|x|<1) \tag{84}$$
$$\int \frac{1}{1-x^2}\,\mathrm{d}x = \operatorname{arcoth} x \quad \text{for } (|x|>1) \tag{85}$$

Spherical coordinates

$$x = r\sin\phi, \cos\theta \tag{86}$$
$$y = r\cos\phi, \cos\theta \tag{87}$$
$$z = r\sin\theta \tag{88}$$

Integration in spherical coordinates

$$\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \int_0^\infty \int_0^{2\pi} \int_0^\pi \mathrm{d}r\,\mathrm{d}\phi\,\mathrm{d}\theta\, r^2 \sin\theta \tag{89}$$

Riemann Zeta Function

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \frac{1}{(1-2^{(1-s)})\Gamma(s)} \int_0^\infty \mathrm{d}\eta \frac{\eta^{(s-1)}}{\mathrm{e}^\eta + 1} \tag{90}$$

TODO:differential equation solutions

4 Probability theory

Mean
Expectation value

$$\langle x \rangle = \int w(x)\, x\, \mathrm{d}x \tag{91}$$

Variance
Square of the Standard deviation

$$\sigma^2 = (\Delta\hat{x})^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 = \langle (x - \langle x \rangle)^2 \rangle \tag{92}$$

Covariance

$$\operatorname{cov}(x,y) = \sigma(x,y) = \sigma_{XY} = \langle (x - \langle x \rangle)\,(y - \langle y \rangle) \rangle \tag{93}$$

Standard deviation

$$\sigma = \sqrt{\sigma^2} = \sqrt{(\Delta x)^2} \tag{94}$$

Median
Value separating lower half from top half

$$\operatorname{med}(x) = \begin{cases} x_{(n+1)/2} & n \text{ odd} \\ \frac{x_{(n/2)} + x_{((n/2)+1)}}{2} & n \text{ even} \end{cases} \tag{95}$$

x dataset with n elements

Probability density function
Random variable has density f. The integral gives the probability of X taking a value $x \in [a, b]$.

$$P([a,b]) := \int_a^b f(x)\,\mathrm{d}x \tag{96}$$

f normalized: $\int_{-\infty}^{\infty} f(x)\,\mathrm{d}x = 1$

Cumulative distribution function

$$F(x) = \int_{-\infty}^{x} f(t)\,\mathrm{d}t \tag{97}$$

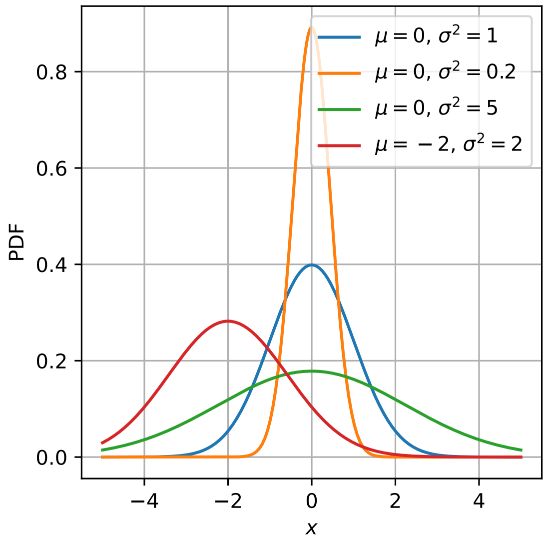
f probability density function

Autocorrelation
Correlation of f to itself at an earlier point in time, C is a covariance function

$$C_A(\tau) = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} f(t+\tau) f(t)\,\mathrm{d}t) = \langle f(t+\tau) \cdot f(t) \rangle \tag{98}$$

4.1 Distributions

4.1.1 Gauß/Normal distribution

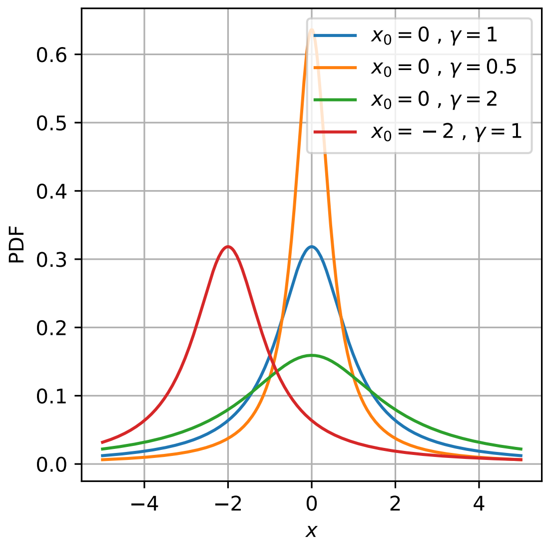


parameters	$\mu \in \mathbb{R}, \quad \sigma^2 \in \mathbb{R}$
support	$x \in \mathbb{R}$
pdf	$\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$
cdf	$\frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{x-\mu}{\sqrt{2}\sigma}\right)\right]$
mean	μ
median	μ
variance	σ^2

Density function of the standard normal distribution
$\mu = 0, \sigma = 1$

$$\varphi(x) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-\frac{1}{2}x^2} \tag{99}$$

4.1.2 Cauchys / Lorentz distribution

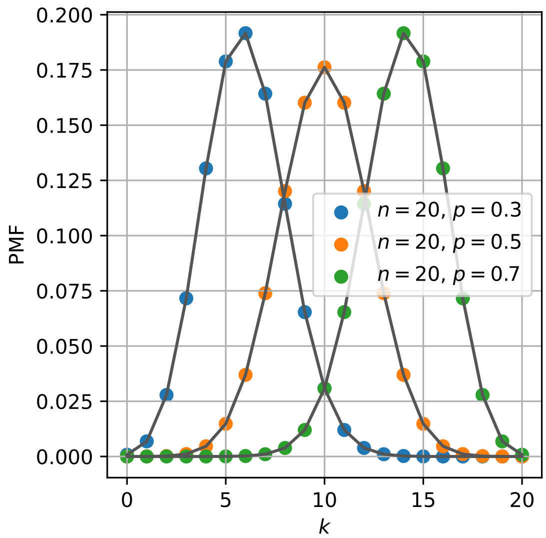


parameters	$x_0 \in \mathbb{R}, \quad \gamma \in \mathbb{R}$
support	$x \in \mathbb{R}$
pdf	$\dfrac{1}{\pi\gamma\left[1+\left(\frac{x-x_0}{\gamma}\right)^2\right]}$
cdf	$\dfrac{1}{\pi}\arctan\left(\dfrac{x-x_0}{\gamma}\right)+\dfrac{1}{2}$
mean	undefined
median	x_0
variance	undefined

Also known as **Cauchy-Lorentz distribution**, **Lorentz(ian) function**, **Breit-Wigner distribution**.

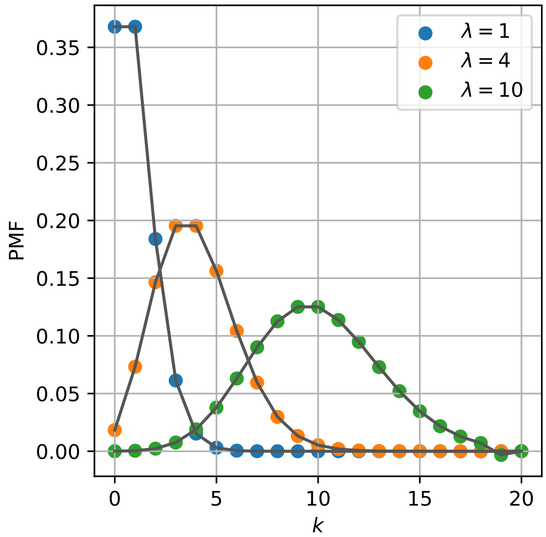
4.1.3 Binomial distribution

For the number of trials going to infinity ($n \to \infty$), the binomial distribution converges to the poisson distribution



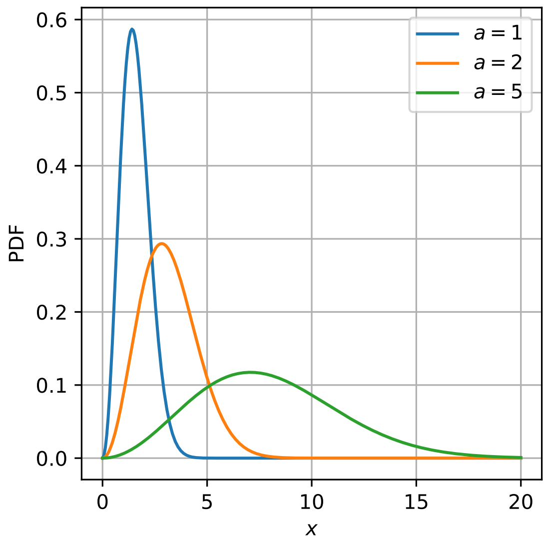
parameters	$n \in \mathbb{Z}, \quad p \in [0,1], \quad q = 1-p$
support	$k \in \{0,\, 1,\, \dots,\, n\}$
pmf	$\binom{n}{k} p^k q^{n-k}$
mean	np
median	$\lfloor np \rfloor$ or $\lceil np \rceil$
variance	$npq = np(1-p)$

4.1.4 Poisson distribution



parameters	$\lambda \in (0, \infty)$
support	$k \in \mathbb{N}$
pmf	$\frac{\lambda^k e^{-\lambda}}{k!}$
cdf	$e^{-\lambda} \sum_{j=0}^{\lfloor k \rfloor} \frac{\lambda^j}{j!}$
mean	λ
median	$\approx \left\lfloor \lambda + \frac{1}{3} - \frac{1}{50\lambda} \right\rfloor$
variance	λ

4.1.5 Maxwell-Boltzmann distribution



parameters	$a > 0$
support	$x \in (0, \infty)$
pdf	$\sqrt{\frac{2}{\pi}} \frac{x^2}{a^3} \exp\left(-\frac{x^2}{2a^2}\right)$
cdf	$\text{erf}\left(\frac{x}{\sqrt{2}a}\right) - \sqrt{\frac{2}{\pi}} \frac{x}{a} \exp\left(\frac{-x^2}{2a^2}\right)$
mean	$2a\frac{2}{\pi}$
median	
variance	$\frac{a^2(3\pi - 8)}{\pi}$

4.2 Central limit theorem

Suppose $X_1, X_2, \dots$ is a sequence of independent and identically distributed random variables with $\langle X_i \rangle = \mu$ and $(\Delta X_i)^2 = \sigma^2 < \infty$. As N approaches infinity, the random variables $\sqrt{N}(\bar{X}_N - \mu)$ converge to a normal distribution $\mathcal{N}(0, \sigma^2)$.
That means that the variance scales with $\frac{1}{\sqrt{N}}$ and statements become accurate for large N.

4.3 Propagation of uncertainty / error

Generalized error propagation

$$V_y = J(x) \cdot V_x \cdot J^{\mathrm{T}}(x) \tag{100}$$

V Covariance matrix, J math:cal:jacobi-matrix

Propagation of uncorrelated errors Linear approximation	$$u_y = \sqrt{\sum_i \left(\frac{\partial y}{\partial x_i} \cdot u_i \right)^2} \quad (101)$$
Weight Variance is a possible choice for a weight	$$w_i = \frac{1}{\sigma_i^2} \quad (102)$$ σ Variance
Weighted mean	$$\overline{x} = \frac{\sum_i (x_i w_i)}{\sum_i w_i} \quad (103)$$ w_i Weight
Variance of weighted mean	$$\sigma_{\overline{x}}^2 = \frac{1}{\sum_i w_i} \quad (104)$$ w_i Weight

Part II
Mechanics

5 Misc

Hooke's law	$$F = D\Delta l \qquad (105)$$ F Force, D Spring constant, Δl spring length

6 Lagrange formalism

The Lagrange formalism is often the most simple approach the get the equations of motion, because with suitable generalied coordinates obtaining the Lagrange function is often relatively easy. The generalized coordinates are choosen so that the cronstraints are automatically fullfilled. For example, the generalized coordinate for a 2D pendelum is $q = \varphi$, with $\vec{x} = \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix}$.

Lagrange function	$$\mathcal{L} = T - V \qquad (106)$$ T kinetic energy, V potential energy
Lagrange equations (2nd type)	$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i} = 0 \qquad (107)$$ q generalized coordinates
Canocial Momentum	$$p = \frac{\partial \mathcal{L}}{\partial \dot{q}} \qquad (108)$$
Hamiltonian Hamiltonian can be derived from the Lagrangian using a Legendre transformation	$$H(q, p) = p\dot{q} - \mathcal{L}\big(q, \dot{q}(q, p)\big) \qquad (109)$$

TODO:Legendre trafo

Part III

Statistichal Mechanics

Extensive quantities: Additive for subsystems (system size dependent): $S(\lambda E, \lambda V, \lambda N) = \lambda S(E, V, N)$
Intensive quantities: Independent of system size, ratio of two extensive quantities

Liouville equation

$$\frac{\partial \rho}{\partial t} = -\sum_{i=1}^{N} \left(\frac{\partial \rho}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial q_i} \right) = \{H, \rho\} \tag{110}$$

$\{\}$ poisson bracket

7 Entropy

Positive-definite and additive

$$S \geq 0 \tag{111}$$

$$S(E_1, E_2) = S_1 + S_2 \tag{112}$$

Von-Neumann

$$S = -k_{\mathrm{B}} \langle \log \rho \rangle = -k_{\mathrm{B}} \operatorname{tr}(\rho \log \rho) \tag{113}$$

ρ density matrix

Gibbs

$$S = -k_{\mathrm{B}} \sum_n p_n \log p_n \tag{114}$$

p_n probability for micro state n

Boltzmann

$$S = k_{\mathrm{B}} \log \Omega \tag{115}$$

Ω #micro states

Temperature

$$\frac{1}{T} := \left(\frac{\partial S}{\partial E} \right)_V \tag{116}$$

Pressure

$$p = T \left(\frac{\partial S}{\partial V} \right)_E \tag{117}$$

Part IV
Thermodynamics

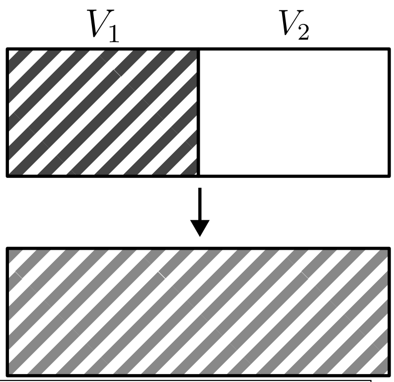
Thermal wavelength	$$\lambda = \frac{\hbar}{\sqrt{2\pi m k_\mathrm{B} T}} \quad (118)$$

8 Processes

- **isobaric**: constant pressure $p = \text{const}$
- **isochoric**: constant volume $V = \text{const}$
- **isothermal**: constant temperature $T = \text{const}$
- **isentropic**: constant entropy $S = \text{const}$
- **isenthalpic**: constant entalphy $H = \text{const}$
- **adiabatic**: no heat transfer $\Delta Q = 0$
- **quasistatic**: happens so slow, the system always stays in td. equilibrium
- **reversivle**: reversible processes are always quasistatic and no entropie is created $\Delta S = 0$

8.1 Irreversible gas expansion (Gay-Lussac experiment)

A classical gas in a system with volume V_1 is separated from another system with volume V_2. In the Gay-Lussac experiment, the separation is removed and the gas flows into V_2.



Entropy change	$$\Delta S = N k_\mathrm{B} \ln\left(\frac{V_1 + V_2}{V_1}\right) > 0 \quad (119)$$

TODO:Reversible
TODO:Quasistatischer T-Ausgleich
TODO:Joule-Thompson Prozess

9 Phase transitions

A phase transition is a discontinuity in the free energy F or Gibbs energy G or in one of their derivatives. The degree of the phase transition is the degree of the derivative which exhibits the discontinuity.

Latent heat Heat required to bring substance from phase 1 to phase 2	$$Q_\mathrm{L} = T\Delta S \quad (120)$$ ΔS entropy change of the phase transition

Clausius-Clapeyron equation Slope of the coexistence curve	$$\frac{\mathrm{d}p}{\mathrm{d}T} = \frac{Q_{\mathrm{L}}}{T\Delta V} \quad (121)$$ ΔV Volume change of the phase transition
Phase transition At the coexistence curve	$$G_1 = G_2 \quad (122)$$ and therefore $$\mu_1 = \mu_2 \quad (123)$$
Gibbs rule / Phase rule	$$f = c - p + 2 \quad (124)$$ c #components, f #degrees of freedom, p #phases

9.0.1 Osmosis

Osmosis is the spontaneous net movement or diffusion of solvent molecules through a selectively-permeable membrane, which allows through the solvent molecules, but not the solute molecules. The direction of the diffusion is from a region of high water potential (region of lower solute concentration) to a region of low water potential (region of higher solute concentration), in the direction that tends to equalize the solute concentrations on the two sides.

Osmotic pressure	$$p_{\mathrm{osm}} = k_{\mathrm{B}}T\frac{N_c}{V} \quad (125)$$ N_c #dissolved particles

9.1 Material properties

Heat capacity	$$c = \frac{Q}{\Delta T} \quad (126)$$ Q heat
Isochoric heat capacity	$$c_v = \left(\frac{\partial Q}{\partial T}\right)_V = \left(\frac{\partial U}{\partial T}\right)_V \quad (127)$$ U internal energy
Isobaric heat capacity	$$c_p = \left(\frac{\partial Q}{\partial T}\right)_P = \left(\frac{\partial H}{\partial T}\right)_P \quad (128)$$ H enthalpy
Bulk modules	$$K = -V\frac{\mathrm{d}p}{\mathrm{d}V} \quad (129)$$ p pressure, V initial volume
Compressibility	$$\kappa = -\frac{1}{V}\frac{\partial V}{\partial p} \quad (130)$$

Isothermal compressibility	$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T = \frac{1}{K} \quad (131)$$
Adiabatic compressibility	$$\kappa_S = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_S \quad (132)$$
Thermal expansion coefficient	$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{p,N} \quad (133)$$

10 Laws of thermodynamics

10.1 Zeroeth law

If two systems are each in thermal equilibrium with a third, they are also in thermal equilibrium with each other.

$$A \overset{th.eq.}{\leftrightarrow} C \quad \wedge \quad B \overset{th.eq.}{\leftrightarrow} C \quad \Rightarrow \quad A \overset{th.eq.}{\leftrightarrow} B \tag{134}$$

10.2 First law

In a process without transfer of matter, the change in internal energy, ΔU, of a thermodynamic system is equal to the energy gained as heat, Q, less the thermodynamic work, W, done by the system on its surroundings.

Internal energy change	$$\Delta U = \delta Q - \delta W \quad (135)$$ $$\mathrm{d}U = T\,\mathrm{d}S - p\,\mathrm{d}V \quad (136)$$

10.3 Second law

Clausius: Heat can never pass from a colder to a warmer body without some other change, connected therewith, occurring at the same time.
Kelvin: It is impossible for a self-acting machine, unaided by any external agency, to convey heat from one body to another at a higher temperature.

10.4 Third law

It is impussible to cool a system to absolute zero.

Entropy density	$$\lim_{T\to 0} s(T) = 0 \quad (137)$$ and therefore also $$\lim_{T\to 0} c_V = 0 \quad (138)$$ $s = \frac{S}{N}$

11 Ensembles

Table 1: caption

	\fqname :mk	\fqname :k	\fqname :gk
variables	E, V, N	T, V, N	T, V, μ
partition_sum	$\Omega = \sum_n 1$	$Z = \sum_n \mathrm{e}^{-\beta E_n}$	$Z_\mathrm{g} = \sum_n \mathrm{e}^{-\beta(E_n - \mu N_n)}$
probability	$p_n = \frac{1}{\Omega}$	$p_n = \frac{\mathrm{e}^{-\beta E_n}}{Z}$	$p_n = \frac{\mathrm{e}^{-\beta(E_n - \mu N_n)}}{Z_\mathrm{g}}$
td_pot	$S = k_\mathrm{B} \ln \Omega$	$F = -k_\mathrm{B} T \ln Z$	$\Phi = -k_\mathrm{B} T \ln Z$
pressure	$p = T\left(\frac{\partial S}{\partial V}\right)_{E,N}$	$p = -\left(\frac{\partial F}{\partial V}\right)_{T,N}$	$p = -\left(\frac{\partial \Phi}{\partial V}\right)_{T,\mu} = -\frac{\Phi}{V}$
entropy	$S = k_\mathrm{B} = \ln \Omega$	$S = -\left(\frac{\partial F}{\partial T}\right)_{V,N}$	$S = -\left(\frac{\partial \Phi}{\partial T}\right)_{V,\mu}$

Ergodic hypothesis
Over a long periode of time, all accessible microstates in the phase space are equiprobable

$$\langle A \rangle_\text{Time} = \langle A \rangle_\text{Ensemble} \tag{139}$$

A Observable

11.1 Potentials

Internal energy

$$\mathrm{d}U(S,V,N) = T\,\mathrm{d}S - p\,\mathrm{d}V + \mu\,\mathrm{d}N \tag{140}$$

Free energy / Helmholtz energy

$$\mathrm{d}F(T,V,N) = -S\,\mathrm{d}T - p\,\mathrm{d}V + \mu\,\mathrm{d}N \tag{141}$$

Enthalpy

$$\mathrm{d}H(S,p,N) = T\,\mathrm{d}S + V\,\mathrm{d}p + \mu\,\mathrm{d}N \tag{142}$$

Free enthalpy / Gibbs energy

$$\mathrm{d}G(T,p,N) = -S\,\mathrm{d}T + V\,\mathrm{d}p + \mu\,\mathrm{d}N \tag{143}$$

Grand canonical potential

$$\mathrm{d}\Phi(T,V,\mu) = -S\,\mathrm{d}T - p\,\mathrm{d}V - N\,\mathrm{d}\mu \tag{144}$$

TODO:Maxwell Relationen, TD Quadrat

Thermodynamic squre

$-S$	U	V
H		F
$-p$	G	T

The corners opposite from the potential are the coefficients and each coefficients differential is opposite to it.

12 Ideal gas

The ideal gas consists of non-interacting, undifferentiable particles.

Phase space volume
$3N$ sphere

$$\Omega(E) = \int_V \mathrm{d}^3 q_1 \ldots \int_V \mathrm{d}^3 q_N \int \mathrm{d}^3 p_1 \ldots \int \mathrm{d}^3 p_N \frac{1}{N!\, h^{3N}} \Theta\left(E - \sum_i \frac{\vec{p}_i^{\,2}}{2m}\right) \tag{145}$$

$$= \left(\frac{V}{N}\right)^N \left(\frac{4\pi m E}{3h^2 N}\right)^{\frac{3N}{2}} \mathrm{e}^{\frac{5N}{2}} \tag{146}$$

N #particles, h^{3N} volume of a microstate, $N!$ particles are undifferentiable

Entropy

$$S = \frac{5}{2} N k_\mathrm{B} + N k_\mathrm{B} \ln\left(\frac{V}{N}\left(\frac{2\pi m E}{3h^2 N}\right)^{\frac{3}{2}}\right) \tag{147}$$

Ideal gas equation

$$pV = nRT \tag{148}$$

$$= N k_\mathrm{B} T \tag{149}$$

Equation of state

$$U = \frac{3}{2} N k_\mathrm{B} T \tag{150}$$

Equipartitiontheorem
Each degree of freedom contributes U_D (for classical particle systems)

$$U_\mathrm{D} = \frac{1}{2} k_\mathrm{B} T \tag{151}$$

Maxwell velocity distribution
See also ??

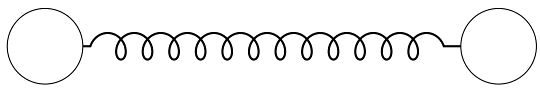
$$w(v)\,\mathrm{d}v = 4\pi \left(\frac{\beta m}{2\pi}\right)^{\frac{3}{2}} v^2\, \mathrm{e}^{-\frac{\beta m v^2}{2}}\, \mathrm{d}v \tag{152}$$

Average quadratic velocity per particle in a 3D gas

$$\langle v^2 \rangle = \int_0^\infty \mathrm{d}v\, v^2 w(v) = \frac{3 k_\mathrm{B} T}{m} \tag{153}$$

12.0.1 Molecule gas

Molecule gas
2 particles of mass M connected by a “spring” with distance L



Translation

$$p_i = \frac{2\pi\hbar}{L} n_i \tag{154}$$

$$E_\mathrm{kin} = \frac{\vec{p}_r^{\,2}}{2M} \tag{155}$$

$n_i \in \mathbb{N}_0$, $i = x, y, z$

Vibration

$$E_\mathrm{vib} = \hbar\omega\left(n + \frac{1}{2}\right) \tag{156}$$

$n \in \mathbb{N}_0$

Rotation

$$E_{\text{rot}} = \frac{\hbar^2}{2I} j(j+1) \quad (157)$$

$j \in \mathbb{N}_0$

TODO:Diagram für verschiedene Temperaturen, Weiler Skript p.83

13 Real gas

13.1 Virial expansion

Expansion of the pressure p in a power series of the density ρ.

Virial expansion
The 2$^{\text{nd}}$ and 3$^{\text{d}}$ virial coefficient are tabelated for many substances

$$p = k_B T \rho \left[1 + B(T)\rho + C(T)\rho^2 + \dots\right] \quad (158)$$

B and C 2$^{\text{nd}}$ and 3$^{\text{d}}$ virial coefficient, $\rho = \frac{N}{V}$

Mayer function

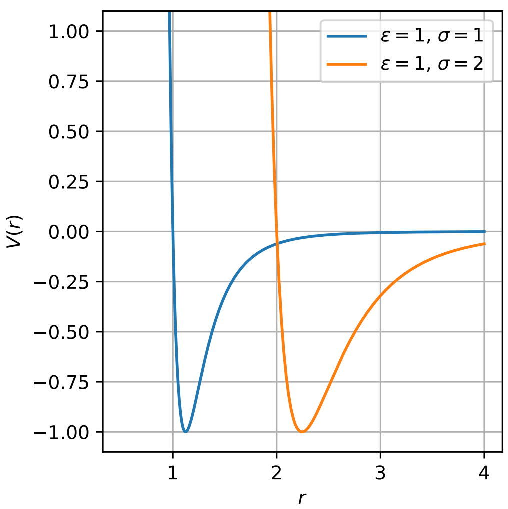
$$f(\vec{r}) = \mathrm{e}^{-\beta V(i,j)} - 1 \quad (159)$$

$V(i,j)$ pair potential

Second virial coefficient
Depends on pair potential between two molecules

$$B = -\frac{1}{2} \int_V \mathrm{d}^3\vec{r} f(\vec{r}) \quad (160)$$

Lennard-Jones potential
Potential between two molecules. Attractive for $r > \sigma$, repulsive for $r < \sigma$. In condensed matter: Attraction due to Landau Dispersion TODO:verify and repulsion due to Pauli exclusion principle.



$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \quad (161)$$

13.2 Van der Waals equation

Assumes a hard-core potential with a weak attraction.

Partition sum

$$Z_N = \frac{(V - V_0)^N}{\lambda^{3N} N!} \mathrm{e}^{\frac{\beta N^2 a}{V}} \quad (162)$$

a internal pressure

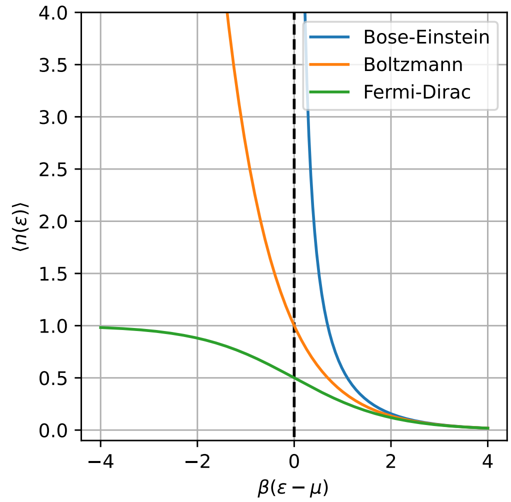
Van der Waals equation	$$p = \frac{N k_{\mathrm{B}} T}{V - b} - \frac{N^2 a}{V^2} \quad (163)$$ b co-volume?

TODO:sometimes N is included in a, b

14 Ideal quantum gas

Fugacity	$$z = \mathrm{e}^{\mu\beta} = \mathrm{e}^{\frac{\mu}{k_{\mathrm{B}}T}} \quad (164)$$
Occupation number	$$\sum_r n_r = N \quad (165)$$ r states
Undifferentiable particles	$$\lvert p_1, p_2, \dots, p_N \rangle = \lvert p_1 \rangle \lvert p_2 \rangle \dots \lvert p_N \rangle \quad (166)$$ p_i state
Applying the parity operator yields a *symmetric* (Bosons) and a *antisymmetic* (Fermions) solution	$$\hat{P}_{12}\psi(p_i(\vec{r}_1), p_j(\vec{r}_2)) = \pm\psi(p_i(\vec{r}_1), p_j(\vec{r}_2)) \quad (167)$$ $\hat{P}_{12}$ parity operator swaps 1 and 2, $\pm$: $\substack{\text{bos} \\ \text{fer}}$
Spin degeneracy factor	$$g_s = 2s + 1 \quad (168)$$ s spin
Density of states	$$g(\epsilon) = g_s \frac{V}{4\pi} \left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{\epsilon} \quad (169)$$ g_s Spin degeneracy factor
Occupation number per energy	$$n(\epsilon)\,\mathrm{d}\epsilon = \frac{g(\epsilon)}{\mathrm{e}^{\beta(\epsilon-\mu)} \mp 1}\,\mathrm{d}\epsilon \quad (170)$$ Density of states, $\pm$: $\substack{\text{bos} \\ \text{fer}}$

Occupation number



$$\langle n(\epsilon)\rangle = \frac{1}{\mathrm{e}^{\beta(\epsilon-\mu)} \mp 1} \tag{171}$$

for $\epsilon - \mu \gg k_{\mathrm{B}}T$

$$= \frac{1}{\mathrm{e}^{\beta(\epsilon-\mu)}} \tag{172}$$

$\pm$: $\substack{\text{bos}\\ \text{fer}}$

Number of particles

$$\langle N\rangle = \int_0^\infty n(\epsilon)\,\mathrm{d}\epsilon \tag{173}$$

Energy
Equal to the classical ideal gas

$$\langle E\rangle = \int_0^\infty \epsilon n(\epsilon)\;\mathrm{d}\epsilon = \frac{3}{2}pV \tag{174}$$

Equation of state
Bosons: decreased pressure, they like to cluster
Fermions: increased pressure because of the Pauli principle

$$pV = k_{\mathrm{B}}T \ln Z_g \tag{175}$$

after Virial expansion

$$= Nk_{\mathrm{B}}T\left[1 \mp \frac{\lambda^3}{2^{5/2}gv} + \mathcal{O}\left(\left(\frac{\lambda^3}{v}\right)^2\right)\right] \tag{176}$$

$\pm$: $\substack{\text{bos}\\ \text{fer}}$, $v = \frac{V}{N}$ specific volume

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Relevance of qm. corrections
Corrections become relevant when the particle distance is in the order of the thermal wavelength

$$\left(\frac{V}{N}\right)^{\frac{1}{3}} \sim \frac{\lambda}{g_s^{\frac{1}{3}}} \tag{177}$$

Generalized zeta function

$$\left.\begin{matrix} g_\nu(z) \\ f_\nu(z) \end{matrix}\right\} := \frac{1}{\Gamma(\nu)} \int_0^\infty \mathrm{d}x\, \frac{x^{\nu-1}}{\mathrm{e}^x\, z^{-1} \mp 1} \tag{178}$$

14.1 Bosons

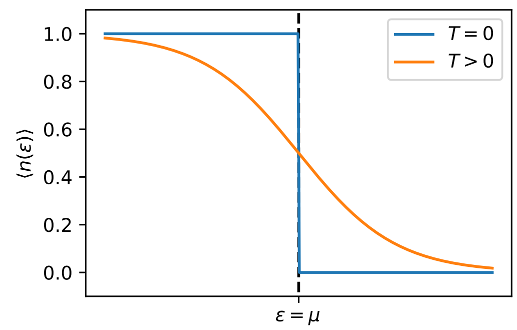
Partition sum

$$Z_{\mathrm{g}} = \prod_p \frac{1}{1 - \mathrm{e}^{-\beta(\epsilon_p - \mu)}} \tag{179}$$

$p \in \mathbb{N}_0$

Occupation number Bose-Einstein distribution	$$\langle n_p \rangle = \frac{1}{e^{\beta(\epsilon-\mu)} - 1} \quad (180)$$

14.2 Fermions

Partition sum	$$Z_g = \prod_p \left(1 + e^{-\beta(\epsilon_p - \mu)}\right) \quad (181)$$ $p = 0, 1$
Occupation number Fermi-Dirac distribution. At $T = 0$ *Fermi edge* at $\epsilon = \mu$	 $$\langle n_p \rangle = \frac{1}{e^{\beta(\epsilon-\mu)} + 1} \quad (182)$$
Slater determinant	$$\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} p_1(\vec{r}_1) & p_2(\vec{r}_1) & \dots & p_N(\vec{r}_1) \\ p_1(\vec{r}_2) & p_2(\vec{r}_2) & \dots & p_N(\vec{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ p_1(\vec{r}_N) & p_2(\vec{r}_N) & \dots & p_N(\vec{r}_N) \end{vmatrix} \quad (183)$$
Fermi energy	$$\epsilon_F := \mu(T = 0) \quad (184)$$
Fermi temperature	$$T_F := \frac{\epsilon_F}{k_B} \quad (185)$$
Fermi impulse Radius of the *Fermi sphere* in impulse space. States with p_F are in the *Fermi surface*	$$p_F = \hbar k_F = (2mE_F)^{\frac{1}{2}} \quad (186)$$
Specific density	$$v = \frac{N}{V} = \frac{g}{\lambda^3} f_{3/2}(z) \quad (187)$$ f Generalized zeta function, g degeneracy factor, z Fugacity

14.2.1 Strong degeneracy

Sommerfeld expansion for low temperatures $T \ll T_F$	$$f_\nu(z) = \frac{(\ln z)^\nu}{\Gamma(\nu+1)} \left(1 + \frac{\pi^6}{6} \frac{\nu(\nu-1)}{(\ln z)^2} + \dots\right) \quad (188)$$

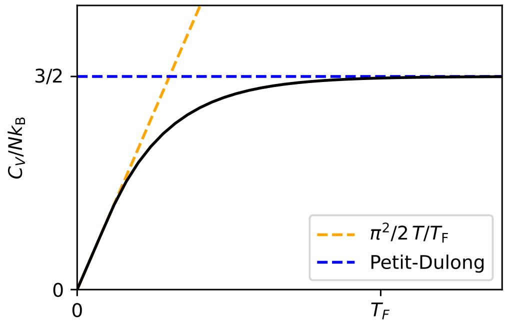
Energy density

$$\frac{E}{V} = \frac{3}{2}\frac{g}{\lambda^3} k_B T f_{5/2}(z) \tag{189}$$

Sommerfeld expansion

$$\approx \frac{3}{5}\frac{N}{V} E_F \left(1 + \frac{5\pi^2}{12}\left(\frac{k_B T}{E_F}\right)^2\right) \tag{190}$$

Heat capacity
for low temperatures $T \ll T_F$



$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = N k_B \frac{\pi}{2}\left(\frac{T}{T_F}\right) \tag{191}$$

differs from td:TODO:petit_dulong

TODO:Entartung und Sommerfeld TODO:DULONG-PETIT Gesetz

Part V
Electrodynamics

15 Hall-Effect

Cyclontron frequency	$$\omega_\text{c} = \frac{eB}{m_\text{e}} \quad (192)$$

TODO:Move

15.1 Classical Hall-Effect

Current flowing in x direction in a conductor $(l \times b \times d)$ with a magnetic field B in z direction leads to a hall voltage U_H in y direction.

Hall voltage	$$U_\text{H} = \frac{IB}{ned} \quad (193)$$ n charge carrier density
Hall coefficient Sometimes R_H	$$A_\text{H} := -\frac{E_y}{j_x B_z} \overset{\text{metals}}{\downarrow}{=} \frac{1}{ne} = \frac{\rho_{xy}}{B_z} \quad (194)$$
Resistivity	$$\rho_{xx} = \frac{m_\text{e}}{ne^2\tau} \quad (195)$$ $$\rho_{xy} = \frac{B}{ne} \quad (196)$$

15.2 Integer quantum hall effect

Conductivity tensor	$$\sigma = \begin{pmatrix} \sigma_{xy} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \quad (197)$$
Resistivity tensor	$$\rho = \sigma^{-1} \quad (198)$$
Resistivity	$$\rho_{xy} = \frac{2\pi\hbar}{e^2}\frac{1}{\nu} \quad (199)$$ $\nu \in \mathbb{Z}$ filing factor
Fractional quantum hall effect	$$\nu = \frac{1}{3}, \frac{2}{5}, \frac{3}{7}, \frac{2}{3} \dots \quad (200)$$ ν fraction of two numbers without shared divisors

- **Integer** (QHE): filling factor ν is an integer
- **Fractional** (FQHE): filling factor ν is a fraction
- **Spin** (QSHE): spin currents instead of charge currents
- **Anomalous** (QAHE): symmetry breaking by internal effects instead of external magnetic fields

TODO:sort

Impedance of a capacitor	$$Z_C = \frac{1}{i\omega C} \quad (201)$$
Impedance of an inductor	$$Z_L = i\omega L \quad (202)$$

TODO:impedance addition for parallel / linear

16 Dipole-stuff

Dipole radiation Poynting vector	$$\vec{S} = \left(\frac{\mu_0 p_0^2 \omega^4}{32\pi^2 c}\right) \frac{\sin^2\theta}{r^2} \vec{r} \quad (203)$$
Time-average power	$$P = \frac{\mu_0 \omega^4 p_0^2}{12\pi c} \quad (204)$$

17 Electric field

Electric field Surrounds charged particles	Symbol: $\vec{\mathcal{E}}$ Unit: $1\,\mathrm{V\,m^{-1}} = 1\,\mathrm{kgm/s^3A}$
Gauss's law for electric fields Electric flux through a closed surface is proportional to the electric charge	$$\Phi_E = \iint_S \vec{\mathcal{E}} \cdot d\vec{S} = \frac{Q}{\varepsilon_0} \quad (205)$$ S closed surface
Permittivity Electric polarizability of a dielectric material	Symbol: ϵ Unit: $1\,\mathrm{A\,s\,V^{-1}\,m} = 1\,\mathrm{F\,m^{-1}} = 1\,\mathrm{C\,V^{-1}\,m} = 1\,\mathrm{C^2/Nm^2} = 1\,\mathrm{A^2s^4/kgm^3}$
Relative permittivity / Dielectric constant	$$\epsilon(\omega)_r = \frac{\epsilon(\omega)}{\epsilon_0} \quad (206)$$ ϵ Permittivity, ϵ_0 Vacuum permittivity
Vacuum permittivity Electric constant	Symbol: ϵ_0 Experimental value $8.8541878188(14) \cdot 10^{-1}\,\mathrm{A\,s\,V^{-1}\,m}$
Electric susceptibility Describes how polarized a dielectric material becomes when an electric field is applied	Symbol: χ_e Unit: $$\epsilon_r = 1 + \chi_e \quad (207)$$ ϵ_r Relative permittivity / Dielectric constant

Dielectric polarization density	$$\vec{P} = \epsilon_0 \chi_e \vec{\mathcal{E}} \quad (208)$$ ϵ_0 Vacuum permittivity, χ_e Electric susceptibility, $\vec{\mathcal{E}}$ Electric field

18 Magnetic field

Magnetic flux	Symbol: Φ_B Unit: $1\,\mathrm{Wb} = 1\,\mathrm{V\,s^{-1}} = 1\,\mathrm{kgm^2/s^2A}$ $$\Phi_B = \iint_A \vec{B} \cdot d\vec{A} \quad (209)$$ $\vec{A}$ area
Magnetic flux density Defined by Lorentz force law	Symbol: $\vec{B}$ Unit: $1\,\mathrm{T} = 1\,\mathrm{Vs/m^2} = 1\,\mathrm{N\,A^{-1}\,m} = 1\,\mathrm{kg/As^2}$ $$\vec{B} = \mu_0(\vec{H} + \vec{M}) \quad (210)$$ $\vec{H}$ Magnetic field intensity, $\vec{M}$ Magnetization, μ_0 Magnetic vauum permeability
Magnetic field intensity	Symbol: $\vec{H}$ Unit: $1\,\mathrm{A\,m^{-1}}$ $$\vec{H} \equiv \frac{1}{\mu_0}\vec{B} - \vec{M} \quad (211)$$
Lorentz force law Force on charged particle	$$\vec{F} = q\vec{\mathcal{E}} + q\vec{v} \times \vec{B} \quad (212)$$
Magnetic permeability	Symbol: μ Unit: $1\,\mathrm{H\,m^{-1}} = 1\,\mathrm{V\,s\,A^{-1}\,m}$ $$\mu = \frac{B}{H} \quad (213)$$ B Magnetic flux density, H Magnetic field intensity
Magnetic vauum permeability	Symbol: μ_0 Experimental value $1.25663706127(20)\,\mathrm{H/m} = \mathrm{N/A^2}$
Relative permeability	$$\mu_r = \frac{\mu}{\mu_0} \quad (214)$$
Gauss's law for magnetism Magnetic flux through a closed surface is 0 ⇒there are no magnetic monopoles	$$\Phi_B = \iint_S \vec{B} \cdot d\vec{S} = 0 \quad (215)$$ S closed surface

Magnetization Vector field describing the density of magnetic dipoles	Symbol: $\vec{M}$ Unit: $1\,\mathrm{A\,m^{-1}}$ $$\vec{M} = \frac{\mathrm{d}\vec{m}}{\mathrm{d}V} = \chi_\mathrm{m} \cdot \vec{H} \quad (216)$$
Magnetic moment Strength and direction of a magnetic dipole	Symbol: $\vec{m}$ Unit: $1\,\mathrm{Am^2}$
Torque	$$\vec{\tau} = \vec{m} \times \vec{B} \quad (217)$$ m Magnetic moment
Susceptibility	$$\chi_\mathrm{m} = \frac{\partial M}{\partial B} = \mu_\mathrm{r} - 1 \quad (218)$$ μ_r Relative permeability

18.1 Magnetic materials

Paramagnetism Magnetic field strengthend in the material	$$\mu_\mathrm{r} > 1 \quad (219)$$ $$\chi_\mathrm{m} > 0 \quad (220)$$ μ Magnetic permeability, χ_m Susceptibility
Diamagnetism Magnetic field expelled from material	$$0 < \mu_\mathrm{r} < 1 \quad (221)$$ $$-1 < \chi_\mathrm{m} < 0 \quad (222)$$ μ Magnetic permeability, χ_m Susceptibility
Ferromagnetism Magnetic moments align to external magnetic field and stay aligned when the field is turned off (Remanescence)	$$\mu_\mathrm{r} \gg 1 \quad (223)$$ μ Magnetic permeability, χ_m Susceptibility

19 Electromagnetism

Speed of light in the vacuum	Symbol: c Experimental value $299792458\,\mathrm{m\,s^{-1}}$
Vacuum permittivity - permeability relation TODO:Does this have a name?	$$\epsilon_0 \mu_0 = \frac{1}{c^2} \quad (224)$$ ϵ_0 Vacuum permittivity, μ_0 Magnetic vauum permeability, c Speed of light

Poisson equation for electrostatics	$$\triangle\Phi(\vec{r}) = -\frac{\rho(\vec{r})}{\epsilon} \quad (225)$$ TODO:double check Φ ρ Charge density, ϵ Permittivity, Φ Potential
Poynting vector Directional energy flux or power flow of an electromagnetic field [W/m^2]	$$\vec{S} = \vec{E} \times \vec{H} \quad (226)$$

19.1 Maxwell-Equations

Vacuum microscopic formulation	$$\vec{\nabla}\cdot\vec{\mathcal{E}} = \frac{\rho_{\text{el}}}{\epsilon_0} \quad (227)$$ $$\vec{\nabla}\cdot\vec{B} = 0 \quad (228)$$ $$\vec{\nabla}\times\vec{\mathcal{E}} = -\frac{\mathrm{d}\vec{B}}{\mathrm{d}t} \quad (229)$$ $$\vec{\nabla}\times\vec{B} = \mu_0\vec{j} + \frac{1}{c^2}\frac{\mathrm{d}\vec{\mathcal{E}}}{\mathrm{d}t} \quad (230)$$
Matter Macroscopic formulation	$$\vec{\nabla}\cdot\vec{D} = \rho_{\text{el}} \quad (231)$$ $$\vec{\nabla}\cdot\vec{B} = 0 \quad (232)$$ $$\vec{\nabla}\times\vec{\mathcal{E}} = -\frac{\mathrm{d}\vec{B}}{\mathrm{d}t} \quad (233)$$ $$\vec{\nabla}\times\vec{H} = \vec{j} + \frac{\mathrm{d}\vec{D}}{\mathrm{d}t} \quad (234)$$

TODO:Polarization

19.2 Induction

Faraday's law of induction	$$U_{\text{ind}} = -\frac{\mathrm{d}}{\mathrm{d}t}\Phi_{\text{B}} = -\frac{\mathrm{d}}{\mathrm{d}t}\iint_A \vec{B}\cdot\mathrm{d}\vec{A} \quad (235)$$
Lenz's law	Change of magnetic flux through a conductor induces a current that counters that change of magnetic flux.

Part VI

Quantum Mechanics

20 Basics

20.1 Operators

Dirac notation	$\langle x \|$ "Bra" Row vector	(236)
	$\| x \rangle$ "Ket" Column vector	(237)
	$\hat{A} \| \beta \rangle = \| \alpha \rangle \Rightarrow \langle \alpha \| = \langle \beta \| \hat{A}^\dagger$	(238)
Dagger	$\hat{A}^\dagger = (\hat{A}^*)^\mathrm{T}$	(239)
	$(c\hat{A})^\dagger = c^* \hat{A}^\dagger$	(240)
	$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$	(241)
		(242)
Adjoint operator	$\langle \alpha \| \hat{A}^\dagger \| \beta \rangle = \langle \beta \| \hat{A} \| \alpha \rangle^*$	(243)
Hermitian operator	$\hat{A} = \hat{A}^\dagger$	(244)

20.1.1 Measurement

An observable is a hermition operator acting on $\hat{H}$. The measurement randomly yields one of the eigenvalues of $\hat{O}$ (all real).

Measurement probability Probability to measure ψ in state λ	$p(\lambda) = \langle \psi \| \hat{P}_\lambda \| \psi \rangle$	(245)
State after measurement	$\| \psi \rangle_\text{post} = \frac{1}{\sqrt{p(\lambda)}} \hat{P}_\lambda \| \psi \rangle$	(246)

20.1.2 Pauli matrices

Pauli matrices	*TODO* : remove macro2	(247)

20.2 Probability theory

Continuity equation	$\frac{\partial \rho(\vec{x},t)}{\partial t} + \nabla \cdot \vec{j}(\vec{x},t) = 0$ ρ density of a conserved quantity q, j flux density of q	(248)
State probability	*TODO*	(249)

Dispersion	$$\Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle \quad (250)$$
Generalized uncertainty principle	$$\sigma_A\sigma_B \geq \frac{1}{4}\langle[\hat{A},\hat{B}]\rangle^2 \quad (251)$$ $$\sigma_A\sigma_B \geq \frac{1}{2}\lvert\langle[\hat{A},\hat{B}]\rangle\rvert \quad (252)$$

20.3 Commutator

Commutator	$$[A,B] = AB - BA \quad (253)$$
Anticommutator	$$\{A,B\} = AB + BA \quad (254)$$
Commutation relations	$$[A,BC] = [A,B]C - B[A,C] \quad (255)$$
TODO:add some more? Commutator involving a function	$$[f(A),B] = [A,B]\frac{\partial f}{\partial A} \quad (256)$$ given $[A,[A,B]] = 0$
Jacobi identity	$$[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0 \quad (257)$$
Hadamard's Lemma	$$\mathrm{e}^A B \mathrm{e}^{-A} = B + [A,B] + \frac{1}{2!}[A,[A,B]] + \frac{1}{3!}[A,[A,[A,B]]] + \dots \quad (258)$$
Canonical commutation relation	$$[x_i,x_j] = 0 \quad (259)$$ $$[p_i,p_j] = 0 \quad (260)$$ $$[x_i,p_j] = i\hbar\delta_{ij} \quad (261)$$ x, p canonical conjugates

21 Schrödinger equation

Energy operator	$$E = i\hbar\frac{\partial}{\partial t} \quad (262)$$
Momentum operator	$$\vec{p} = -i\hbar\vec{\nabla}_x \quad (263)$$
Space operator	$$\vec{x} = i\hbar\vec{\nabla}_p \quad (264)$$
Stationary Schrödingerequation	$$\hat{H}\lvert\psi\rangle = E\lvert\psi\rangle \quad (265)$$

Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = (-\frac{\hbar^2}{2m}\vec{\nabla}^2 + \vec{V}(x))\psi(x) \quad (266)$$

21.1 Time evolution

The time evolution of the Hamiltonian is given by:

Time evolution operator

$$|\psi(t)\rangle = \hat{U}(t,t_0)\,|\psi(t_0)\rangle \quad (267)$$

U unitary

Von-Neumann Equation
Time evolution of the density operator in the Schrödinger picture. Qm analog to the Liouville equation ??

$$\frac{\partial\hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] \quad (268)$$

Lindblad master equation
Generalization of von-Neummann equation for open quantum systems

$$\dot{\rho} = \underbrace{-\frac{i}{\hbar}[\hat{H},\rho]}_{\text{reversible}} + \underbrace{\sum_{n.m} h_{nm}\left(\hat{A}_n\rho\hat{A}_{m^\dagger} - \frac{1}{2}\left\{\hat{A}_m^\dagger\hat{A}_n,\rho\right\}\right)}_{\text{irreversible}} \quad (269)$$

h positive semidifnite matrix, $\hat{A}$ arbitrary operator

Hellmann-Feynman-Theorem
Derivative of the energy to a parameter

$$\frac{\mathrm{d}E_\lambda}{\mathrm{d}\lambda} = \int \mathrm{d}^3r\psi_\lambda^*\frac{\mathrm{d}\hat{H}_\lambda}{\mathrm{d}\lambda}\psi_\lambda = \left\langle\psi(\lambda)\middle|\frac{\mathrm{d}\hat{H}_\lambda}{\mathrm{d}\lambda}\middle|\psi(\lambda)\right\rangle \quad (270)$$

TODO:unitary transformation of time dependent H

21.1.1 Schrödinger- and Heisenberg-pictures

In the **Schrödinger picture**, the time dependecy is in the states while in the **Heisenberg picture** the observables (operators) are time dependent.

Schrödinger time evolution

$$|\psi(t)_\mathrm{S}\rangle = \hat{U}(t,t_0)\,|\psi(t_0)\rangle \quad (271)$$

Heisenberg time evolution

$$|\psi_\mathrm{H}\rangle = |\psi_\mathrm{S}(t_0)\rangle \quad (272)$$

$$A_\mathrm{H} = U^\dagger(t,t_0)A_\mathrm{S}U(t,t_0) \quad (273)$$

$$\frac{\mathrm{d}\hat{A}_\mathrm{H}}{\mathrm{d}t} = \frac{1}{i\hbar}[\hat{A}_\mathrm{H},\hat{H}_\mathrm{H}] + \left(\frac{\partial\hat{A}_\mathrm{S}}{\partial t}\right)_\mathrm{H} \quad (274)$$

H and S being the Heisenberg and Schrödinger picture, respectively

21.1.2 Ehrenfest theorem

See also ??

Ehrenfest theorem
applies to both pictures

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle \quad (275)$$

Ehrenfest theorem example Example for x	$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x\rangle = -\langle\nabla V(x)\rangle = \langle F(x)\rangle$$	(276)

21.2 Correspondence principle

The classical mechanics can be derived from quantum mechanics in the limit of large quantum numbers.

22 Pertubation theory

qm:qm_pertubation:desc

Hamiltonian	$$\hat{H} = \hat{H}_0 + \lambda\hat{H}_1$$	(277)
Power series	$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$	(278)
	$$\lvert\psi_n\rangle = \lvert\psi_n^{(0)}\rangle + \lambda\lvert\psi_n^{(1)}\rangle + \lambda^2\lvert\psi_n^{(2)}\rangle + \dots$$	(279)
1. order energy shift	$$E_n^{(1)} = \left\langle\psi_n^{(0)}\middle\vert\hat{H}_1\middle\vert\psi_n^{(0)}\right\rangle$$	(280)
1. order states	$$\lvert\psi_n^{(1)}\rangle = \sum_{k\neq n}\frac{\left\langle\psi_k^{(0)}\middle\vert\hat{H}_1\middle\vert\psi_n^{(0)}\right\rangle}{E_n^{(0)} - E_k^{(0)}}\lvert\psi_k^{(0)}\rangle$$	(281)
2. order energy shift	$$E_n^{(2)} = \sum_{k\neq n}\frac{\left\lvert\left\langle\psi_k^{(0)}\middle\vert\hat{H}_1\middle\vert\psi_n^{(0)}\right\rangle\right\rvert^2}{E_n^{(0)} - E_k^{(0)}}$$	(282)
Fermiś golden rule Transition rate from initial state $\lvert i\rangle$ under a pertubation H^1 to final state $\lvert f\rangle$	$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}\lvert\langle f\rvert H^1\lvert i\rangle\rvert^2\rho(E_f)$$	(283)

23 Harmonic oscillator

Hamiltonian	$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$$	(284)
	$$= \frac{1}{2}\hbar\omega + \omega a^\dagger a$$	(285)
Energy spectrum	$$E_n = \hbar\omega\left(\frac{1}{2} + n\right)$$	(286)

See also ??

23.1 Creation and Annihilation operators / Ladder operators

Particle number operator/occupation number operator	$$\hat{N} := a^\dagger a \quad (287)$$ $$\hat{N}\lvert n\rangle = n\lvert N\rangle \quad (288)$$ $\lvert n\rangle$ = Fock states, $\hat{a}$ = Annihilation operator, $\hat{a}^\dagger$ = Creation operator
Commutator	$$[\hat{a},\hat{a}^\dagger] = 1 \quad (289)$$ $$[N,\hat{a}] = -\hat{a} \quad (290)$$ $$[N,\hat{a}^\dagger] = \hat{a}^\dagger \quad (291)$$
Application on states	$$\hat{a}\lvert n\rangle = \sqrt{n}\lvert n-1\rangle \quad (292)$$ $$\hat{a}^\dagger\lvert n\rangle = \sqrt{n+1}\lvert n+1\rangle \quad (293)$$ $$\lvert n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\lvert 0\rangle \quad (294)$$
Matrix forms	$$\hat{n} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & N \end{pmatrix} \quad (295)$$ $$\hat{a} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \sqrt{N} \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (296)$$ $$\hat{a}^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 \\ 0 & 0 & \sqrt{N} & 0 \end{pmatrix} \quad (297)$$

23.1.1 Harmonischer Oszillator

Harmonic oscillator	$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^\dagger) \quad (298)$$ $$\hat{p} = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}-\hat{a}^\dagger) \quad (299)$$ $$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \quad (300)$$ $$a = \frac{1}{\sqrt{2}}(\tilde{X}+i\tilde{P}) \quad (301)$$ $$a^\dagger = \frac{1}{\sqrt{2}}(\tilde{X}-i\tilde{P}) \quad (302)$$

24 Angular momentum

24.1 Aharanov-Bohm effect

Acquired phase
Electron along a closed loop aquires a phase proportional to the enclosed magnetic flux

$$\delta = \frac{2e}{\hbar} \oint \vec{A} \cdot \mathrm{d}\vec{s} = \frac{2e}{\hbar} \Phi \tag{303}$$

TODO:replace with loop intergral symbol and add more info

25 Periodic potentials

Bloch waves
Solve the stat. SG in periodic potential with period $\vec{R}$: $V(\vec{r}) = V(\vec{r} + \vec{R})$

$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \cdot u_{\vec{k}}(\vec{r}) \tag{304}$$

$\vec{k}$ arbitrary, u periodic function

Periodicity

$$u_{\vec{k}}(\vec{r} + \vec{R}) = u_{\vec{k}}(\vec{r}) \tag{305}$$
$$\psi_{\vec{k}+\vec{G}}(\vec{r}) = \psi_{\vec{k}}(\vec{r}) \tag{306}$$

$\vec{R}$ Lattice vector, $\vec{G}$ Reciprokal attice vector

26 Symmetries

Most symmetry operators are unitary **??** because the norm of a state must be invariant under transformations of space, time and spin.

Invariance
$\hat{H}$ is invariant under a symmetrie described by $\hat{U}$ if this holds

$$\hat{U}\hat{H}\hat{U}^\dagger = \hat{H} \Leftrightarrow [\hat{U}, \hat{H}] = 0 \tag{307}$$

26.1 Time-reversal symmetry

Time-reversal symmetry

$$T : t \to -t \tag{308}$$

Anti-unitary

$$T^2 = -1 \tag{309}$$

27 Two-level systems (TLS)

James-Cummings Hamiltonian
TLS interacting with optical cavity

$$H = \underbrace{\hbar\omega_c \hat{a}^\dagger \hat{a}}_{\text{field}} + \underbrace{\hbar\omega_a \frac{\hat{\sigma}_z}{2}}_{\text{atom}} + \underbrace{\frac{\hbar\Omega}{2}\hat{E}\hat{S}}_{\text{int}} \tag{310}$$

after RWA:

$$\tag{311}$$

$$= \hbar\omega_c \hat{a}^\dagger \hat{a} + \hbar\omega_a \hat{\sigma}^\dagger \hat{\sigma} + \frac{\hbar\Omega}{2}(\hat{a}\hat{\sigma}^\dagger + \hat{a}^\dagger \hat{\sigma}) \tag{312}$$

$\hat{E} = E_{\text{ZPF}}(\hat{a} + \hat{a}^\dagger)$ field operator with bosonic ladder operators, $\hat{S} = \hat{\sigma}^\dagger + \hat{\sigma}$ polarization operator with ladder operators of the TLS

28 Other

Rotating Wave Approximation (RWS)
Rapidly oscilating terms are neglected

$$\Delta\omega := |\omega_0 - \omega_\mathrm{L}| \ll |\omega_0 + \omega_\mathrm{L}| \approx 2\omega_0 \tag{313}$$

ω_L light frequency, ω_0 transition frequency

Slater determinant
Construction of a fermionic (antisymmetric) many-particle wave function from single-particle wave functions

$$\Psi(q_1,\dots,q_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_a(q_1) & \phi_a(q_2) & \cdots & \phi_a(q_N) \\ \phi_b(q_1) & \phi_b(q_2) & \cdots & \phi_b(q_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_z(q_1) & \phi_z(q_2) & \cdots & \phi_z(q_N) \end{vmatrix} \tag{314}$$

29 Hydrogen Atom

Reduced mass

$$\mu = \frac{m_\mathrm{e} m_\mathrm{K}}{m_\mathrm{e} + m_\mathrm{K}} \overset{m_\mathrm{e} \ll m_\mathrm{K}}{\approx} m_\mathrm{e} \tag{315}$$

Coulumb potential
For a single electron atom

$$V(\vec{r}) = \frac{Z\,e^2}{4\pi\epsilon_0 r} \tag{316}$$

Z atomic number

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2\mu}\vec{\nabla}_{\vec{r}}^2 - V(\vec{r}) \tag{317}$$

$$= \frac{\hat{p}_r^2}{2\mu} + \frac{\hat{L}^2}{2\mu r} + V(r) \tag{318}$$

Wave function

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r) Y_{lm}(\theta,\phi) \tag{319}$$

$R_{nl}(r)$ Radial part, Y_{lm} qm:spherical_harmonics

Radial part

$$R_{nl} = -\sqrt{\frac{(n-l-1)!(2\kappa)^3}{2n[(n+l)!]^3}}(2\kappa r)^l\,\mathrm{e}^{-\kappa r}\,L_{n+1}^{2l+1}(2\kappa r) \tag{320}$$

with

$$\kappa = \frac{\sqrt{2\mu|E|}}{\hbar} = \frac{Z}{n a_\mathrm{B}} \tag{321}$$

$L_r^s(x)$ Laguerre-polynomials

Energy eigenvalues

$$E_n = \frac{Z^2 \mu e^4}{n^2 (4\pi\epsilon_0)^2 2\hbar^2} = -E_\mathrm{H}\frac{Z^2}{n^2} \tag{322}$$

Rydberg energy

$$E_\mathrm{H} = h\,c\,R_\mathrm{H} = \frac{\mu e^4}{(4\pi\epsilon_0)^2 2\hbar^2} \tag{323}$$

29.1 Corrections

29.1.1 Darwin term

Relativisitc correction: Because of the electrons zitterbewegung, it is not entirely localised. TODO:fact check

Energy shift

$$\Delta E_{\text{rel}} = -E_n \frac{Z^2\alpha^2}{n}\left(\frac{3}{4n} - \frac{1}{l+\frac{1}{2}}\right) \tag{324}$$

Fine-structure constant
Sommerfeld constant

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137} \tag{325}$$

29.1.2 Spin-orbit coupling (LS-coupling)

The interaction of the electron spin with the electrostatic field of the nuclei lead to energy shifts.

Energy shift

$$\Delta E_{\text{LS}} = \frac{\mu_0 Z e^2}{8\pi m_e^2 r^3}\langle \vec{S}\cdot\vec{L}\rangle \tag{326}$$

TODO:name

$$\begin{aligned}\langle \vec{S}\cdot\vec{L}\rangle &= \frac{1}{2}\langle [J^2 - L^2 - S^2]\rangle \\ &= \frac{\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)] \end{aligned} \tag{327}$$

29.1.3 Fine-structure

The fine-structure combines relativistic corrections 29.1.1 and the spin-orbit coupling 29.1.2.

Energy shift

$$\Delta E_{\text{FS}} = \frac{Z^2\alpha^2}{n}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right) \tag{328}$$

29.1.4 Lamb-shift

The interaction of the electron with virtual photons emitted/absorbed by the nucleus leads to a (very small) shift in the energy level.

Potential energy

$$\langle E_{\text{pot}}\rangle = -\frac{Ze^2}{4\pi\epsilon_0}\left\langle\frac{1}{r+\delta r}\right\rangle \tag{329}$$

δr pertubation of r

29.1.5 Hyperfine structure

Interaction of the nucleus spin with the magnetic field created by the electron leads to energy shifts. (Lifts degeneracy)

Nuclear spin

$$\vec{F} = \vec{J} + \vec{I} \tag{330}$$

$$|\vec{I}| = \sqrt{i(i+1)}\hbar \tag{331}$$

$$I_z = m_i\hbar \tag{332}$$

$$m_i = -i, -i+1, \dots, i-1, i \tag{333}$$

Combined angular momentum	$$\vec{F} = \vec{J} + \vec{I} \quad (334)$$ $$\lvert\vec{F}\rvert = \sqrt{f(f+1)}\hbar \quad (335)$$ $$F_z = m_f \hbar \quad (336)$$
Selection rule	$$f = j \pm i \quad (337)$$ $$m_f = -f, -f+1, \dots, f-1, f \quad (338)$$
Hyperfine structure constant	$$A = \frac{g_i \mu_K B_{HFS}}{\sqrt{j(j+1)}} \quad (339)$$ B_{HFS} hyperfine field, μ_K nuclear magneton, g_i nuclear g-factor ??
Energy shift	$$\Delta H_{HFS} = \frac{A}{2}[f(f+1) - j(j+1) - i(i+1)] \quad (340)$$

TODO:landé factor

29.2 Effects in magnetic field

TODO:all
TODO:Hunds rules

29.3 misc

Auger-Meitner-Effekt Auger-Effect	An excited electron relaxes into a lower, unoccupied energy level. The released energy causes the emission of another electron in a higher energy level (Auger-Electron)

Part VII
Condensed matter physics

TODO:Bonds, hybridized orbitals

30 Crystals

30.1 Bravais lattice

Table 2: In 2D, there are 5 different Bravais lattices

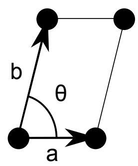
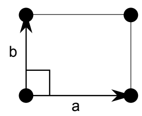
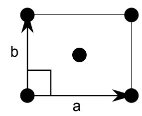
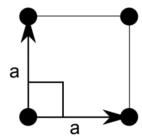
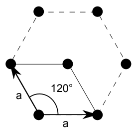
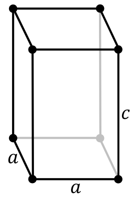
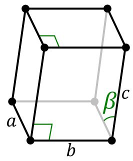
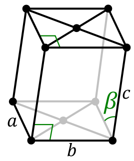
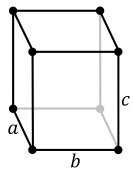
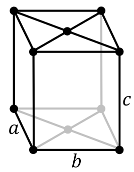
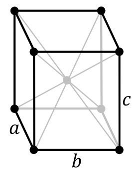
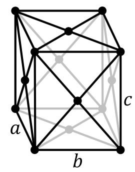
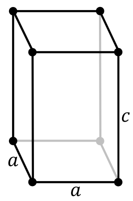
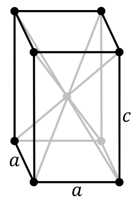
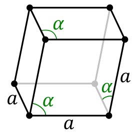
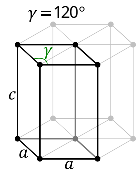
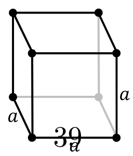
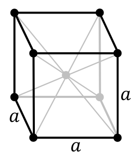
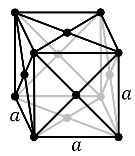
Lattice system	Point group	5 Bravais lattices	
		primitive (p)	centered (c)
monoclinic (m)	C_2		
orthorhombic (o)	D_2		
tetragonal (t)	D_4		
hexagonal (h)	D_6		

Table 3: In 3D, there are 14 different Bravais lattices

Crystal system	Lattice system	Point group	14 Bravais lattices			
			primitive (P)	base_centered (S)	body_centered (I)	face_centered (F)
triclinic (a)		C_i				
monoclinic (m)		C_{2h}				
orthorhombic (o)		D_{2h}				
tetragonal (t)		D_{4h}				
hexagonal (h)	rhombohedral	D_{3d}				
	hexagonal	D_{6h}				
cubic (c)		O_h				

Lattice constant Parameter (length or angle) describing the smallest unit cell	Symbol: a Unit:
Lattice vector	Symbol: $\vec{R}$ Unit: $$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \quad (341)$$ $n_i \in \mathbb{Z}$

TODO:primitive unit cell: contains one lattice point

Miller index	$$(hkl)\text{plane} \quad (342)$$ $$[hkl]\text{direction} \quad (343)$$ $$\{hkl\}\text{millerFamily} \quad (344)$$ Miller family: planes that are equivalent due to crystal symmetry

30.2 Reciprocal lattice

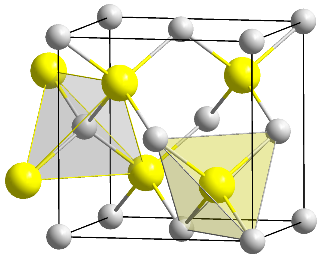
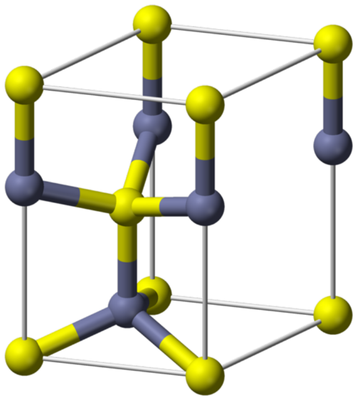
The reciprokal lattice is made up of all the wave vectors $\vec{k}$ that ressemble standing waves with the periodicity of the Bravais lattice.

Reciprocal lattice vectors	$$\vec{b_1} = \frac{2\pi}{V_c}\vec{a}_2 \times \vec{a}_3 \quad (345)$$ $$\vec{b_2} = \frac{2\pi}{V_c}\vec{a}_3 \times \vec{a}_1 \quad (346)$$ $$\vec{b_3} = \frac{2\pi}{V_c}\vec{a}_1 \times \vec{a}_2 \quad (347)$$ a_i real-space lattice vectors, V_c volume of the primitive lattice cell
Reciprokal attice vector	Symbol: $\vec{G}$ Unit: $$\vec{G}_{hkl} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3} \quad (348)$$ $n_i \in \mathbb{Z}$

30.3 Scattering processes

Matthiessen's rule Approximation, only holds if the processes are independent of each other	$$\frac{1}{\mu} = \sum_{i=\text{Scattering processes}} \frac{1}{\mu_i} \quad (349)$$ $$\frac{1}{\tau} = \sum_{i=\text{Scattering processes}} \frac{1}{\tau_i} \quad (350)$$ μ Electrical mobility, τ Scattering time

30.4 Lattices

Simple cubic (SC) Reciprocal: Simple cubic	$$\vec{a}_1 = a \begin{pmatrix}1\\0\\0\end{pmatrix}, \vec{a}_2 = a \begin{pmatrix}0\\1\\0\end{pmatrix}, \vec{a}_3 = a \begin{pmatrix}0\\0\\1\end{pmatrix} \quad (351)$$ a Lattice constant
Body centered cubic (BCC) Reciprocal: cm:bravais:fcc	$$\vec{a}_1 = \frac{a}{2} \begin{pmatrix}-1\\1\\1\end{pmatrix}, \vec{a}_2 = \frac{a}{2} \begin{pmatrix}1\\-1\\1\end{pmatrix}, \vec{a}_3 = \frac{a}{2} \begin{pmatrix}1\\1\\-1\end{pmatrix} \quad (352)$$ a Lattice constant
Face centered cubic (FCC) Reciprocal: cm:bravais:bcc	$$\vec{a}_1 = \frac{a}{2} \begin{pmatrix}0\\1\\1\end{pmatrix}, \vec{a}_2 = \frac{a}{2} \begin{pmatrix}1\\0\\1\end{pmatrix}, \vec{a}_3 = \frac{a}{2} \begin{pmatrix}1\\1\\0\end{pmatrix} \quad (353)$$ a Lattice constant
Diamond lattice	cm:bravais:fcc with basis $\begin{pmatrix}0 & 0 & 0\end{pmatrix}$ and $\begin{pmatrix}\frac{1}{4} & \frac{1}{4} & \frac{1}{4}\end{pmatrix}$
Zincblende lattice	 Like cm:bravais:diamond but with different species on each basis
Wurtzite structure hP4	 Placeholder cm:crystal:lat:wurtzite:desc

31 Free electron gas

Assumptions: electrons can move freely and independent of each other.

Drift velocity Velocity component induced by an external force (eg. electric field)	$$\vec{v}_\text{D} = \vec{v} - \vec{v}_\text{th} \quad (354)$$ v_th thermal velocity

Mean free path	$$\ell = \langle v \rangle \tau \quad (355)$$
Electrical mobility How quickly a particle moves through a material when moved by an electric field	Symbol: μ Unit: $1\,\mathrm{cm^2/Vs}$ $$\mu = \frac{q\tau}{m} \quad (356)$$ q Charge, m Mass, τ Scattering time

31.1 2D electron gas

Lower dimension gases can be obtained by restricting a 3D gas with infinetly high potential walls on a narrow area with the width L.

Confinement energy Raises ground state energy	$$\Delta E = \frac{\hbar^2 \pi^2}{2 m_\mathrm{e} L^2} \quad (357)$$
Energy	$$E_n = \underbrace{\frac{\hbar^2 k_\parallel^2}{2 m_\mathrm{e}}}_{x\text{-}y\text{: plain wave}} + \underbrace{\frac{\hbar^2 \pi^2}{2 m_\mathrm{e} L^2} n^2}_{z} \quad (358)$$

31.2 1D electron gas / quantum wire

Energy	$$E_n = \frac{\hbar^2 k_x^2}{2 m_\mathrm{e}} + \frac{\hbar^2 \pi^2}{2 m_\mathrm{e} L_z^2} n_1^2 + \frac{\hbar^2 \pi^2}{2 m_\mathrm{e} L_y^2} n_2^2 \quad (359)$$

TODO:conduntance

31.3 0D electron gas / quantum dot

TODO:TODO

32 Charge transport

32.1 Drude model

Classical model describing the transport properties of electrons in materials (metals): The material is assumed to be an ion lattice and with freely moving electrons (electron gas). The electrons are accelerated by an electric field and decelerated through collisions with the lattice ions. The model disregards the Fermi-Dirac partition of the conducting electrons.

Equation of motion	$$m_\mathrm{e} \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} + \frac{m_\mathrm{e}}{\tau} \vec{v}_\mathrm{D} = -e\vec{\mathcal{E}} \quad (360)$$ v electron speed, $\vec{v}_\mathrm{D}$ drift velocity, τ mean free time between collisions

Scattering time Momentum relaxation time	Symbol: τ Unit: $1\,\mathrm{s}$ τ the average time between scattering events weighted by the characteristic momentum change cause by the scattering process.
Current density Ohm's law	Symbol: $\vec{j}$ Unit: $1\,\mathrm{A/m^2}$ $$\vec{j} = -ne\vec{v}_\mathrm{D} = ne\mu\vec{\mathcal{E}} \quad (361)$$ n charge particle density
Drude-conductivity	$$\sigma = \frac{\vec{j}}{\vec{\mathcal{E}}} = \frac{e^2\tau n}{m_\mathrm{e}} = ne\mu \quad (362)$$

32.2 Sommerfeld model

Assumes a gas of free fermions underlying the pauli-exclusion principle. Only electrons in an energy range of $k_\mathrm{B}T$ around the Fermi energy E_F participate in scattering processes.

Electrical current density	$$\vec{j} = -en\langle v\rangle = -en\frac{\hbar}{m_\mathrm{e}}\langle\vec{k}\rangle = -e\frac{1}{V}\sum_{\vec{k},\sigma}\frac{\hbar\vec{k}}{m_\mathrm{e}} \quad (363)$$

TODO:The formula for the conductivity is the same as in the drude model?

32.3 Boltzmann-transport

Semiclassical description using a probability distribution (stat:todo:fermi_dirac) to describe the particles.

Boltzmann Transport equation for charge transport	$$\frac{\partial f(\vec{r},\vec{k},t)}{\partial t} = -\vec{v}\cdot\vec{\nabla}_{\vec{r}}f - \frac{e}{\hbar}(\vec{\mathcal{E}} + \vec{v}\times\vec{B})\cdot\vec{\nabla}_{\vec{k}}f + \left(\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right)_\mathrm{scatter} \quad (364)$$ f ??

32.4 misc

Tsu-Esaki tunneling current Describes the current $I_{\mathrm{L}\leftrightarrow\mathrm{R}}$ through a barrier	$$I_\mathrm{T} = \frac{2e}{h}\int_{U_\mathrm{L}}^{\infty}\left(f(E,\mu_\mathrm{L}) - f(E,\mu_\mathrm{R})\right)T(E)\,\mathrm{d}E \quad (365)$$ μ_i ???:chemical_pot at left/right side, U_i voltage on left/right side. Electrons occupy region between U_i and μ_i
Charge continuity equation Electric charge can only change by the amount of electric current	$$\frac{\partial\rho}{\partial t} = -\nabla\vec{j} \quad (366)$$ ρ Charge density, $\vec{j}$ Current density

33 Superconductivity

Materials for which the electric resistance jumps to 0 under a critical temperature T_c. Below T_c they have perfect conductivity and perfect diamagnetism, up until a critical magnetic field B_c.
Type I: Has a single critical magnetic field at which the superconutor becomes a normal conductor.
Type II: Has two critical

Perfect conductor	In contrast to a superconductor, perfect conductors become diamagnetic only when the external magnetic field is turned on **after** the material was cooled below the critical temperature. (ed:fields:mag:induction:lenz)
Meißner-Ochsenfeld effect Perfect diamagnetism	External magnetic field decays exponetially inside the superconductor below a critical temperature and a critical magnetic field.

33.1 London equations

Quantitative description of the Meißner-Ochsenfeld effect.

First London Equation	$$\frac{\partial \vec{j}_s}{\partial t} = \frac{n_s q_s^2}{m_s} \vec{E} - \mathcal{O}\left(\vec{j}_s^2\right) \quad (367)$$ $\vec{j}$ current density, n_s, m_s, q_s density, mass and charge of superconduticng particles
Second London Equation Describes the Meißner-Ochsenfeld effect	$$\vec{\nabla} \times \vec{j}_s = -\frac{n_s q_s^2}{m_s} \vec{B} \quad (368)$$ $\vec{j}$ current density, n_s, m_s, q_s density, mass and charge of superconduticng particles
London penetration depth	$$\lambda_L = \sqrt{\frac{m_s}{\mu_0 n_s q_s^2}} \quad (369)$$

33.2 Ginzburg-Landau Theory (GLAG)

Ginzburg-Landau Coherence Length	$$\xi_{GL} = \frac{\hbar}{\sqrt{2m\lvert\alpha\rvert}} \quad (370)$$ $$\xi_{GL}(T) = \xi_{GL}(0) \frac{1}{\sqrt{1 - \frac{T}{T_c}}} \quad (371)$$
Ginzburg-Landau Penetration Depth / Field screening length	$$\lambda_{GL} = \sqrt{\frac{m_s \beta}{\mu_0 \lvert\alpha\rvert q_s^2}} \quad (372)$$ $$\lambda_{GL}(T) = \lambda_{GL}(0) \frac{1}{\sqrt{1 - \frac{T}{T_c}}} \quad (373)$$

First Ginzburg-Landau Equation	$$\alpha\Psi + \beta\|\Psi\|^2\Psi + \frac{1}{2m}(-i\hbar\vec{\nabla} + 2e\vec{A})^2\Psi = 0 \quad (374)$$ ξ_{GL} Ginzburg-Landau Coherence Length, λ_{GL} Ginzburg-Landau Penetration Depth / Field screening length
Second Ginzburg-Landau Equation	$$\vec{j}_s = \frac{ie\hbar}{m}(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*) - \frac{4e^2}{m}\|\Psi\|^2\vec{A} \quad (375)$$

TODO:proximity effect

33.3 Microscopic theory

33.4 BCS-Theory

34 Semiconductors

Intrinsic/extrinsic	Intrinsic: pure, electron density determiend only by thermal excitation and $n_i^2 = n_0 p_0$ Extrinsic: doped n, p Equilibrium charge densitites
Equilibrium charge densitites Holds when $\frac{E_c - E_F}{k_B T} > 3.6$ and $\frac{E_F - E_v}{k_B T} > 3.6$	$$n_0 \approx N_c(T)\exp\left(-\frac{E_c - E_F}{k_B T}\right) \quad (376)$$ $$p_0 \approx N_v(T)\exp\left(-\frac{E_F - E_v}{k_B T}\right) \quad (377)$$
Intrinsic charge density	$$n_i \approx \sqrt{n_0 p_0} = \sqrt{N_c(T)N_v(T)}\exp\left(-\frac{E_{gap}}{2k_B T}\right) \quad (378)$$
Mass action law Charge densities at thermal equilibrium, independent of doping	$$np = n_i^2 \quad (379)$$

	$E_{gap}(0\,K)[eV]$	$E_{gap}(300\,K)[eV]$	
Diamond	5,48	5,47	indirect
Si	1,17	1,12	indirect
Ge	0,75	0,66	indirect
GaP	2,32	2,26	indirect
GaAs	1,52	1,43	direct
InSb	0,24	0,18	direct
InP	1,42	1,35	direct
CdS	2.58	2.42	direct

Minority / Majority charge carriers	Majority carriers: higher number of particles (e^- in n-type, h^+ in p-type) Minority carriers: lower number of particles (h^+ in n-type, e^- in p-type)

35 Band theory

35.1 Hybrid orbitals

Hybrid orbitals are linear combinations of other atomic orbitals.

sp3 Orbital
eg CH_4

$$1s + 3p = sp3 \tag{380}$$

---

sp2 Orbital

$$1s + 2p = sp2 \tag{381}$$

---

sp Orbital

$$1s + 1p = sp \tag{382}$$

---

36 Diffusion

Diffusion coefficient

Symbol: D
Unit: $1\,\mathrm{m^2/s}$

Particle current density
Number of particles through an area

Symbol: J
Unit: $1\,1/\mathrm{s}^2$

Einstein relation
Classical

$$D = \frac{\mu k_\mathrm{B} T}{q} \tag{383}$$

D Diffusion coefficient, μElectrical mobility, T Temperature, q Charge

---

Concentration
A quantity per volume

Symbol: c
Unit: $1\,\mathrm{x/m^3}$

Fick's first law
Particle movement is proportional to concentration gradient

$$J = -D\frac{c}{x} \tag{384}$$

J Particle current density, D Diffusion coefficient, c Concentration

---

Fick's second law

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{385}$$

J Particle current density, D Diffusion coefficient, c Concentration

---

37 misc

Exciton

Quasi particle, excitation in condensed matter as bound electron-hole pair.

Work function Lowest energy required to remove an electron into the vacuum	Symbol: W Unit: 1 eV $$-e\phi - E_\text{F} \quad (386)$$

38 Measurement techniques

38.1 ARPES

what? in? how? plot

38.2 Scanning probe microscopy SPM

Images of surfaces are taken by scanning the specimen with a physical probe.

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Application	\fqname :amf:application
how	\fqname :amf:how

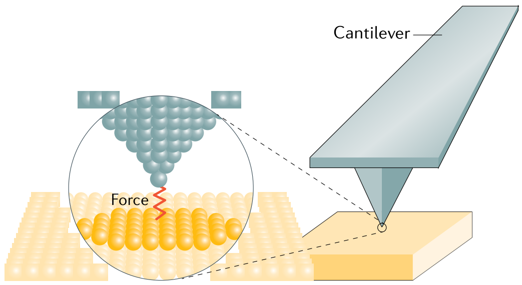

Figure 1: [?]

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how	\fqname :stm:how

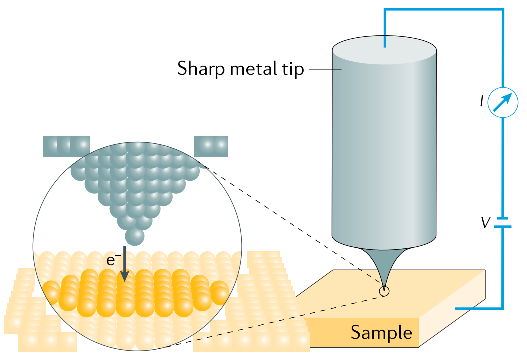

Figure 2: [?]

39 Fabrication techniques

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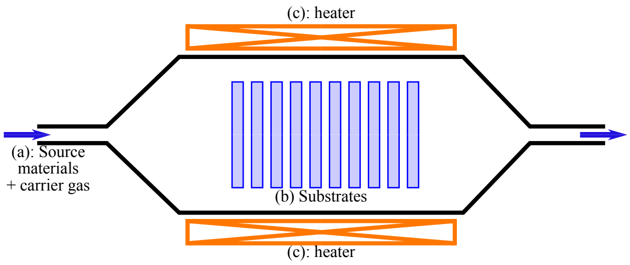
Application	\fqname :cvd:application



39.1 Epitaxy

A type of crystal groth in which new layers are formed with well-defined orientations with respect to the crystalline seed layer.

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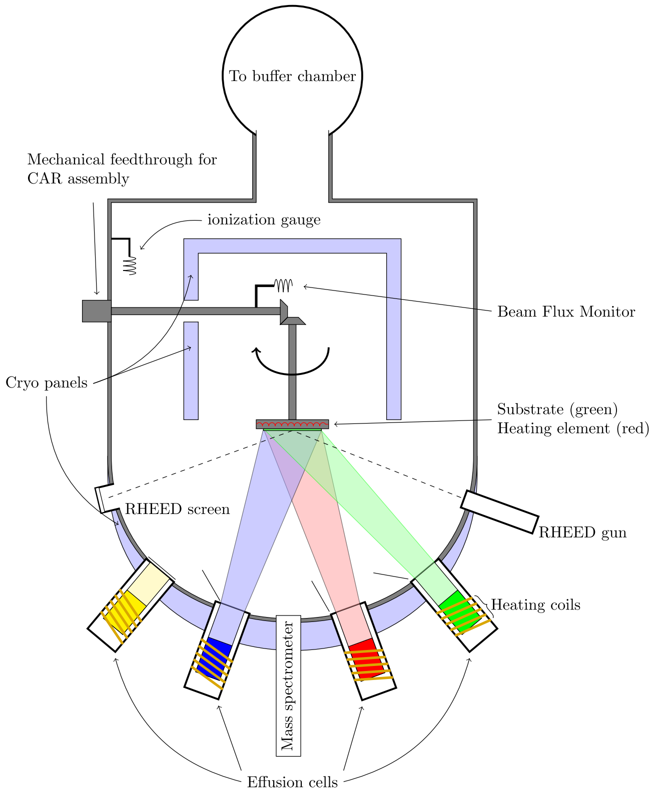


Part VIII

Topological Materials

40 Berry phase / Geometric phase

While adiabatically traversing a closed through the parameter space $R(t)$, the wave function of a systems may pick up an additional phase γ.
If $\vec{R}(t)$ varies adiabatically (slowly) and the system is initially in eigenstate $|n\rangle$, it will stay in an Eigenstate throughout the process (quantum adiabtic theorem).

Schrödinger equation

$$H(\vec{R}(t))\,|n(\vec{R}(t))\rangle = \epsilon(\vec{R}(t))\,|n(\vec{R}(t))\rangle \tag{387}$$

Wave function
After full adiabtic loop in $\vec{R}$

$$|\psi_n(t)\rangle = \underbrace{e^{i\gamma_n(t)}}_{\text{Berry Phase}} \underbrace{e^{\frac{-i}{\hbar}\int^{r} \epsilon_n(\vec{R}(t'))\,dt}}_{\text{Dynamical Phase}} |n(\vec{R}(t))\rangle \tag{388}$$

Berry connection

$$A_n(\vec{R}) = i\,\langle\psi|\nabla_R|\psi\rangle \tag{389}$$

Berry curvature
Gauge invariant

$$\vec{\Omega}_n = \vec{\nabla}_R \times A_n(\vec{R}) \tag{390}$$

Berry phase
Gauge invariant up to 2π

$$\gamma_n = \oint_C d\vec{R}\cdot A_n(\vec{R}) = \int_S d\vec{S}\cdot\vec{\Omega}_n(\vec{R}) \tag{391}$$

The Berry flux through any 2D closed surface is quantized by the **Chern number**. If there is time-reversal symmetry, the Chern-number is 0.

Chern number
The Berry flux through any 2D closed surface is quantized by the **Chern number**. If there is time-reversal symmetry, the Chern-number is 0.

$$C_n = \frac{1}{2\pi}\oint d\vec{S}\,\cdot\vec{\Omega}_n(\vec{R}) \tag{392}$$

$\vec{S}$ closed surface in $\vec{R}$-space. A *Chern insulator* is a 2D insulator with $C_n \neq 0$

Hall conductance of a 2D band insulator

$$\vec{\sigma}_{xy} = \sum_n \frac{e^2}{h}\int_{\text{occupied}} d^2k\,\frac{\Omega_{xy}^n}{2\pi} = \sum_n C_n\frac{e^2}{h} \tag{393}$$

While adiabatically traversing a closed through the parameter space $R(t)$, the wave function of a systems may pick up an additional phase γ.
If $\vec{R}(t)$ varies adiabatically (slowly) and the system is initially in eigenstate $|n\rangle$, it will stay in an Eigenstate throughout the process (quantum adiabtic theorem).

Part IX
Quantum Computing

41 Qubits

Bloch sphere

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \tag{394}$$
$$= \cos\frac{\theta}{2}\,e^{i\phi_\alpha}|0\rangle + \sin\frac{\theta}{2}\,e^{i\phi_\beta}|1\rangle \tag{395}$$
$$= e^{i\phi_\alpha}\cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}\,e^{i\phi}|1\rangle \tag{396}$$

42 Gates

\fqname :gates

$$TODO: \text{remove macro}2 \tag{397}$$

43 Superconducting qubits

43.1 Building blocks

43.1.1 Josephson Junction

When two superconductors are separated by a thin isolator, Cooper pairs can tunnel through the insulator. The Josephson junction is a non-linear inductor.

Josephson-Hamiltonian

$$\hat{H}_\text{J} = -\frac{E_\text{J}}{2}\sum_n [|n\rangle\langle n+1| + |n+1\rangle\langle n|] \tag{398}$$

1. Josephson relation
Dissipationless supercurrent accros junction at zero applied voltage

$$\hat{I}|\delta\rangle = I_\text{C}\sin\delta|\delta\rangle \tag{399}$$

$I_\text{C} = \frac{2e}{\hbar}E_\text{J}$ critical current, δ phase difference accross junction

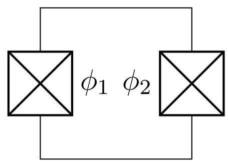
2. Josephson relation
superconducting phase change is proportional to applied voltage

$$\frac{\mathrm{d}\hat{\delta}}{\mathrm{d}t} = \frac{1}{i\hbar}[\hat{H},\hat{\delta}] = -\frac{2eU}{i\hbar}[\hat{n},\hat{\delta}] = \frac{1}{\varphi_0}U \tag{400}$$

$\varphi_0 = \frac{\hbar}{2e}$ reduced flux quantum

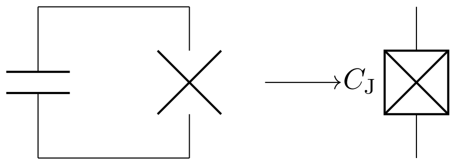
43.1.2 SQUID

SQUID
Superconducting quantum interference device, consists of parallel can be used to measure extremely weak magnetic fields

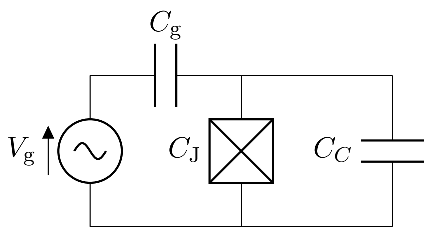


Hamiltonian	$$\hat{H} = -E_{\mathrm{J}1}\cos\hat{\phi}_1 - E_{\mathrm{J}2}\cos\hat{\phi}_2 \quad (401)$$ $\hat{\phi}$ phase difference across the junction

43.2 Josephson Qubit??



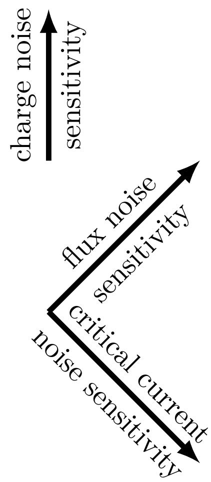
TODO:Include schaltplan



Charging energy / electrostatic energy	$$E_{\mathrm{C}} = \frac{(2e)^2}{C} \quad (402)$$
Josephson energy	$$E_{\mathrm{J}} = \frac{I_0\phi_0}{2\pi} \quad (403)$$
TODO:Was ist I0 Inductive energy	$$E_{\mathrm{L}} = \frac{\varphi_0^2}{L} \quad (404)$$
Gate charge or offset charge	$$n_{\mathrm{g}} = \frac{C_g V_{\mathrm{g}}}{2e} \quad (405)$$
Anharmonicity	$$\alpha := \omega_{1\leftrightarrow 2} - \omega_{0\leftrightarrow 1} \quad (406)$$

$E_L/(E_J - E_L)$

$\frac{E_J}{E_C}$		0	$\ll 1$	~ 1	$\gg 1$
	$\ll 1$	cooper-pair box			
	~ 1	quantronium	fluxonium		
	$\gg 1$	transmon			flux qubit
	$\ggg 1$			phase qubit	

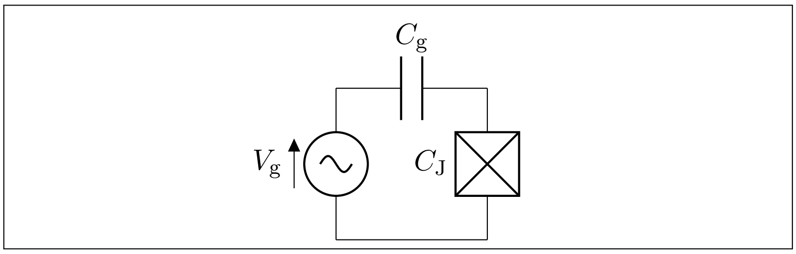


43.3 Cooper Pair Box (CPB) qubit

= voltage bias junction
= charge qubit?

Cooper Pair Box / Charge qubit

- large anharmonicity
- sensitive to charge noise



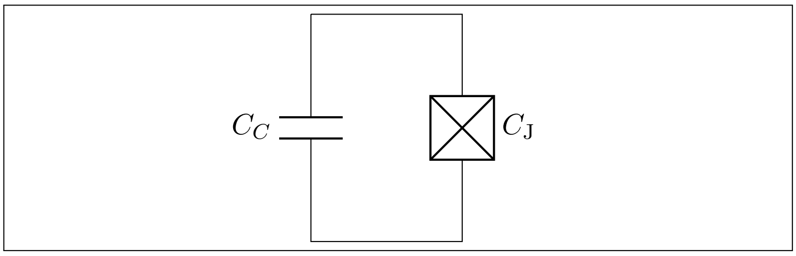
Hamiltonian

$$\hat{H} = 4E_C(\hat{n} - n_g)^2 - E_J \cos\hat{\phi} \tag{407}$$
$$= \sum_n \left[4E_C(n - n_g)^2 |n\rangle\langle n| - \frac{E_J}{2} |n\rangle\langle n+1| + |n+1\rangle\langle n|\right] \tag{408}$$

43.4 Transmon qubit

Transmon qubit
Josephson junction with a shunt **capacitance**.

- charge noise insensitive
- small anharmonicity

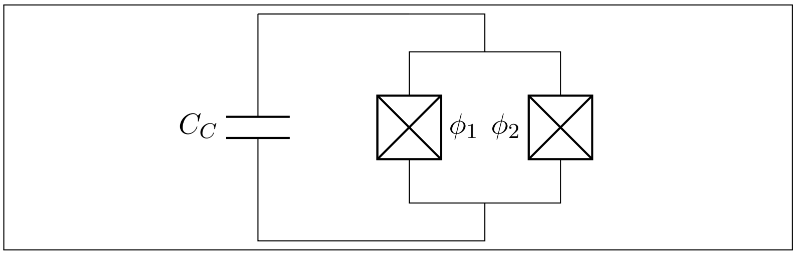


Hamiltonian

$$\hat{H} = 4E_C\hat{n}^2 - E_J \cos\hat{\phi} \tag{409}$$

43.4.1 Tunable Transmon qubit

Frequency tunable transmon
By using a SQUID instead of a Josephson Junction, the qubit is frequency tunable through an external field



Josephson energy

$$E_{J,\text{eff}}(\Phi_{\text{ext}}) = (E_{J1} + E_{J2})\sqrt{\cos^2\left(\pi\frac{\Phi_{\text{ext}}}{\Phi_0}\right) + d^2 \sin\left(\pi\frac{\Phi_{\text{ext}}}{\Phi_0}\right)} \tag{410}$$

$d = (E_{J1} - E_{J2})/(E_{J1} + E_{J2})$ asymmetry

Hamiltonian

$$\hat{H} = 4E_C\hat{n}^2 - \frac{1}{2}E_{J,\text{eff}}(\Phi_{\text{ext}}) \sum_n [|n\rangle\langle n+1| + |n+1\rangle\langle n|] \tag{411}$$

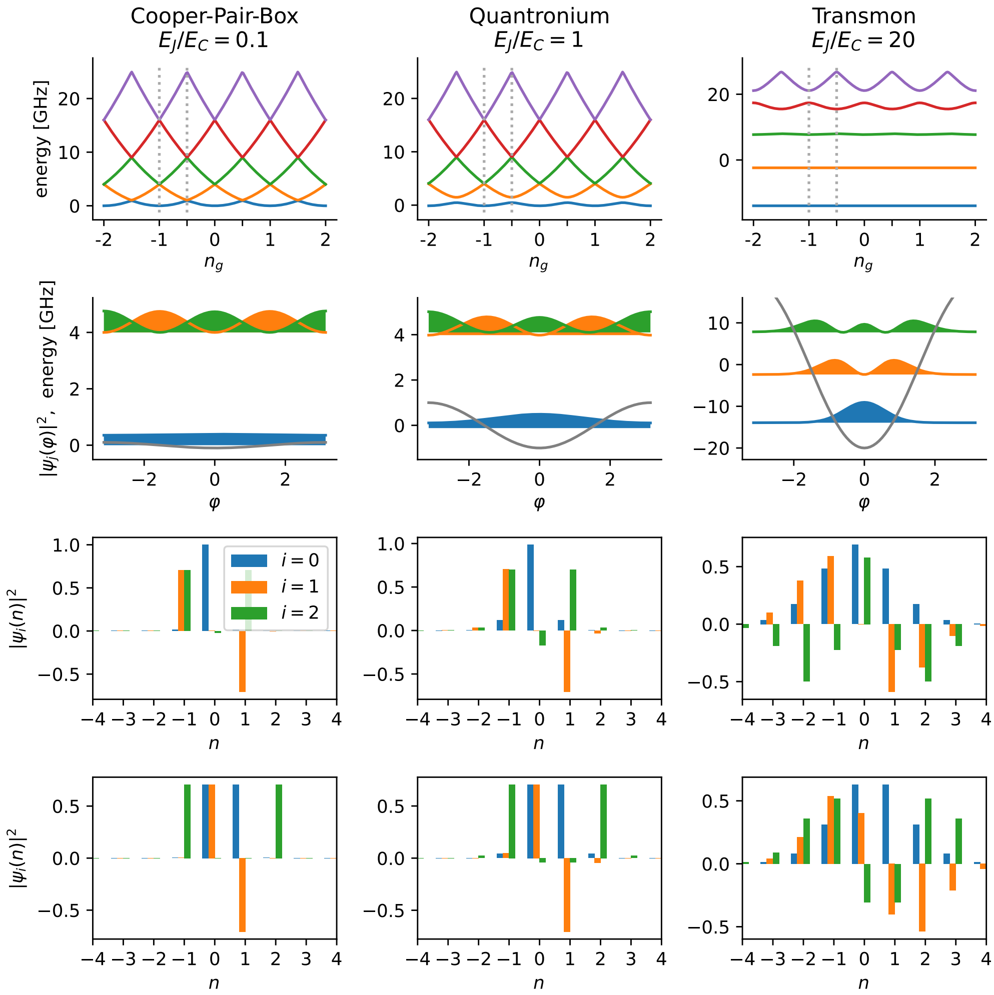
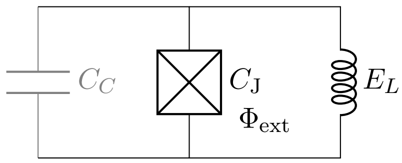


Figure 3: Transmon and so TODO

43.5 Phase qubit

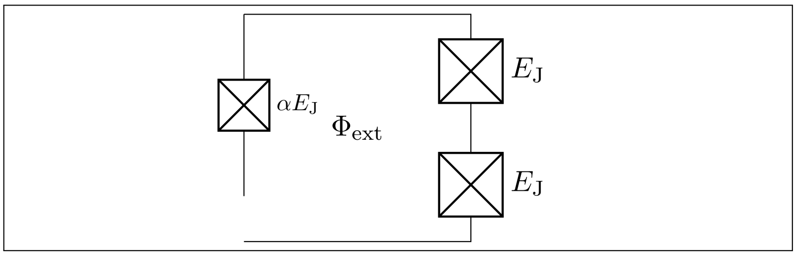
Phase qubit	 TODO:Ist beim Fluxonium noch die Voltage source dran?
Hamiltonian	$$\hat{H} = E_C \hat{n}^2 - E_J \cos\hat{\delta} + E_L(\hat{\delta} - \delta_s)^2 \quad (412)$$ $\delta = \frac{\phi}{\phi_0}$

This is only a test

43.6 Flux qubit

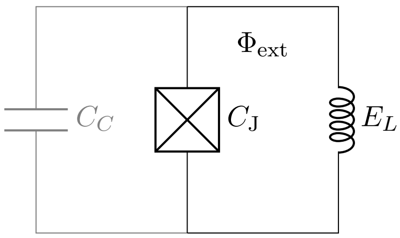
TODO:TODO

Flux qubit / Persistent current qubit



43.7 Fluxonium qubit

Fluxonium qubit
Josephson junction with a shunt **inductance**. Instead of having to tunnel, cooper pairs can move to the island via the inductance. The inductance consists of many parallel Josephson Junctions to avoid parasitic capacitances.



TODO:Ist beim Fluxonium noch die Voltage source dran?

Hamiltonian

$$\hat{H} = 4E_C\hat{n}^2 - E_J\cos\hat{\delta} + E_L(\hat{\delta} - \delta_s)^2 \tag{413}$$

$E_C = \frac{(2e)^2}{2C}, E_L = \frac{\varphi_0^2}{2L}, \delta_s = \frac{\varphi_s}{\varphi_0}$

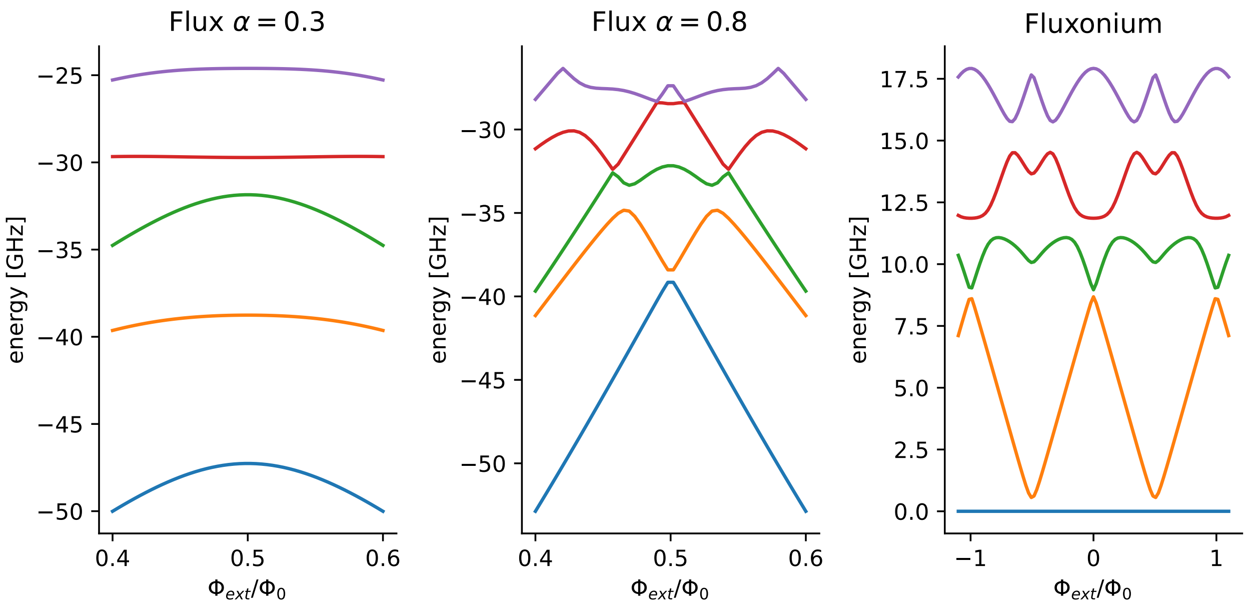


Figure 4: img/

44 Two-level system

Resonance frequency

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} \tag{414}$$

TODO:sollte das nicht 10 sein?

Rabi oscillations	$$\Omega_T ODO \quad (415)$$ ω_{21} resonance frequency of the energy transition, Ω Rabi frequency

44.1 Ramsey interferometry

$|0\rangle \xrightarrow{\frac{\pi}{2}\text{ pulse}}$ precession in xy plane for time $\tau \xrightarrow{\frac{\pi}{2}\text{ pulse}}$ measurement

45 Noise and decoherence

Longitudinal relaxation rate $\Gamma_{1\downarrow}$: $\lvert 1\rangle \to \lvert 0\rangle$ $\Gamma_{1\uparrow}$: $\lvert 0\rangle \to \lvert 1\rangle$	$$\Gamma_1 = \frac{1}{T_1} = \Gamma_{1\uparrow} + \Gamma_{1\downarrow} \quad (416)$$
Longitudinal relaxation rate Pure dephasing rate	$$\Gamma_\phi \quad (417)$$
Transversal relaxation rate	$$\Gamma_2 = \frac{1}{T_2} = \frac{\Gamma_1}{2} + \Gamma_\phi \quad (418)$$
Bloch-Redfield density matrix 2-level System weakly coupled to noise sources with short correlation time	$$\rho_{\text{BR}} = \begin{pmatrix} 1 + (\lvert\alpha\rvert^2 - 1)\,\mathrm{e}^{-\Gamma_1 t} & \alpha\beta^*\,\mathrm{e}^{-\Gamma_2 t} \\ \alpha^*\beta\,\mathrm{e}^{-\Gamma_2 t} & \lvert\beta\rvert^2\,\mathrm{e}^{-\Gamma_1 t} \end{pmatrix} \quad (419)$$

Part X
Computational Physics

46 Quantum many-body physics

TODO:TODO

46.1 Importance sampling

TODO:Monte Carlo

46.2 Matrix product states

47 Electronic structure theory

Electronic structure Hamiltonian

$$\hat{H} = \hat{T}_\text{e} + \hat{T}_\text{n} + V_{\text{e}\leftrightarrow\text{e}} + V_{\text{n}\leftrightarrow\text{e}} + V_{\text{n}\leftrightarrow\text{n}} \tag{420}$$

with

$$\hat{T}_i = -\sum_{n=1}^{N_i} \frac{\hbar^2}{2m_i} \vec{\nabla}_n^2 \tag{421}$$

$$\hat{V}_{i\leftrightarrow j} = -\sum_{k,l} \frac{Z_i Z_j \, \text{e}^2}{|\vec{r}_k - \vec{r}_l|} \tag{422}$$

$\hat{T}$ kinetic energy, $\hat{V}$ electrostatic potential, e electrons, n nucleons

---

Mean field approximation
Replaces 2-particle operator by 1-particle operator

$$\frac{1}{2} \sum_{i\neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \approx \sum_i V_\text{eff}(\vec{r}_i) \tag{423}$$

Example for Coulumb interaction between many electrons

47.1 Tight-binding

47.2 Density functional theory (DFT)

47.2.1 Hartree-Fock

- comp:misc:mean_field theory
- Self-interaction free: Self interaction is cancelled out by the Fock-term

Hartree-Fock equation

$$\left(\hat{T} + \hat{V}_\text{en} + \hat{V}_\text{HF}^\xi\right) \varphi_\xi(x) = \epsilon_\xi \varphi_\xi(x) \tag{424}$$

φ_ξ single particle wavefunction of ξth orbital, $\hat{T}$ kinetic electron energy, $\hat{V}_\text{en}$ electron-nucleus attraction, $\hat{V}_\text{HF}$ comp:dft:hf:potential,

---

Hartree-Fock potential

$$V_\text{HF}^\xi(\vec{r}) = \sum_\vartheta \int \text{d}x' \frac{e^2}{|\vec{r} - \vec{r}'|} \left(\underbrace{|\varphi_\xi(x')|^2}_\text{Hartree-Term} - \underbrace{\frac{\varphi_\vartheta^*(x')\varphi_\xi(x')\varphi_\vartheta(x)}{\varphi_\xi(x)}}_\text{Fock-Term} \right) \tag{425}$$

Self-consistend field cycle	1. Initial guess for ψ 2. Solve SG for each particle 3. Make new guess for ψ

48 Atomic dynamics

48.1 Kohn-Sham

TODO:TODO

48.2 Born-Oppenheimer Approximation

TODO:TODO, BO surface

48.3 Molecular Dynamics

Statistical method

TODO:ab-initio MD, force-field MD

49 Gradient descent

TODO:TODO

50 Physical quantities

50.1 SI quantities

Time	Symbol: t Unit: $1\,\mathrm{s}$
Length	Symbol: l Unit: $1\,\mathrm{m}$
Mass	Symbol: m Unit: $1\,\mathrm{kg}$
Temperature	Symbol: T Unit: $1\,\mathrm{K}$
Electric current	Symbol: I Unit: $1\,\mathrm{A}$
Amount of substance	Symbol: n Unit: $1\,\mathrm{mol}$
Luminous intensity	Symbol: I_V Unit: $1\,\mathrm{cd}$

50.2 Mechanics

Force	Symbol: $\vec{F}$ Unit: $1\,\mathrm{N} = 1\,\mathrm{kgm/s^2}$
Spring constant	Symbol: k Unit: $1\,\mathrm{N\,m^{-1}} = 1\,\mathrm{kg/s^2}$
Velocity	Symbol: $\vec{v}$ Unit: $1\,\mathrm{m\,s^{-1}}$
Torque	Symbol: τ Unit: $1\,\mathrm{N\,m} = 1\,\mathrm{kgm^2/s^2}$

50.3 Thermodynamics

Volume d dimensional Volume	Symbol: V Unit: $1\,\mathrm{m}^d$
Heat capacity	Symbol: C Unit: $1\,\mathrm{J\,K^{-1}}$

50.4 Electrodynamics

Charge	Symbol: q Unit: $1\,\mathrm{C} = 1\,\mathrm{A\,s}$
Charge density	Symbol: ρ Unit: $1\,\mathrm{C/m^3}$

50.5 Others

51 Constants

Planck Constant	Symbol: h Defined value $6.62607015 \cdot 10^{-34}\,\mathrm{J\,s}$ $4.135667969\ldots \cdot 10^{-15}\,\mathrm{eV\,s}$
Universal gas constant Proportionality factor for ideal gases	Symbol: R Defined value $8.31446261815324\,\mathrm{J\,mol^{-1}\,K}$ $N_\mathrm{A} \cdot k_\mathrm{B}$ N_A Avogadro constant, k_B Boltzmann constant
Avogadro constant Number of molecules per mole	Symbol: N_A Defined value $6.02214076 \cdot 10^{23}\,1/\mathrm{mol}$

Boltzmann constant Temperature-Energy conversion factor	Symbol: k_B Defined value $1.380649 \cdot 10^{-23}\,\mathrm{J\,K^{-1}}$
Faraday constant Electric charge of one mol of single-charged ions	Symbol: F Defined value $9.64853321233100184\,\mathrm{C\,mol^{-1}}$ $N_\mathrm{A}\,e$ N_A Avogadro constant, k_B Boltzmann constant

Part XI
Chemie

52 Periodic table

- metalloid
- halogen
- metal
- lanthanoide
- alkalimetal
- transitionmetal
- noblegas
- alkalineearthmetal
- nonmetal

1	1 H 1.008																	2 He 4.003
2	3 Li 6.946	4 Be 9.012											5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
3	11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.085	15 P 30.974	16 S 32.063	17 Cl 35.453	18 Ar 39.948
4	19 K 39.098	20 Ca 40.078	21 Sc 44.956	22 Ti 47.867	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.693	29 Cu 63.546	30 Zn 65.382	31 Ga 69.723	32 Ge 72.631	33 As 74.922	34 Se 78.972	35 Br 79.905	36 Kr 83.798
5	37 Rb 85.468	38 Sr 87.621	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.951	43 Tc 98.906	44 Ru 101.072	45 Rh 102.906	46 Pd 106.421	47 Ag 107.868	48 Cd 112.414	49 In 114.818	50 Sn 118.711	51 Sb 121.760	52 Te 127.603	53 I 126.904	54 Xe 131.294
6	55 Cs 132.905	56 Ba 137.328	57 La 138.905	72 Hf 178.492	73 Ta 180.948	74 W 183.841	75 Re 186.207	76 Os 190.233	77 Ir 192.217	78 Pt 195.085	79 Au 196.967	80 Hg 200.592	81 Tl 204.382	82 Pb 207.210	83 Bi 208.980	84 Po 209.980	85 At 209.987	86 Rn 222.000
7	87 Fr 223.020	88 Ra 226.025	89 Ac 227.028	104 Rf 261.109	105 Db 262.114	106 Sg 263.118	107 Bh 262.123	108 Hs 265.269	109 Mt 268.000	110 Ds 281.000	111 Rg 280.000	112 Cn 277.000	113 Nh 287.000	114 Fl 289.000	115 Mc 288.000	116 Lv 293.000	117 Ts 292.000	118 Og 294.000
				58 Ce 140.116	59 Pr 140.908	60 Nd 144.242	61 Pm 146.915	62 Sm 150.362	63 Eu 151.964	64 Gd 157.253	65 Tb 158.925	66 Dy 162.500	67 Ho 164.930	68 Er 167.259	69 Tm 168.934	70 Yb 173.045	71 Lu 174.967	
				90 Th 232.038	91 Pa 231.036	92 U 238.029	93 Np 237.048	94 Pu 244.064	95 Am 243.061	96 Cm 247.070	97 Bk 247.000	98 Cf 251.000	99 Es 252.000	100 Fm 257.095	101 Md 258.000	102 No 259.000	103 Lr 266.000	

53 stuff

Covalent bond	Bonds that involve sharing of electrons to form electron pairs between atoms.

Part XII

Appendix

List of Figures

List of Tables

54 List of elements

Hydrogen colorless gas (H2)	Symbol: H Number: 1 atomic_mass: 1.0081 Crystal structure: hex set: nonmetal magnetic_ordering: diamagnetic Electronic configuration: 1s[1]
Helium colorless gas, exhibiting a gray, cloudy glow	Symbol: He Number: 2 atomic_mass: 4.0026022 Crystal structure: hcp set: noblegas magnetic_ordering: diamagnetic Electronic configuration: 1s[1]
Lithium silvery-white	Symbol: Li Number: 3 atomic_mass: 6.946 Crystal structure: bcc set: alkalimetal magnetic_ordering: paramagnetic Electronic configuration: He 2s[1]
Beryllium white-gray metallic	Symbol: Be Number: 4 atomic_mass: 9.01218315 Crystal structure: hcp set: alkalineearthmetal magnetic_ordering: diamagnetic Electronic configuration: He 2s[2]

Boron black-brown	Symbol: B Number: 5 atomic_mass: 10.811 Crystal structure: rho set: metalloid magnetic_ordering: diamagnetic Electronic configuration: He 2s[2] 2p[1]
Carbon black, metallic-looking (graphite); clear (diamond)	Symbol: C Number: 6 atomic_mass: 12.01112 Crystal structure: hex set: nonmetal magnetic_ordering: diamagnetic Electronic configuration: He 2s[2] 2p[2]
Nitrogen colorless gas, liquid or solid	Symbol: N Number: 7 atomic_mass: 14.006714 Crystal structure: hex set: nonmetal magnetic_ordering: diamagnetic Electronic configuration: He 2s[2] 2p[3]
Oxygen colorless (gas); pale blue (liquid and solid)	Symbol: O Number: 8 atomic_mass: 15.99915 Crystal structure: sc set: nonmetal magnetic_ordering: paramagnetic Electronic configuration: He 2s[2] 2p[4]
Fluorine very pale yellow (gas); bright yellow (liquid); alpha is opaque, beta is transparent (solid)	Symbol: F Number: 9 atomic_mass: 18.9984031636 Crystal structure: sc set: halogen magnetic_ordering: diamagnetic Electronic configuration: He 2s[2] 2p[5] refractive_index: 1.000195
Neon colorless gas exhibiting an orange-red glow when placed in an electric field	Symbol: Ne Number: 10 atomic_mass: 20.17976 Crystal structure: fcc set: noblegas magnetic_ordering: diamagnetic Electronic configuration: He 2s[2] 2p[6] refractive_index: 1.000067

Sodium silvery white metallic	Symbol: Na Number: 11 atomic_mass: 22.989769282 Crystal structure: bcc set: alkalimetal magnetic_ordering: paramagnetic Electronic configuration: Ne 3s[1]
Magnesium shiny grey solid	Symbol: Mg Number: 12 atomic_mass: 24.30524 Crystal structure: hcp set: alkalineearthmetal magnetic_ordering: paramagnetic Electronic configuration: Ne 3s[2]
Aluminum silvery gray metallic	Symbol: Al Number: 13 atomic_mass: 26.98153857 Crystal structure: fcc set: metal magnetic_ordering: paramagnetic Electronic configuration: Ne 3s[2] 3p[1]
Silicon crystalline, reflective with bluish-tinged faces	Symbol: Si Number: 14 atomic_mass: 28.08528 Crystal structure: dc set: metalloid magnetic_ordering: diamagnetic Electronic configuration: Ne 3s[2] 3p[2]
Phosphorus white, red and violet are waxy, black is metallic-looking	Symbol: P Number: 15 atomic_mass: 30.9737619985 Crystal structure: orth set: nonmetal magnetic_ordering: diamagnetic Electronic configuration: Ne 3s[2] 3p[3] refractive_index: 1.001212
Sulfur yellow sintered microcrystals	Symbol: S Number: 16 atomic_mass: 32.0632 Crystal structure: orth set: nonmetal magnetic_ordering: diamagnetic Electronic configuration: Ne 3s[2] 3p[4] refractive_index: 1.001111

Chlorine pale yellow-green gas	Symbol: Cl Number: 17 atomic_mass: 35.4535 Crystal structure: orth set: halogen magnetic_ordering: diamagnetic Electronic configuration: Ne 3s[2] 3p[5] refractive_index: 1.000773
Argon colorless gas exhibiting a lilac/violet glow when placed in an electric field	Symbol: Ar Number: 18 atomic_mass: 39.9481 Crystal structure: fcc set: noblegas magnetic_ordering: diamagnetic Electronic configuration: Ne 3s[2] 3p[6] refractive_index: 1.000281
Potassium silvery white, faint bluish-purple hue when exposed to air	Symbol: K Number: 19 atomic_mass: 39.09831 Crystal structure: bcc set: alkalimetal magnetic_ordering: paramagnetic Electronic configuration: Ar 4s[1]
Calcium dull gray, silver; with a pale yellow tint	Symbol: Ca Number: 20 atomic_mass: 40.0784 Crystal structure: fcc set: alkalineearthmetal magnetic_ordering: diamagnetic Electronic configuration: Ar 4s[2]
Scandium silvery white	Symbol: Sc Number: 21 atomic_mass: 44.9559085 Crystal structure: hcp set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Ar 3d[1] 4s[2]
Titanium silvery grey-white metallic	Symbol: Ti Number: 22 atomic_mass: 47.8671 Crystal structure: hcp set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Ar 3d[2] 4s[2]

Vanadium blue-silver-grey metal	Symbol: V Number: 23 atomic_mass: 50.94151 Crystal structure: bcc set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Ar 3d[3] 4s[2]
Chromium silvery metallic	Symbol: Cr Number: 24 atomic_mass: 51.99616 Crystal structure: bcc set: transitionmetal magnetic_ordering: antiferromagnetic Electronic configuration: Ar 3d[5] 4s[1]
Manganese silvery metallic	Symbol: Mn Number: 25 atomic_mass: 54.9380443 Crystal structure: bcc set: transitionmetal magnetic_ordering: antiferromagnetic Electronic configuration: Ar 3d[5] 4s[2]
Iron lustrous metallic with a grayish tinge	Symbol: Fe Number: 26 atomic_mass: 55.8452 Crystal structure: bcc set: transitionmetal magnetic_ordering: ferromagnetic Electronic configuration: Ar 3d[6] 4s[2]
Cobalt hard lustrous bluish gray metal	Symbol: Co Number: 27 atomic_mass: 58.9331944 Crystal structure: hcp set: transitionmetal magnetic_ordering: ferromagnetic Electronic configuration: Ar 3d[7] 4s[2]
Nickel glänzend, metallisch, silbrig	Symbol: Ni Number: 28 atomic_mass: 58.69344 Crystal structure: fcc set: transitionmetal magnetic_ordering: ferromagnetic Electronic configuration: Ar 3d[8] 4s[2]

Copper red-orange metallic luster	Symbol: Cu Number: 29 atomic_mass: 63.5463 Crystal structure: fcc set: transitionmetal magnetic_ordering: diamagnetic Electronic configuration: Ar 3d[10] 4s[1]
Zinc silver-gray	Symbol: Zn Number: 30 atomic_mass: 65.382 Crystal structure: hcp set: transitionmetal magnetic_ordering: diamagnetic Electronic configuration: Ar 3d[10] 4s[2] refractive_index: 1.00205
Gallium silvery blue	Symbol: Ga Number: 31 atomic_mass: 69.7231 Crystal structure: orth set: metal magnetic_ordering: diamagnetic Electronic configuration: Ar 3d[10] 4s[2] 4p[1]
Germanium grayish-white	Symbol: Ge Number: 32 atomic_mass: 72.6308 Crystal structure: dc set: metalloid magnetic_ordering: diamagnetic Electronic configuration: Ar 3d[10] 4s[2] 4p[2]
Arsenic metallic grey	Symbol: As Number: 33 atomic_mass: 74.9215956 Crystal structure: rho set: metalloid magnetic_ordering: diamagnetic Electronic configuration: Ar 3d[10] 4s[2] 4p[3] refractive_index: 1.001552
Selenium grey metallic-looking, red, and vitreous black allotropes	Symbol: Se Number: 34 atomic_mass: 78.9718 Crystal structure: hex set: metalloid magnetic_ordering: diamagnetic Electronic configuration: Ar 3d[10] 4s[2] 4p[4] refractive_index: 1.000895

Bromine reddish-brown	Symbol: Br Number: 35 atomic_mass: 79.90479 Crystal structure: orth set: halogen magnetic_ordering: diamagnetic Electronic configuration: Ar 3d[10] 4s[2] 4p[5] refractive_index: 1.001132
Krypton colorless gas, exhibiting a whitish glow in an electric field	Symbol: Kr Number: 36 atomic_mass: 83.7982 Crystal structure: fcc set: noblegas magnetic_ordering: diamagnetic Electronic configuration: Ar 3d[10] 4s[2] 4p[6] refractive_index: 1.000427
Rubidium grey white	Symbol: Rb Number: 37 atomic_mass: 85.46783 Crystal structure: bcc set: alkalimetal magnetic_ordering: paramagnetic Electronic configuration: Kr 5s[1]
Strontium silvery white metallic; with a pale yellow tint	Symbol: Sr Number: 38 atomic_mass: 87.621 Crystal structure: fcc set: alkalineearthmetal magnetic_ordering: paramagnetic Electronic configuration: Kr 5s[2]
Yttrium silvery white	Symbol: Y Number: 39 atomic_mass: 88.905842 Crystal structure: hcp set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Kr 4d[1] 5s[2]
Zirconium silvery white	Symbol: Zr Number: 40 atomic_mass: 91.2242 Crystal structure: hcp set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Kr 4d[2] 5s[2]

Niobium gray metallic, bluish when oxidized	Symbol: Nb Number: 41 atomic_mass: 92.906372 Crystal structure: bcc set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Kr 4d[4] 5s[1]
Molybdenum gray metallic	Symbol: Mo Number: 42 atomic_mass: 95.951 Crystal structure: bcc set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Kr 4d[5] 5s[1]
Technetium shiny gray metal	Symbol: Tc Number: 43 atomic_mass: 98.9063 Crystal structure: hcp set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Kr 4d[5] 5s[2]
Ruthenium silvery white metallic	Symbol: Ru Number: 44 atomic_mass: 101.072 Crystal structure: hcp set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Kr 4d[7] 5s[1]
Rhodium silvery white metallic	Symbol: Rh Number: 45 atomic_mass: 102.905502 Crystal structure: fcc set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Kr 4d[8] 5s[1]
Palladium silvery white	Symbol: Pd Number: 46 atomic_mass: 106.421 Crystal structure: fcc set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Kr 4d[10]

Silver lustrous white metal	Symbol: Ag Number: 47 atomic_mass: 107.86822 Crystal structure: fcc set: transitionmetal magnetic_ordering: diamagnetic Electronic configuration: Kr 4d[10] 5s[1]
Cadmium silvery bluish-gray metallic	Symbol: Cd Number: 48 atomic_mass: 112.4144 Crystal structure: hcp set: transitionmetal magnetic_ordering: diamagnetic Electronic configuration: Kr 4d[10] 5s[2]
Indium silvery lustrous gray	Symbol: In Number: 49 atomic_mass: 114.8181 Crystal structure: tetr set: metal magnetic_ordering: diamagnetic Electronic configuration: Kr 4d[10] 5s[2] 5p[1]
Tin silvery-white (beta); gray (alpha)	Symbol: Sn Number: 50 atomic_mass: 118.7107 Crystal structure: tetr set: metal magnetic_ordering: paramagnetic Electronic configuration: Kr 4d[10] 5s[2] 5p[2]
Antimony silvery lustrous gray	Symbol: Sb Number: 51 atomic_mass: 121.7601 Crystal structure: rho set: metalloid magnetic_ordering: diamagnetic Electronic configuration: Kr 4d[10] 5s[2] 5p[3]
Tellurium silvery lustrous gray (crystalline); brown-black powder (amorphous)	Symbol: Te Number: 52 atomic_mass: 127.603 Crystal structure: hex set: metalloid magnetic_ordering: diamagnetic Electronic configuration: Kr 4d[10] 5s[2] 5p[4] refractive_index: 1.000991

Iodine lustrous metallic gray (solid); black/violet (liquid); violet (gas)	Symbol: I Number: 53 atomic_mass: 126.904473 Crystal structure: orth set: halogen magnetic_ordering: diamagnetic Electronic configuration: Kr 4d[10] 5s[2] 5p[5]
Xenon colorless gas, exhibiting a blue glow when placed in an electric field	Symbol: Xe Number: 54 atomic_mass: 131.2936 Crystal structure: fcc set: noblegas magnetic_ordering: diamagnetic Electronic configuration: Kr 4d[10] 5s[2] 5p[6] refractive_index: 1.000702
Caesium pale gold	Symbol: Cs Number: 55 atomic_mass: 132.905451966 Crystal structure: bcc set: alkalimetal magnetic_ordering: paramagnetic Electronic configuration: Xe 6s[1]
Barium silvery gray; with a pale yellow tint	Symbol: Ba Number: 56 atomic_mass: 137.3277 Crystal structure: bcc set: alkalineearthmetal magnetic_ordering: paramagnetic Electronic configuration: Xe 6s[2]
Lanthanum silvery white	Symbol: La Number: 57 atomic_mass: 138.905477 Crystal structure: dhcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 5d[1] 6s[2]
Cerium silvery white	Symbol: Ce Number: 58 atomic_mass: 140.1161 Crystal structure: dhcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[1] 5d[1] 6s[2]

Praseodymium grayish white	Symbol: Pr Number: 59 atomic_mass: 140.907662 Crystal structure: dhcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[3] 6s[2]
Neodymium silvery white	Symbol: Nd Number: 60 atomic_mass: 144.2423 Crystal structure: dhcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[4] 6s[2]
Promethium metallic	Symbol: Pm Number: 61 atomic_mass: 146.9151 Crystal structure: dhcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[5] 6s[2]
Samarium silvery white	Symbol: Sm Number: 62 atomic_mass: 150.362 Crystal structure: rho set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[6] 6s[2]
Europium silvery white, with a pale yellow tint; but rarely seen without oxide discoloration	Symbol: Eu Number: 63 atomic_mass: 151.9641 Crystal structure: bcc set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[7] 6s[2]
Gadolinium silvery white	Symbol: Gd Number: 64 atomic_mass: 157.253 Crystal structure: hcp set: lanthanoide magnetic_ordering: ferromagnetic Electronic configuration: Xe 4f[7] 5d[1] 6s[2]

Terbium silvery white	Symbol: Tb Number: 65 atomic_mass: 158.925352 Crystal structure: hcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[9] 6s[2]
Dysprosium silbrig weiß	Symbol: Dy Number: 66 atomic_mass: 162.5001 Crystal structure: hcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[10] 6s[2]
Holmium silvery white	Symbol: Ho Number: 67 atomic_mass: 164.930332 Crystal structure: hcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[11] 6s[2]
Erbium silvery white	Symbol: Er Number: 68 atomic_mass: 167.2593 Crystal structure: hcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[12] 6s[2]
Thulium silvery gray	Symbol: Tm Number: 69 atomic_mass: 168.934222 Crystal structure: hcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[13] 6s[2]
Ytterbium silvery white; with a pale yellow tint	Symbol: Yb Number: 70 atomic_mass: 173.0451 Crystal structure: fcc set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[14] 6s[2]

Lutetium silvery white	Symbol: Lu Number: 71 atomic_mass: 174.96681 Crystal structure: hcp set: lanthanoide magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[14] 5d[1] 6s[2]
Hafnium steel gray	Symbol: Hf Number: 72 atomic_mass: 178.492 Crystal structure: hcp set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[14] 5d[2] 6s[2]
Tantalum gray blue	Symbol: Ta Number: 73 atomic_mass: 180.947882 Crystal structure: bcc set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[14] 5d[3] 6s[2]
Tungsten grayish white, lustrous	Symbol: W Number: 74 atomic_mass: 183.841 Crystal structure: bcc set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[14] 5d[4] 6s[2]
Rhenium silvery-grayish	Symbol: Re Number: 75 atomic_mass: 186.2071 Crystal structure: hcp set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[14] 5d[5] 6s[2]
Osmium silvery, blue cast	Symbol: Os Number: 76 atomic_mass: 190.233 Crystal structure: hcp set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[14] 5d[6] 6s[2]

Iridium silvery white	Symbol: Ir Number: 77 atomic_mass: 192.2173 Crystal structure: fcc set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[14] 5d[7] 6s[2]
Platinum silvery white	Symbol: Pt Number: 78 atomic_mass: 195.0849 Crystal structure: fcc set: transitionmetal magnetic_ordering: paramagnetic Electronic configuration: Xe 4f[14] 5d[9] 6s[1]
Gold metallic yellow	Symbol: Au Number: 79 atomic_mass: 196.9665695 Crystal structure: fcc set: transitionmetal magnetic_ordering: diamagnetic Electronic configuration: Xe 4f[14] 5d[10] 6s[1]
Mercury shiny, silvery liquid	Symbol: Hg Number: 80 atomic_mass: 200.5923 Crystal structure: rho set: transitionmetal magnetic_ordering: diamagnetic Electronic configuration: Xe 4f[14] 5d[10] 6s[2] refractive_index: 1.000933
Thallium silvery white	Symbol: Tl Number: 81 atomic_mass: 204.38204 Crystal structure: hcp set: metal magnetic_ordering: diamagnetic Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[1]
Lead metallic gray	Symbol: Pb Number: 82 atomic_mass: 207.21 Crystal structure: fcc set: metal magnetic_ordering: diamagnetic Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[2]

Bismuth lustrous brownish silver	Symbol: Bi Number: 83 atomic_mass: 208.980401 Crystal structure: rho set: metal magnetic_ordering: diamagnetic Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[3]
Polonium silvery	Symbol: Po Number: 84 atomic_mass: 209.98 Crystal structure: sc set: metal magnetic_ordering: nonmagnetic Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[4]
Astatine unknown, probably metallic	Symbol: At Number: 85 atomic_mass: 209.9871 Crystal structure: fcc Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[5] set: halogen
Radon colorless gas	Symbol: Rn Number: 86 atomic_mass: 222 Crystal structure: fcc set: noblegas magnetic_ordering: nonmagnetic Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[6]
Francium	Symbol: Fr Number: 87 atomic_mass: 223.0197 Crystal structure: bcc set: alkalimetal magnetic_ordering: paramagnetic Electronic configuration: Rn 7s[1]
Radium silvery white metallic	Symbol: Ra Number: 88 atomic_mass: 226.0254 Crystal structure: bcc set: alkalineearthmetal magnetic_ordering: nonmagnetic Electronic configuration: Rn 7s[2]

Actinium silvery-white, glowing with an eerie blue light; sometimes with a golden cast	Symbol: Ac Number: 89 atomic_mass: 227.0278 Crystal structure: fcc Electronic configuration: Rn 6d[1] 7s[2] set: actinoide
Thorium silvery	Symbol: Th Number: 90 atomic_mass: 232.03774 Crystal structure: fcc set: actinoide magnetic_ordering: paramagnetic Electronic configuration: Rn 6d[2] 7s[2]
Protactinium bright, silvery metallic luster	Symbol: Pa Number: 91 atomic_mass: 231.035882 Crystal structure: tetr set: actinoide magnetic_ordering: paramagnetic Electronic configuration: Rn 5f[2] 6d[1] 7s[2]
Uranium silvery gray metallic; corrodes to a spalling black oxide coat in air	Symbol: U Number: 92 atomic_mass: 238.028913 Crystal structure: orth set: actinoide magnetic_ordering: paramagnetic Electronic configuration: Rn 5f[3] 6d[1] 7s[2]
Neptunium silvery metallic	Symbol: Np Number: 93 atomic_mass: 237.0482 Crystal structure: orth set: actinoide magnetic_ordering: paramagnetic Electronic configuration: Rn 5f[4] 6d[1] 7s[2]
Plutonium silvery white, tarnishing to dark gray in air	Symbol: Pu Number: 94 atomic_mass: 244.0642 Crystal structure: mon set: actinoide magnetic_ordering: paramagnetic Electronic configuration: Rn 5f[6] 7s[2]

Americium silvery white	Symbol: Am Number: 95 atomic_mass: 243.061375 Crystal structure: dhcp set: actinoide magnetic_ordering: paramagnetic Electronic configuration: Rn 5f[7] 7s[2]
Curium silvery metallic, glows purple in the dark	Symbol: Cm Number: 96 atomic_mass: 247.0703 Crystal structure: dhcp set: actinoide magnetic_ordering: antiferromagnetic Electronic configuration: Rn 5f[7] 6d[1] 7s[2]
Berkelium silvery	Symbol: Bk Number: 97 atomic_mass: 247 Crystal structure: dhcp set: actinoide magnetic_ordering: paramagnetic Electronic configuration: Rn 5f[9] 7s[2]
Californium silvery	Symbol: Cf Number: 98 atomic_mass: 251 Crystal structure: dhcp Electronic configuration: Rn 5f[10] 7s[2] set: actinoide
Einsteinium silvery; glows blue in the dark	Symbol: Es Number: 99 atomic_mass: 252 Crystal structure: fcc set: actinoide magnetic_ordering: paramagnetic Electronic configuration: Rn 5f[11] 7s[2]
Fermium	Symbol: Fm Number: 100 atomic_mass: 257.0951 Crystal structure: fcc Electronic configuration: Rn 5f[12] 7s[2] set: actinoide
Mendelevium	Symbol: Md Number: 101 atomic_mass: 258 Crystal structure: fcc Electronic configuration: Rn 5f[13] 7s[2] set: actinoide

Nobelium	Symbol: No Number: 102 atomic_mass: 259 Crystal structure: fcc Electronic configuration: Rn 5f[14] 7s[2] set: actinoide
Lawrencium	Symbol: Lr Number: 103 atomic_mass: 266 Crystal structure: hcp Electronic configuration: Rn 5f[14] 7s[2] 7p[1] set: actinoide
Rutherfordium	Symbol: Rf Number: 104 atomic_mass: 261.1087 Crystal structure: hcp Electronic configuration: Rn 5f[14] 6d[2] 7s[2] set: transitionmetal
Dubnium	Symbol: Db Number: 105 atomic_mass: 262.1138 Crystal structure: bcc Electronic configuration: Rn 5f[14] 6d[3] 7s[2] set: transitionmetal
Seaborgium	Symbol: Sg Number: 106 atomic_mass: 263.1182 Crystal structure: bcc Electronic configuration: Rn 5f[14] 6d[4] 7s[2] set: transitionmetal
Bohrium	Symbol: Bh Number: 107 atomic_mass: 262.1229 Crystal structure: hcp Electronic configuration: Rn 5f[14] 6d[5] 7s[2] set: transitionmetal
Hassium	Symbol: Hs Number: 108 atomic_mass: 265.269 Crystal structure: hcp Electronic configuration: Rn 5f[14] 6d[6] 7s[2] set: transitionmetal

Meitnerium	Symbol: Mt Number: 109 atomic_mass: 268 Crystal structure: fcc set: unknown magnetic_ordering: paramagnetic Electronic configuration: Rn 5f[14] 6d[7] 7s[2]
Darmstadtium	Symbol: Ds Number: 110 atomic_mass: 281 Crystal structure: bcc Electronic configuration: Rn 5f[14] 6d[8] 7s[2] set: unknown
Roentgenium	Symbol: Rg Number: 111 atomic_mass: 280 Crystal structure: bcc Electronic configuration: Rn 5f[14] 6d[9] 7s[2] set: unknown
Copernicium	Symbol: Cn Number: 112 atomic_mass: 277 Crystal structure: bcc Electronic configuration: Rn 5f[14] 6d[10] 7s[2] set: unknown
Nihonium	Symbol: Nh Number: 113 atomic_mass: 287 Crystal structure: hcp Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[1] set: unknown
Flerovium	Symbol: Fl Number: 114 atomic_mass: 289 Crystal structure: fcc Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[2] set: unknown
Moscovium	Symbol: Mc Number: 115 atomic_mass: 288 Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[3] set: unknown

Livermorium	Symbol: Lv Number: 116 atomic_mass: 293 Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[4] set: unknown
Tennessine semimetallic (predicted)	Symbol: Ts Number: 117 atomic_mass: 292 Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[5] set: unknown
Oganesson metallic (predicted)	Symbol: Og Number: 118 atomic_mass: 294 Crystal structure: fcc Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[6] set: unknown