Formelsammlung

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Contents

Part I

Mathematics

1 Linear algebra

1.1 Matrix basics

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

1.1.1 Transposed matrix

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

1.2 Determinant

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

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

1.3 Misc

Normal equation Solves a linear regression problem	$\underline{\theta} = (\underline{X}^{\mathrm{T}}\underline{X})^{-1}\underline{X}^{\mathrm{T}}\vec{y}$ (16) $\underline{\theta}$ hypothesis / weight matrix, $\underline{X}$ design matrix, $\vec{y}$ output vector
Woodbury matrix identity Inverse of a rank-k correction	$(\underline{A} + \underline{U} + \underline{C} + \underline{V})-1 = \underline{A}^{-1} - \underline{A}^{-1}\underline{U}(\underline{C}^{-1} + \underline{V}\,\underline{A}^{-1}\underline{U})^{-1}\underline{V}\,\underline{A}^{-1}$ (17) $\underline{A}\, n \times n$, $\underline{U}\, n \times k$, $\underline{C}\, k \times k$, $\underline{V}\, k \times n$
Inverse 2×2 matrix	$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad - bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$ (18)
Singular value decomposition Factorization of complex matrices through rotating →rescaling →rotation.	$A = U \Lambda V$ (19) 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	$R = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$ (20)
3D rotation matrices	$R_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}$ (21) $R_y = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$ (22) $R_z = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$ (23)
Properites of rotation matrices	$R^{\mathrm{T}} = R^{-1}$ (24) $\det R = 1$ (25) $R \in \mathrm{SO}(n)$ (26) n dimension, $\mathrm{SO}(n)$ special othogonal group

1.4 Eigenvalues

Eigenvalue equation

$$Av = \lambda v \tag{27}$$

λ eigenvalue, v eigenvector

Characteristic polynomial
Zeros are the eigenvalues of A

$$\chi_A = \det(A - \lambda \mathbb{1}) \overset{!}{=} 0 \tag{28}$$

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

$$THT^\dagger = H \quad \wedge \quad H|\psi\rangle = E|\psi\rangle \quad \Rightarrow \quad HT|\psi\rangle = ET|\psi\rangle \tag{29}$$

Eigendecomposition

$$A = V\Lambda V^{-1} \tag{30}$$

A diagonalizable, columns of V are eigenvectors v_i, Λ diagonal matrix with eigenvalues λ_i on the diagonal

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

2 Geometry

2.1 Trigonometry

Exponential function

$$\exp(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} \tag{31}$$

Sine

$$\sin(x) = \sum_{n=0}^{\infty} (-1)^n \frac{x^{(2n+1)}}{(2n+1)!} \tag{32}$$

$$= \frac{e^{ix} - e^{-ix}}{2i} \tag{33}$$

Cosine

$$\cos(x) = \sum_{n=0}^{\infty} (-1)^n \frac{x^{(2n)}}{(2n)!} \tag{34}$$

$$= \frac{e^{ix} + e^{-ix}}{2} \tag{35}$$

Hyperbolic sine

$$\sinh(x) = -i \sin ix \tag{36}$$

$$= \frac{e^{x} - e^{-x}}{2} \tag{37}$$

Hyperbolic cosine

$$\cosh(x) = \cos ix \tag{38}$$

$$= \frac{e^{x} + e^{-x}}{2} \tag{39}$$

2.2 Various theorems

Hypthenuse in the unit circle

$$1 = \sin^2 x + \cos^2 x \tag{40}$$

Addition theorems

$$\sin(x \pm y) = \sin x \cos y \pm \cos x \sin y \tag{41}$$

$$\cos(x \pm y) = \cos x \cos y \mp \sin x \sin y \tag{42}$$

$$\tan(x \pm y) = \frac{\sin(x \pm y)}{\cos(x \pm y)} = \frac{\tan x \pm \tan y}{1 \mp \tan x \tan y} \tag{43}$$

Double angle

$$\sin 2x = 2 \sin x \cos x \tag{44}$$

$$\cos 2x = \cos^2 x - \sin^2 x = 1 - 2\sin^2 x \tag{45}$$

$$\tan 2x = \frac{2 \tan x}{1 - \tan^2 x} \tag{46}$$

Other

$$\cos x + b \sin x = \sqrt{1 + b^2} \cos(x - \theta) \tag{47}$$

$\tan \theta = b$

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 Fourier analysis

3.1.1 Fourier series

Fourier series
Complex representation

$$f(t) = \sum_{k=-\infty}^{\infty} c_k \exp\left(\frac{2\pi i k t}{T}\right) \tag{48}$$

$f \in \mathcal{L}^2(\mathbb{R}, \mathbb{C})$ T-periodic

Fourier coefficients
Complex representation

$$c_k = \frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} f(t) \exp\left(-\frac{2\pi i}{T} k t\right) \mathrm{d}t \quad \text{for } k \geq 0 \tag{49}$$

$$c_{-k} = \overline{c_k} \quad \text{if } f \text{ real} \tag{50}$$

Fourier series
Sine and cosine representation

$$f(t) = \frac{a_0}{2} + \sum_{k=1}^{\infty}\left(a_k \cos\left(\frac{2\pi}{T}kt\right) + b_k \sin\left(\frac{2\pi}{T}kt\right)\right) \tag{51}$$

$f \in \mathcal{L}^2(\mathbb{R}, \mathbb{C})$ T-periodic

Fourier coefficients
Sine and cosine representation
If f has point symmetry: $a_{k>0} = 0$, if f has axial symmetry: $b_k = 0$

$$a_k = \frac{2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} f(t)\,\cos\left(-\frac{2\pi}{T}kt\right)\mathrm{d}t \quad \text{for } k \geq 0 \tag{52}$$

$$b_k = \frac{2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} f(t)\,\sin\left(-\frac{2\pi}{T}kt\right)\mathrm{d}t \quad \text{for } k \geq 1 \tag{53}$$

$$a_k = c_k + c_{-k} \quad \text{for } k \geq 0 \tag{54}$$

$$b_k = i(c_k - c_{-k}) \quad \text{for } k \geq 1 \tag{55}$$

TODO:cleanup

3.1.2 Fourier transformation

Fourier transform

$$\hat{f}(k) := \frac{1}{\sqrt{2\pi}^n}\int_{\mathbb{R}^n} \mathrm{e}^{-ikx}\, f(x)\,\mathrm{d}x \tag{56}$$

$\hat{f} : \mathbb{R}^n \mapsto \mathbb{C}$, $\forall f \in L^1(\mathbb{R}^n)$

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

3.1.3 Convolution

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

Definition

$$(f * g)(t) = f(t) * g(t) = \int_{-\infty}^{\infty} f(\tau)g(t-\tau)\,\mathrm{d}\tau \tag{57}$$

Notation

$$f(t) * g(t-t_0) = (f * g)(t-t_0) \tag{58}$$

$$f(t-t_0) * g(t-t_0) = (f * g)(t-2t_0) \tag{59}$$

Commutativity

$$f * g = g * f \tag{60}$$

Associativity

$$(f * g) * h = f * (g * h) \tag{61}$$

Distributivity

$$f * (g + h) = f * g + f * h \tag{62}$$

Complex conjugate

$$(f * g)^* = f^* * g^* \tag{63}$$

3.2 Misc

Stirling approximation

$$\ln(N!) \approx N\ln(N) - N + \mathcal{O}(()\ln(N)) \tag{64}$$

Error function
$\mathrm{erf} : \mathbb{C} \to \mathbb{C}$ and
complementary error function
erfc

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\,\mathrm{d}t \tag{65}$$

$$\mathrm{erfc}(x) = 1 - \mathrm{erf}(x) \tag{66}$$

$$= \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2}\,\mathrm{d}t \tag{67}$$

Dirac-Delta of a function

$$\delta(f(x)) = \sum_i \frac{\delta(x - x_i)}{|f'(x_i)|} \tag{68}$$

$f(x_i) = 0$

Geometric series

$$\sum_{k=0}^{\infty} q^k = \frac{1}{1-q} \tag{69}$$

$|q| < 1$

3.3 Logarithm

Logarithm identities

$$\log(xy) = \log(x) + \log(y) \tag{70}$$

$$\log\left(\frac{x}{y}\right) = \log(x) - \log(y) \tag{71}$$

$$\log\left(x^d\right) = d\log(x) \tag{72}$$

$$\log\left(\sqrt[y]{x}\right) = \frac{\log(x)}{y} \tag{73}$$

$$x^{\log(y)} = y^{\log(x)} \tag{74}$$

Integral of natural logarithm

$$\int \ln(x)\,\mathrm{d}x = x\left(\ln(x) - 1\right) \tag{75}$$

$$\int \ln(ax+b)\,\mathrm{d}x = \frac{ax+b}{a}\left(\ln(ax+b) - 1\right) \tag{76}$$

3.4 Vector calculus

Laplace operator

$$\triangle = \vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{77}$$

3.4.1 Spherical symmetry

Spherical coordinates

$$x = r\sin\phi, \cos\theta \tag{78}$$

$$y = r\cos\phi, \cos\theta \tag{79}$$

$$z = r\sin\theta \tag{80}$$

Laplace operator

$$\vec{\nabla}^2 = \triangle = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) \tag{81}$$

p-norm	$\lVert\vec{x}\rVert_p \equiv \left(\sum_{i=1}^{n} \lvert x_i\rvert^p\right)^{\frac{1}{p}}$ (82)

3.5 Integrals

Partial integration	$\int_a^b f'(x)\cdot g(x)\,\mathrm{d}x = [f(x)\cdot g(x)]_a^b - \int_a^b f(x)\cdot g'(x)\,\mathrm{d}x$ (83)
Integration by substitution	$\int_a^b f(g(x))\,g'(x)\,\mathrm{d}x = \int_{g(a)}^{g(b)} f(z)\,\mathrm{d}z$ (84)
Gauss's theorem / Divergence theorem Divergence in a volume equals the flux through the surface	$\iiint_V \vec{\nabla}\cdot\vec{F}\,\mathrm{d}V = \oiint_A \vec{F}\cdot\mathrm{d}\vec{A}$ (85) $A = \partial V$
Stokes's theorem	$\int_A (\vec{\nabla}\times\vec{F})\cdot\mathrm{d}\vec{S} = \oint_S \vec{F}\cdot\mathrm{d}\vec{r}$ (86) $S = \partial A$

3.5.1 List of common integrals

cal:log:integral

Arcsine, arccosine, arctangent	$\int \frac{1}{\sqrt{1-x^2}}\,\mathrm{d}x = \arcsin x$ (87) $\int -\frac{1}{\sqrt{1-x^2}}\,\mathrm{d}x = \arccos x$ (88) $\int \frac{1}{x^2+1}\,\mathrm{d}x = \arctan x$ (89)
Arcsinh, arccosh, arctanh	$\int \frac{1}{\sqrt{x^2+1}}\,\mathrm{d}x = \operatorname{arsinh} x$ (90) $\int \frac{1}{\sqrt{x^2-1}}\,\mathrm{d}x = \operatorname{arcosh} x \quad \text{for } (x > 1)$ (91) $\int \frac{1}{1-x^2}\,\mathrm{d}x = \operatorname{artanh} x \quad \text{for } (\lvert x\rvert < 1)$ (92) $\int \frac{1}{1-x^2}\,\mathrm{d}x = \operatorname{arcoth} x \quad \text{for } (\lvert x\rvert > 1)$ (93)
Integration in spherical coordinates	$\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \int_0^\infty \int_0^{2\pi} \int_0^{\pi} \mathrm{d}r\,\mathrm{d}\phi\,\mathrm{d}\theta\, r^2 \sin\theta$ (94)
Riemann Zeta Function	$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \frac{1}{(1-2^{(1-s)})\Gamma(s)} \int_0^\infty \mathrm{d}\eta \frac{\eta^{(s-1)}}{\mathrm{e}^\eta + 1}$ (95)

Gamma function	$\Gamma(n) = (n-1)!$ (96) $\Gamma(z) = \int_0^\infty t^{z-1}\,\mathrm{e}^{-t}\,\mathrm{d}t$ (97) $\Gamma(z+1) = z\Gamma(z)$ (98)
Upper incomplete gamma function	$\Gamma(s,x) = \int_x -^{\infty} t^{s-1}\,\mathrm{e}^{-t}\,\mathrm{d}t$ (99)
Lower incomplete gamma function	$\gamma(s,x) = \int_0^x t^{s-1}\,\mathrm{e}^{-t}\,\mathrm{d}t$ (100)
Beta function Complete beta function	$\mathrm{B}(z_1,z_2) = \int_0^1 t^{z_1-1}(1-t)^{z_2-1}\,\mathrm{d}t$ (101) $\mathrm{B}(z_1,z_2) = \frac{\Gamma(z_1)\Gamma(z_2)}{\Gamma(z_1+z_2)}$ (102)
Incomplete beta function Complete beta function	$\mathrm{B}(x;z_1,z_2) = \int_0^x t^{z_1-1}(1-t)^{z_2-1}\,\mathrm{d}t$ (103)

TODO:differential equation solutions

4 Probability theory

Mean Expectation value	$\langle x\rangle = \int w(x)\,x\,\mathrm{d}x$ (104)
Variance Square of the Standard deviation	$\sigma^2 = (\Delta\hat{x})^2 = \left\langle\hat{x}^2\right\rangle - \langle\hat{x}\rangle^2 = \langle(x-\langle x\rangle)^2\rangle$ (105)
Covariance	$\mathrm{cov}(x,y) = \sigma(x,y) = \sigma_{XY} = \langle(x-\langle x\rangle)\,(y-\langle y\rangle)\rangle$ (106)
Standard deviation	$\sigma = \sqrt{\sigma^2} = \sqrt{(\Delta x)^2}$ (107)
Median Value separating lower half from top half	$\mathrm{med}(x) = \begin{cases} x_{(n+1)/2} & n \text{ odd} \\ \frac{x_{(n/2)}+x_{((n/2)+1)}}{2} & n \text{ even} \end{cases}$ (108) x dataset with n elements
Probability density function Random variable has density f. The integral gives the probability of X taking a value $x \in [a,b]$.	$P([a,b]) := \int_a^b f(x)\,\mathrm{d}x$ (109) f normalized: $\int_{-\infty}^{\infty} f(x)\,\mathrm{d}x = 1$
Cumulative distribution function	$F(x) = \int_{-\infty}^x f(t)\,\mathrm{d}t$ (110) f probability density function

Probability mass function
Probability p that **discrete** random variable X has exact value x

$$p_X(x) = P(X = x) \tag{111}$$

P probability measure

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

$$\begin{aligned} C_A(\tau) &= \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} f(t+\tau) f(t)\,\mathrm{d}t) \qquad (112) \\ &= \langle f(t+\tau)\cdot f(t)\rangle \qquad (113) \end{aligned}$$

τ lag-time

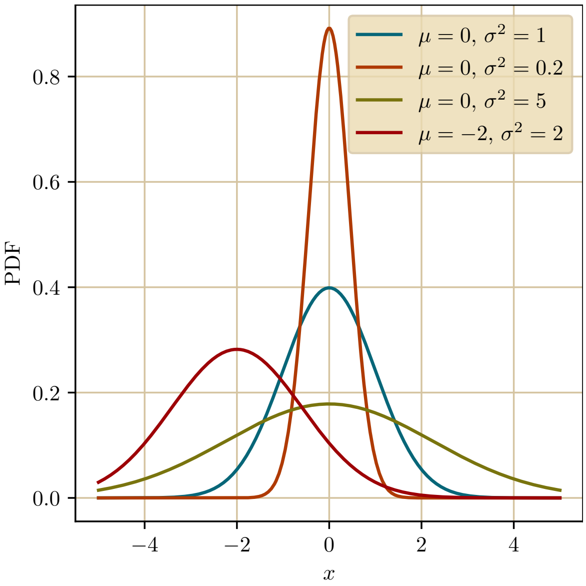
Binomial coefficient
Number of possibilitites of choosing k objects out of n objects

$$\binom{n}{k} = \frac{n!}{k!(n-k)!} \tag{114}$$

4.1 Distributions

4.1.1 Continuous probability distributions

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
$\mu = 0,\ \sigma = 1$

$$\varphi(x) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-\frac{1}{2}x^2} \tag{115}$$

Multivariate normal distribution

: Multivariate Gaussian distribution

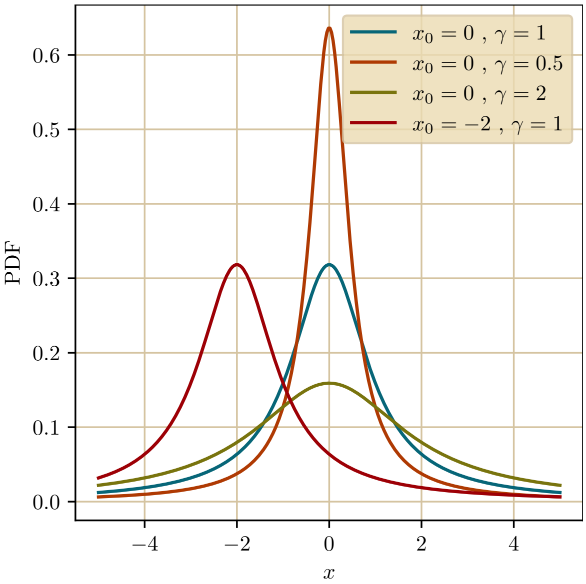
parameters	$\vec{\mu} \in \mathbb{R}^k, + \quad \underline{\Sigma} \in \mathbb{R}^{k \times k}$
support	$\vec{x} \in \vec{\mu} + \mathrm{span}(\underline{\Sigma})$
pdf	$\mathcal{N}(\vec{m}u, \underline{\Sigma}) = \frac{1}{(2\pi)^{k/2}} \frac{1}{\sqrt{\det \Sigma}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^{\mathrm{T}} \underline{\Sigma}^{-1} (\vec{x}-\vec{\mu})\right)$ TODO:k-variate normal plot
mean	$\vec{\mu}$
variance	$\underline{\Sigma}$

$\vec{m}u$ Mean , $\underline{\Sigma}$ Covariance

Laplace-distribution TODO:TODO

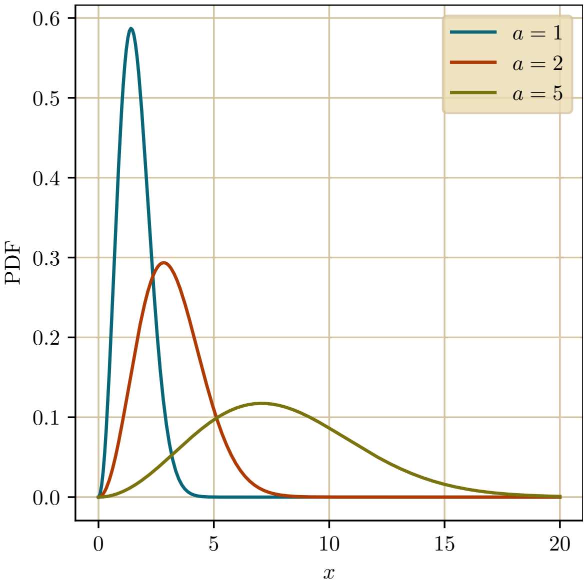
Cauchys / Lorentz distribution

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



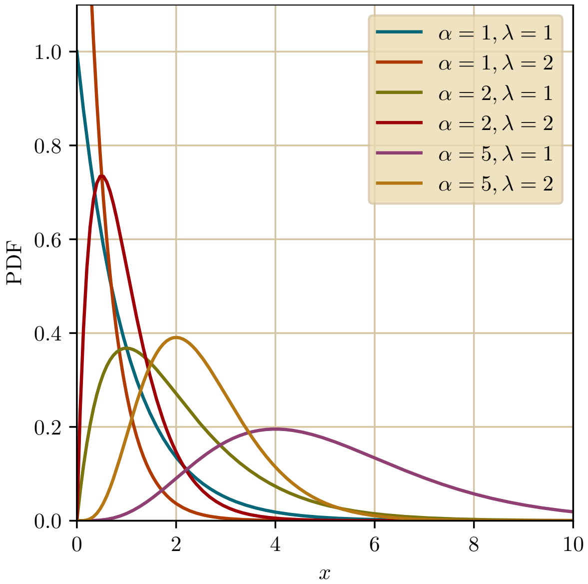
parameters	$x_0 \in \mathbb{R}, \quad \gamma \in \mathbb{R}$
support	$x \in \mathbb{R}$
pdf	$\frac{1}{\pi\gamma\left[1+\left(\frac{x-x_0}{\gamma}\right)^2\right]}$
cdf	$\frac{1}{\pi}\arctan\left(\frac{x-x_0}{\gamma}\right)+\frac{1}{2}$
mean	undefined
median	x_0
variance	undefined

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	$\mathrm{erf}\left(\frac{x}{\sqrt{2}a}\right) - \sqrt{\frac{2}{\pi}\frac{x}{a}}\exp\left(\frac{-x^2}{2a^2}\right)$
mean	$2a\frac{2}{\pi}$
median	
variance	$\frac{a^2(3\pi-8)}{\pi}$

Gamma Distribution : with λ parameter



parameters	$\alpha > 0, \lambda > 0$
support	$x \in (0, 1)$
pdf	$\frac{\lambda^\alpha}{\Gamma(\alpha) x^{\alpha-1} \mathrm{e}^{-\lambda x}}$
cdf	$\frac{1}{\Gamma(\alpha)\gamma(\alpha, \lambda x)}$
mean	$\frac{\alpha}{\lambda}$
variance	$\frac{\alpha}{\lambda^2}$

Γ math:cal:integral:list:gamma, γ Lower incomplete gamma function

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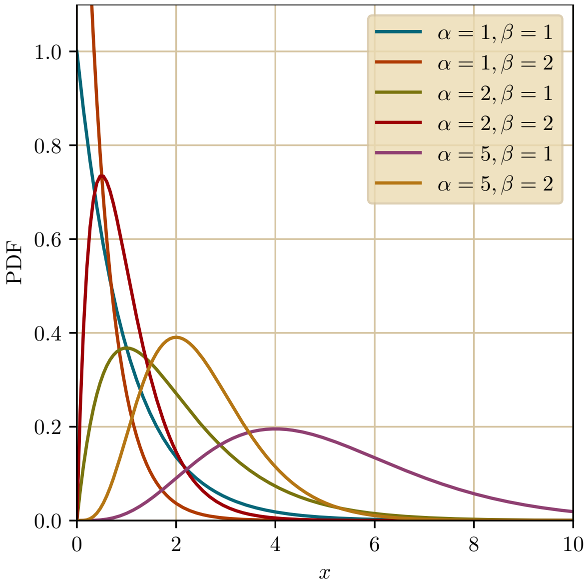
Beta Distribution



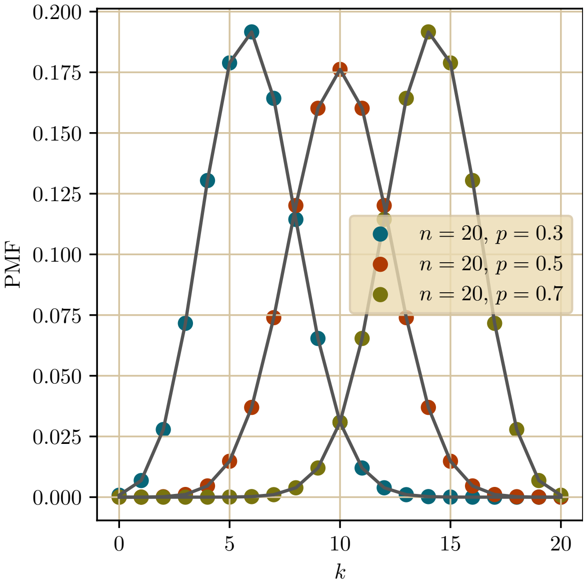
parameters	$\alpha \in \mathbb{R}, \beta \in \mathbb{R}$
support	$x \in [0, 1]$
pdf	$\frac{x^{\alpha-1}(1-x)^{\beta-1}}{\mathrm{B}(\alpha, \beta)}$
cdf	$\frac{\mathrm{B}(x; \alpha, \beta)}{\mathrm{B}(\alpha, \beta)}$
mean	$\frac{\alpha}{\alpha + \beta}$
variance	$\frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$

B Beta function / Incomplete beta function

4.1.2 Discrete probability distributions

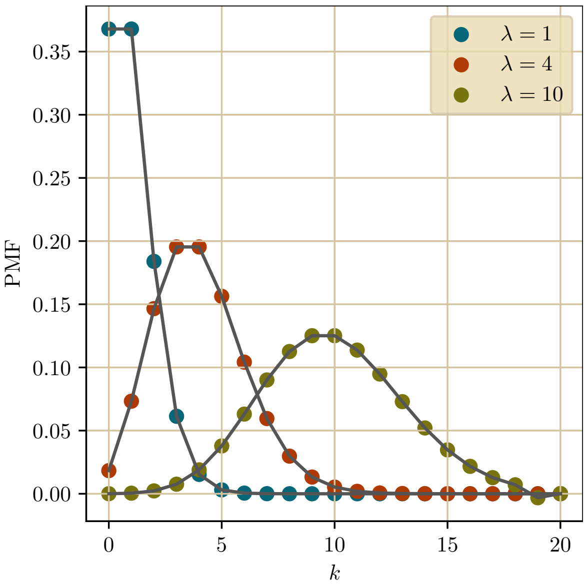
Binomial distribution

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	$npq = np(1-p)$

Poisson distribution



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

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

$$V_y = J(x) \cdot V_x \cdot J^{\mathrm{T}}(x) \tag{116}$$

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

Propagation of uncorrelated errors
Linear approximation

$$u_y = \sqrt{\sum_i \left(\frac{\partial y}{\partial x_i} \cdot u_i \right)^2} \tag{117}$$

Weight
Variance is a possible choice for a weight

$$w_i = \frac{1}{\sigma_i^2} \tag{118}$$

σ Variance

Weighted mean

$$\overline{x} = \frac{\sum_i (x_i w_i)}{\sum_i w_i} \tag{119}$$

w_i Weight

Variance of weighted mean

$$\sigma_{\overline{x}}^2 = \frac{1}{\sum_i w_i} \tag{120}$$

w_i Weight

4.4 Maximum likelihood estimation

Likelihood function
Likelihood of observing x when parameter is θ
in general not normalized!

$$L : \Theta \to [0, 1], \quad \theta \mapsto \rho(x|\theta) \tag{121}$$

ρ Probability density function $x \mapsto \rho(x|\theta)$ depending on parameter θ, Θ parameter space

Likelihood function
for independent and identically distributed random variables

$$L(\theta) = \prod_{i=1}^{n} f(x_i; \theta) \tag{122}$$

x_i n random variables, ρ Probability density function $x \mapsto f(x|\theta)$ depending on parameter θ

Maximum likelihood estimate (MLE)
Paramater for which outcome is most likely

$$\theta_{\text{ML}} = \arg\max_{\theta} L(\theta) \tag{123}$$

$$= \arg\max_{\theta} \log\big(L(\theta)\big) \tag{124}$$

L pt:mle:likelihood, θ parameter of a Probability density function

4.5 Bayesian probability theory

Prior distribution
Expected distribution before conducting the experiment

$$p(\theta) \tag{125}$$

θ parameter

Evidence

$$p(\mathcal{D}) = \int \mathrm{d}\theta \, p(\mathcal{D}|\theta) \, p(\theta) \tag{126}$$

$p(\mathcal{D}|\theta)$ Likelihood function, $p(\theta)$ Prior distribution, $\mathcal{D}$ data set

Bayes’ theorem	$p(\theta \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \theta)\, p(\theta)}{p(\mathcal{D})}$ (127) $p(\theta \mid \mathcal{D})$ posterior distribution, $p(\mathcal{D} \mid \theta)$ Likelihood function, $p(\theta)$ Prior distribution, $p(\mathcal{D})$ Evidence, $\mathcal{D}$ data set
Maximum a posterior estimation (MAP)	$\theta_{\mathrm{MAP}} = \arg\max_{\theta} p(\theta \mid \mathcal{D}) = \arg\max_{\theta} p(\mathcal{D} \mid \theta)\, p(\theta)$ (128)

Part II

Mechanics

5 Newton

Newton's laws	1. A body remains at rest, or in motion at a constant speed in a straight line, except insofar as it is acted upon by a force 2. $\vec{F} = m \cdot \vec{a}$ 3. If two bodies exert forces on each other, these force have the same magnitude but opposite directions $\vec{F}_{\mathrm{A}\to\mathrm{B}} = -\vec{F}_{\mathrm{B}\to\mathrm{A}}$

6 Misc

Hooke's law	$F = D\Delta l \qquad (129)$ F Force, D Spring constant, Δl spring length

7 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	$\mathcal{L} = T - V \qquad (130)$ T kinetic energy, V potential energy
Lagrange equations (2nd type)	$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{q}_i} - \frac{\partial\mathcal{L}}{\partial q_i} = 0 \qquad (131)$ q generalized coordinates
Canocial Momentum	$p = \frac{\partial\mathcal{L}}{\partial\dot{q}} \qquad (132)$
Hamiltonian Hamiltonian can be derived from the Lagrangian using a Legendre transformation	$H(q,p) = p\dot{q} - \mathcal{L}\big(q, \dot{q}(q,p)\big) \qquad (133)$

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	$\frac{\partial \rho}{\partial t} = -\sum_{i=1}^{N}\left(\frac{\partial \rho}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i}\frac{\partial H}{\partial q_i}\right) = \{H, \rho\}$ (134) $\{\}$ poisson bracket

8 Entropy

Positive-definite and additive	$S \geq 0$ (135) $S(E_1, E_2) = S_1 + S_2$ (136)
Von-Neumann	$S = -k_\mathrm{B} \langle \log \rho \rangle = -k_\mathrm{B} \operatorname{tr}(\rho \log \rho)$ (137) ρ density matrix
Gibbs	$S = -k_\mathrm{B} \sum_n p_n \log p_n$ (138) p_n probability for micro state n
Boltzmann	$S = k_\mathrm{B} \log \Omega$ (139) Ω #micro states
Temperature	$\frac{1}{T} := \left(\frac{\partial S}{\partial E}\right)_V$ (140)
Pressure	$p = T\left(\frac{\partial S}{\partial V}\right)_E$ (141)

Part IV

Thermodynamics

Thermal wavelength

$$\lambda = \frac{\hbar}{\sqrt{2\pi m k_\mathrm{B} T}} \tag{142}$$

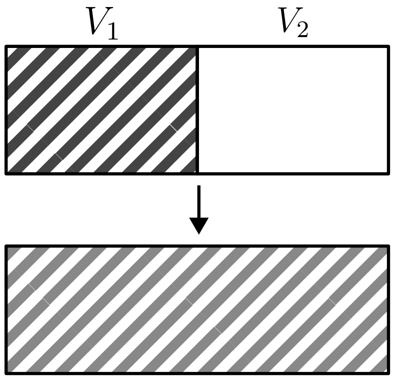
9 Processes

- **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 $\Delta S = 0$

9.1 Irreversible gas expansion (Gay-Lussac experiment)

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

$$\Delta S = N k_\mathrm{B} \ln\left(\frac{V_1 + V_2}{V_1}\right) > 0 \tag{143}$$

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

10 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

$$Q_\mathrm{L} = T\Delta S \tag{144}$$

ΔS entropy change of the phase transition

Clausius-Clapeyron equation
Slope of the coexistence curve

$$\frac{\mathrm{d}p}{\mathrm{d}T} = \frac{Q_\mathrm{L}}{T\Delta V} \tag{145}$$

ΔV Volume change of the phase transition

Phase transition
At the coexistence curve

$$G_1 = G_2 \tag{146}$$

and therefore

$$\mu_1 = \mu_2 \tag{147}$$

Gibbs rule / Phase rule

$$f = c - p + 2 \tag{148}$$

c #components, f #degrees of freedom, p #phases

10.0.1 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

$$p_\mathrm{osm} = k_\mathrm{B} T \frac{N_c}{V} \tag{149}$$

N_c #dissolved particles

10.1 Material properties

Heat capacity

$$c = \frac{Q}{\Delta T} \tag{150}$$

Q heat

Isochoric heat capacity

$$c_v = \left(\frac{\partial Q}{\partial T}\right)_V = \left(\frac{\partial U}{\partial T}\right)_V \tag{151}$$

U internal energy

Isobaric heat capacity

$$c_p = \left(\frac{\partial Q}{\partial T}\right)_P = \left(\frac{\partial H}{\partial T}\right)_P \tag{152}$$

H enthalpy

Bulk modules

$$K = -V \frac{\mathrm{d}p}{\mathrm{d}V} \tag{153}$$

p pressure, V initial volume

Compressibility

$$\kappa = -\frac{1}{V}\frac{\partial V}{\partial p} \tag{154}$$

Isothermal compressibility

$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T = \frac{1}{K} \tag{155}$$

Adiabatic compressibility

$$\kappa_S = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_S \tag{156}$$

Thermal expansion coefficient

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{p,N} \tag{157}$$

11 Laws of thermodynamics

11.1 Zeroeth law

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

$$A \overset{th.eq.}{\leftrightarrow} C \quad \wedge \quad B \overset{th.eq.}{\leftrightarrow} C \quad \Rightarrow \quad A \overset{th.eq.}{\leftrightarrow} B \tag{158}$$

11.2 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

$$\Delta U = \delta Q - \delta W \tag{159}$$

$$\mathrm{d}U = T\,\mathrm{d}S - p\,\mathrm{d}V \tag{160}$$

11.3 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.

11.4 Third law

It is impussible to cool a system to absolute zero.

Entropy density

$$\lim_{T\to 0} s(T) = 0 \tag{161}$$

and therefore also

$$\lim_{T\to 0} c_V = 0 \tag{162}$$

$s = \frac{S}{N}$

12 Ensembles

Microcanonical ensemble

Constant variables	$E,\ V,\ N$
partition sum	$\Omega = \sum_n 1$
probability	$p_n = \frac{1}{\Omega}$
td pot	$S = k_\mathrm{B} \ln \Omega$
pressure	$p = T \left(\frac{\partial S}{\partial V}\right)_{E,N}$
entropy	$S = k_\mathrm{B} = \ln \Omega$

Canonical ensemble

Constant variables	$T,\ V,\ N$
partition sum	$Z = \sum_n \mathrm{e}^{-\beta E_n}$
probability	$p_n = \frac{\mathrm{e}^{-\beta E_n}}{Z}$
td pot	$F = -k_\mathrm{B} T \ln Z$
pressure	$p = -\left(\frac{\partial F}{\partial V}\right)_{T,N}$
entropy	$S = -\left(\frac{\partial F}{\partial T}\right)_{V,N}$

Grand canonical ensemble

Constant variables	$T,\ V,\ \mu$
partition sum	$Z_\mathrm{g} = \sum_n \mathrm{e}^{-\beta(E_n - \mu N_n)}$
probability	$p_n = \frac{\mathrm{e}^{-\beta(E_n - \mu N_n}}{Z_\mathrm{g}}$
td pot	$\Phi = -k_\mathrm{B} T \ln Z$
pressure	$p = -\left(\frac{\partial \Phi}{\partial V}\right)_{T,\mu} = -\frac{\Phi}{V}$
entropy	$S = -\left(\frac{\partial \Phi}{\partial T}\right)_{V,\mu}$

Isobaric-isothermal : Gibbs ensemble

Constant variables	N, p, T
partition sum	
probability	$p_n ? \frac{\mathrm{e}^{-\beta(E_n+pV_n)}}{Z}$
td pot	
pressure	
entropy	

Isonthalpic-isobaric ensemble : Enthalpy ensemble

Constant variables	
partition sum	
probability	
td pot	
pressure	
entropy	

TODO:complete, link potentials

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

$$\langle A\rangle_{\text{Time}} = \langle A\rangle_{\text{Ensemble}} \tag{163}$$

A Observable

12.1 Potentials

Internal energy

$$\mathrm{d}U(S,V,N) = T\,\mathrm{d}S - p\,\mathrm{d}V + \mu\,\mathrm{d}N \tag{164}$$

Free energy / Helmholtz energy

$$\mathrm{d}F(T,V,N) = -S\,\mathrm{d}T - p\,\mathrm{d}V + \mu\,\mathrm{d}N \tag{165}$$

Enthalpy

$$\mathrm{d}H(S,p,N) = T\,\mathrm{d}S + V\,\mathrm{d}p + \mu\,\mathrm{d}N \tag{166}$$

Free enthalpy / Gibbs energy

$$\mathrm{d}G(T,p,N) = -S\,\mathrm{d}T + V\,\mathrm{d}p + \mu\,\mathrm{d}N \tag{167}$$

Grand canonical potential

$$\mathrm{d}\Phi(T,V,\mu) = -S\,\mathrm{d}T - p\,\mathrm{d}V - N\,\mathrm{d}\mu \tag{168}$$

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.

13 Ideal gas

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

Phase space volume
$3N$ sphere

$$\Omega(E) = \int_V \mathrm{d}^3 q_1 \ldots \int_V \mathrm{d}^3 q_N \int \mathrm{d}^3 p_1 \ldots \int \mathrm{d}^3 p_N \frac{1}{N!\, h^{3N}} \Theta\left(E - \sum_i \frac{\vec{p}_i^{\,2}}{2m}\right) \tag{169}$$

$$= \left(\frac{V}{N}\right)^N \left(\frac{4\pi m E}{3h^2 N}\right)^{\frac{3N}{2}} \mathrm{e}^{\frac{5N}{2}} \tag{170}$$

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

Entropy

$$S = \frac{5}{2} N k_\mathrm{B} + N k_\mathrm{B} \ln\left(\frac{V}{N}\left(\frac{2\pi m E}{3h^2 N}\right)^{\frac{3}{2}}\right) \tag{171}$$

Ideal gas equation

$$pV = nRT \tag{172}$$

$$= N k_\mathrm{B} T \tag{173}$$

Equation of state

$$U = \frac{3}{2} N k_\mathrm{B} T \tag{174}$$

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

$$U_\mathrm{D} = \frac{1}{2} k_\mathrm{B} T \tag{175}$$

Maxwell velocity distribution

See Maxwell-Boltzmann distribution

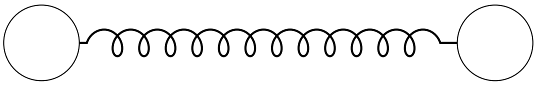
$$w(v)\,\mathrm{d}v = 4\pi \left(\frac{\beta m}{2\pi}\right)^{\frac{3}{2}} v^2\, \mathrm{e}^{-\frac{\beta m v^2}{2}}\, \mathrm{d}v \tag{176}$$

Average quadratic velocity
per particle in a 3D gas

$$\langle v^2 \rangle = \int_0^\infty \mathrm{d}v\, v^2 w(v) = \frac{3 k_\mathrm{B} T}{m} \tag{177}$$

13.0.1 Molecule gas

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



Translation	$p_i = \frac{2\pi\hbar}{L} n_i \qquad (178)$ $E_{\text{kin}} = \frac{\vec{p}_r^{\,2}}{2M} \qquad (179)$ $n_i \in \mathbb{N}_0$, $i = x, y, z$
Vibration	$E_{\text{vib}} = \hbar\omega\left(n + \frac{1}{2}\right) \qquad (180)$ $n \in \mathbb{N}_0$
Rotation	$E_{\text{rot}} = \frac{\hbar^2}{2I} j(j+1) \qquad (181)$ $j \in \mathbb{N}_0$

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

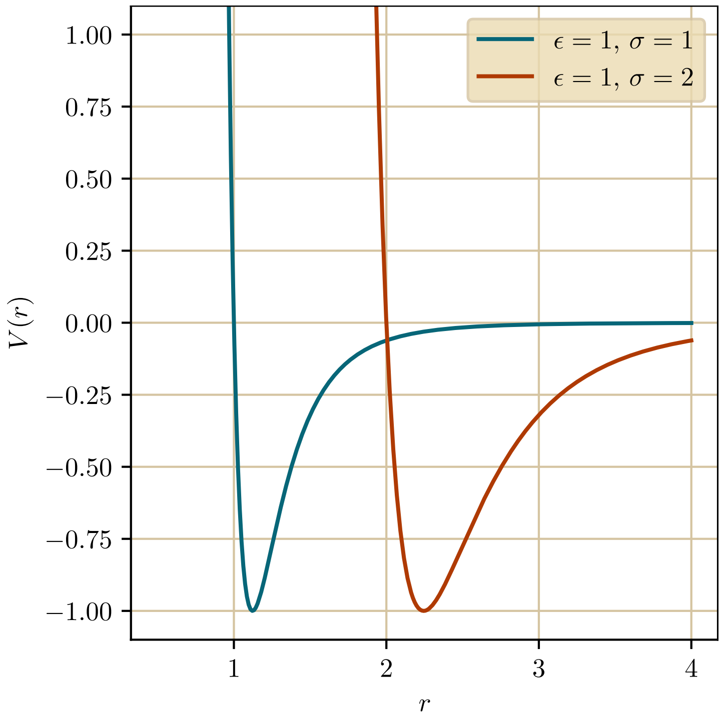
14 Real gas

14.1 Virial expansion

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

Virial expansion The 2nd and 3d virial coefficient are tabelated for many substances	$p = k_{\mathrm{B}} T \rho \left[1 + B(T)\rho + C(T)\rho^2 + \dots\right] \qquad (182)$ B and C 2nd and 3d virial coefficient, $\rho = \frac{N}{V}$
Mayer function	$f(\vec{r}) = \mathrm{e}^{-\beta V(i,j)} - 1 \qquad (183)$ $V(i,j)$ pair potential
Second virial coefficient Depends on pair potential between two molecules	$B = -\frac{1}{2}\int_V \mathrm{d}^3\vec{r}\, f(\vec{r}) \qquad (184)$

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.



$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{185}$$

14.2 Van der Waals equation

Assumes a hard-core potential with a weak attraction.

Partition sum

$$Z_N = \frac{(V - V_0)^N}{\lambda^{3N} N!} \mathrm{e}^{\frac{\beta N^2 a}{V}} \tag{186}$$

a internal pressure

Van der Waals equation

$$p = \frac{N k_\mathrm{B} T}{V - b} - \frac{N^2 a}{V^2} \tag{187}$$

b co-volume?

TODO:sometimes N is included in a, b

15 Ideal quantum gas

Fugacity

$$z = \mathrm{e}^{\mu\beta} = \mathrm{e}^{\frac{\mu}{k_\mathrm{B} T}} \tag{188}$$

Occupation number

$$\sum_r n_r = N \tag{189}$$

r states

Undifferentiable particles

$$|p_1, p_2, \dots, p_N\rangle = |p_1\rangle\,|p_2\rangle \dots |p_N\rangle \tag{190}$$

p_i state

Applying the parity operator yields a *symmetric* (Bosons) and a *antisymmetic* (Fermions) solution

$$\hat{P}_{12}\psi(p_i(\vec{r}_1), p_j(\vec{r}_2)) = \pm\psi(p_i(\vec{r}_1), p_j(\vec{r}_2)) \tag{191}$$

$\hat{P}_{12}$ parity operator swaps 1 and 2, ±: $\substack{\text{bos} \\ \text{fer}}$

Spin degeneracy factor

$$g_s = 2s + 1 \tag{192}$$

s spin

Density of states

$$g(\epsilon) = g_s \frac{V}{4\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\epsilon} \tag{193}$$

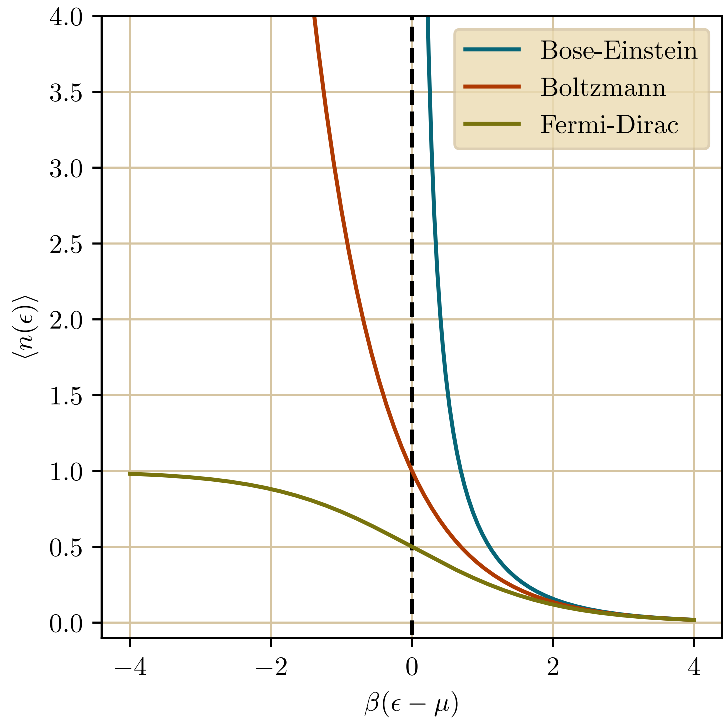
g_s Spin degeneracy factor

Occupation number per energy

$$n(\epsilon)\,\mathrm{d}\epsilon = \frac{g(\epsilon)}{\mathrm{e}^{\beta(\epsilon-\mu)} \mp 1}\,\mathrm{d}\epsilon \tag{194}$$

Density of states, ±: $\substack{\text{bos} \\ \text{fer}}$

Occupation number



$$\langle n(\epsilon)\rangle = \frac{1}{\mathrm{e}^{\beta(\epsilon-\mu)} \mp 1} \tag{195}$$

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

$$= \frac{1}{\mathrm{e}^{\beta(\epsilon-\mu)}} \tag{196}$$

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

Number of particles

$$\langle N\rangle = \int_0^\infty n(\epsilon)\,\mathrm{d}\epsilon \tag{197}$$

Energy
Equal to the classical ideal gas

$$\langle E\rangle = \int_0^\infty \epsilon n(\epsilon)\,\mathrm{d}\epsilon = \frac{3}{2}pV \tag{198}$$

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

$$pV = k_\mathrm{B} T \ln Z_g \tag{199}$$

after Virial expansion

$$= N k_\mathrm{B} T \left[1 \mp \frac{\lambda^3}{2^{5/2} g v} + \mathcal{O}\left(\left(\frac{\lambda^3}{v} \right)^2 \right) \right] \tag{200}$$

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

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

$$\left(\frac{V}{N} \right)^{\frac{1}{3}} \sim \frac{\lambda}{g_s^{\frac{1}{3}}} \tag{201}$$

Generalized zeta function

$$\left.\begin{matrix} g_\nu(z) \\ f_\nu(z) \end{matrix}\right\} := \frac{1}{\Gamma(\nu)} \int_0^\infty \mathrm{d}x \, \frac{x^{\nu-1}}{\mathrm{e}^x \, z^{-1} \mp 1} \tag{202}$$

15.1 Bosons

Partition sum

$$Z_\mathrm{g} = \prod_p \frac{1}{1 - \mathrm{e}^{-\beta(\epsilon_p - \mu)}} \tag{203}$$

$p \in \mathbb{N}_0$

Occupation number
Bose-Einstein distribution

$$\langle n_p \rangle = \frac{1}{\mathrm{e}^{\beta(\epsilon - \mu)} - 1} \tag{204}$$

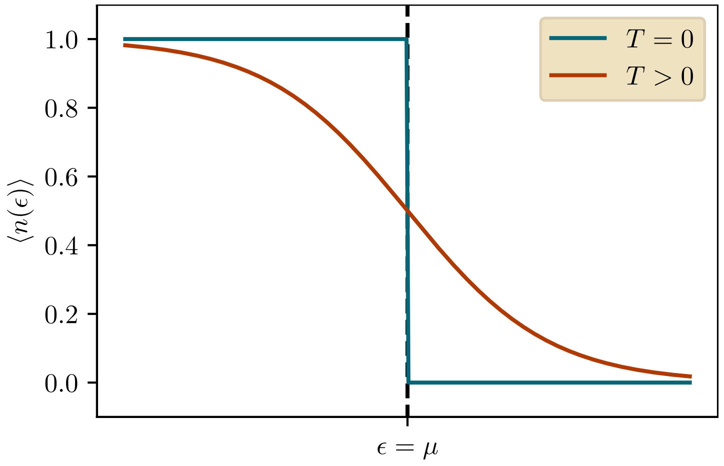
15.2 Fermions

Partition sum

$$Z_\mathrm{g} = \prod_p \left(1 + \mathrm{e}^{-\beta(\epsilon_p - \mu)} \right) \tag{205}$$

$p = 0, 1$

Occupation number
Fermi-Dirac distribution. At $T = 0$ *Fermi edge* at $\epsilon = \mu$



$$\langle n_p \rangle = \frac{1}{\mathrm{e}^{\beta(\epsilon - \mu)} + 1} \tag{206}$$

Slater determinant

$$\psi(\vec{r}_1,\vec{r}_2,\dots,\vec{r}_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} p_1(\vec{r}_1) & p_2(\vec{r}_1) & \dots & p_N(\vec{r}_1) \\ p_1(\vec{r}_2) & p_2(\vec{r}_2) & \dots & p_N(\vec{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ p_1(\vec{r}_N) & p_2(\vec{r}_N) & \dots & p_N(\vec{r}_N) \end{vmatrix} \tag{207}$$

Fermi energy

$$\epsilon_\text{F} := \mu(T = 0) \tag{208}$$

Fermi temperature

$$T_\text{F} := \frac{\epsilon_\text{F}}{k_\text{B}} \tag{209}$$

Fermi impulse
Radius of the *Fermi sphere* in impulse space. States with p_F are in the *Fermi surface*

$$p_\text{F} = \hbar k_\text{F} = (2mE_\text{F})^{\frac{1}{2}} \tag{210}$$

Specific density

$$v = \frac{N}{V} = \frac{g}{\lambda^3} f_{3/2}(z) \tag{211}$$

f Generalized zeta function, g degeneracy factor, z Fugacity

15.2.1 Strong degeneracy

Sommerfeld expansion
for low temperatures $T \ll T_\text{F}$

$$f_\nu(z) = \frac{(\ln z)^\nu}{\Gamma(\nu+1)}\left(1 + \frac{\pi^6}{6}\frac{\nu(\nu-1)}{(\ln z)^2} + \dots\right) \tag{212}$$

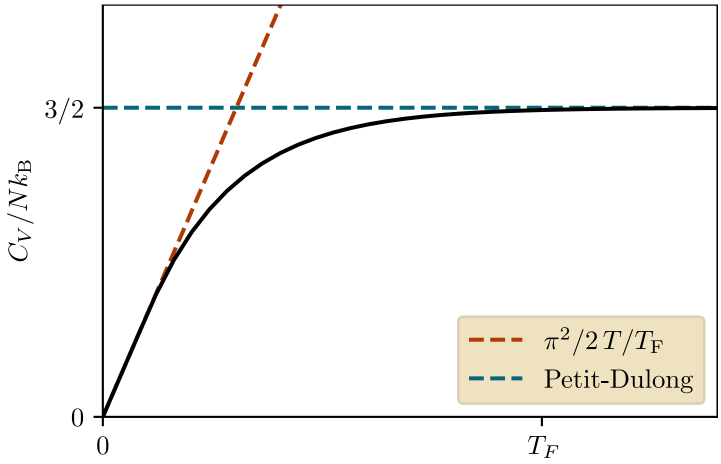
Energy density

$$\frac{E}{V} = \frac{3}{2}\frac{g}{\lambda^3} k_\text{B} T f_{5/2}(z) \tag{213}$$

Sommerfeld expansion

$$\approx \frac{3}{5}\frac{N}{V} E_\text{F}\left(1 + \frac{5\pi^2}{12}\left(\frac{k_\text{B}T}{E_\text{F}}\right)^2\right) \tag{214}$$

Heat capacity
for low temperatures $T \ll T_\text{F}$



$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = Nk_\text{B}\frac{\pi}{2}\left(\frac{T}{T_\text{F}}\right) \tag{215}$$

differs from td:TODO:petit dulong

TODO:Entartung und Sommerfeld TODO:DULONG-PETIT Gesetz

Part V

Electrodynamics

16 Electric field

Electric field
Surrounds charged particles

Symbol: $\vec{\mathcal{E}}$ Unit: $1\,\mathrm{V\,m^{-1}} = 1\,\mathrm{kgm/s^3A}$

Electric potential
Work required to move a unit of charge between two points

Symbol: ϕ Unit: $1\,\mathrm{V} = 1\,\mathrm{kgm^2/s^3A}$

$$\phi = -\int \vec{\mathcal{E}} \cdot \mathrm{d}\vec{r} \tag{216}$$

Gauss's law for electric fields
Electric flux through a closed surface is proportional to the electric charge

$$\Phi_\mathrm{E} = \iint_S \vec{\mathcal{E}} \cdot \mathrm{d}\vec{S} = \frac{Q}{\varepsilon_0} \tag{217}$$

S closed surface

Permittivity
Dieletric function
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

$$\epsilon(\omega)_\mathrm{r} = \frac{\epsilon(\omega)}{\epsilon_0} \tag{218}$$

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:

$$\epsilon_\mathrm{r} = 1 + \chi_\mathrm{e} \tag{219}$$

ϵ_r Relative permittivity / Dielectric constant

Dielectric polarization density

Symbol: $\vec{P}$ Unit: $1\,\mathrm{C/m^2}$

$$\vec{P} = \epsilon_0 \chi_\mathrm{e} \vec{\mathcal{E}} \tag{220}$$

ϵ_0 Vacuum permittivity, χ_e Electric susceptibility, $\vec{\mathcal{E}}$ Electric field

---

Electric displacement field

Symbol: $\vec{D}$ Unit: $1\,\mathrm{C/m^2} = 1\,\mathrm{As/m^2}$

$$\vec{D} = \epsilon_0 \vec{\mathcal{E}} + \vec{P} \tag{221}$$

ϵ_0 Vacuum permittivity, $\vec{\mathcal{E}}$ Electric field, $\vec{P}$ Dielectric polarization density

Electric flux through area $\vec{A}$	$\Phi_\mathrm{E} = \int_A \vec{D} \cdot \mathrm{d}\vec{A}$ (222) $\vec{D}$ Electric displacement field
Electric power	$P_\mathrm{el} = U\,I$ (223) U Electric potential, I Electric current

17 Magnetic field

Magnetic flux	Symbol: Φ_B Unit: $1\,\mathrm{Wb} = 1\,\mathrm{V\,s}^{-1} = 1\,\mathrm{kgm}^2/\mathrm{s}^2\mathrm{A}$ $\Phi_\mathrm{B} = \iint_A \vec{B} \cdot \mathrm{d}\vec{A}$ (224) $\vec{A}$ area
Magnetic flux density Defined by Lorentz force law	Symbol: $\vec{B}$ Unit: $1\,\mathrm{T} = 1\,\mathrm{Vs/m}^2 = 1\,\mathrm{N\,A}^{-1}\,\mathrm{m} = 1\,\mathrm{kg/As}^2$ $\vec{B} = \mu_0(\vec{H} + \vec{M})$ (225) $\vec{H}$ Magnetic field intensity, $\vec{M}$ Magnetization, μ_0 Magnetic vauum permeability
Magnetic vector potential	Symbol: $\vec{A}$ Unit: $1\,\mathrm{T\,m} = 1\,\mathrm{V\,s\,m}^{-1} = 1\,\mathrm{kgm/s}^2\mathrm{A}$ $\vec{\nabla} \times \vec{A}(\vec{r}) = \vec{B}(\vec{r})$ (226)
Magnetic field intensity	Symbol: $\vec{H}$ Unit: $1\,\mathrm{A\,m}^{-1}$ $\vec{H} \equiv \frac{1}{\mu_0}\vec{B} - \vec{M}$ (227)
Lorentz force law Force on charged particle	$\vec{F} = q\vec{\mathcal{E}} + q\vec{v} \times \vec{B}$ (228)
Magnetic permeability	Symbol: μ Unit: $1\,\mathrm{H\,m}^{-1} = 1\,\mathrm{V\,s\,A}^{-1}\,\mathrm{m}$ $\mu = \frac{B}{H}$ (229) 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	$\mu_\mathrm{r} = \frac{\mu}{\mu_0}$ (230)

Gauss's law for magnetism
Magnetic flux through a closed surface is 0 ⇒there are no magnetic monopoles

$$\Phi_{\mathrm{B}} = \iint_S \vec{B} \cdot \mathrm{d}\vec{S} = 0 \tag{231}$$

S closed surface

Magnetization
Vector field describing the density of magnetic dipoles

Symbol: $\vec{M}$ Unit: $1\,\mathrm{A\,m^{-1}}$

$$\vec{M} = \frac{\mathrm{d}\vec{m}}{\mathrm{d}V} = \chi_{\mathrm{m}} \cdot \vec{H} \tag{232}$$

Magnetic moment
Strength and direction of a magnetic dipole

Symbol: $\vec{m}$ Unit: $1\,\mathrm{Am^2}$

Torque

$$\vec{\tau} = \vec{m} \times \vec{B} \tag{233}$$

m Magnetic moment

Susceptibility

$$\chi_{\mathrm{m}} = \frac{\partial M}{\partial B} = \mu_{\mathrm{r}} - 1 \tag{234}$$

μ_{r} Relative permeability

17.1 Magnetic materials

Paramagnetism
Magnetic field strengthend in the material

$$\mu_{\mathrm{r}} > 1 \tag{235}$$

$$\chi_{\mathrm{m}} > 0 \tag{236}$$

μ Magnetic permeability, χ_{m} Susceptibility

Diamagnetism
Magnetic field expelled from material

$$0 < \mu_{\mathrm{r}} < 1 \tag{237}$$

$$-1 < \chi_{\mathrm{m}} < 0 \tag{238}$$

μ Magnetic permeability, χ_{m} Susceptibility

Ferromagnetism
Magnetic moments align to external magnetic field and stay aligned when the field is turned off (Remanescence)

$$\mu_{\mathrm{r}} \gg 1 \tag{239}$$

μ Magnetic permeability, χ_{m} Susceptibility

18 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?

$$\epsilon_0\mu_0 = \frac{1}{c^2} \tag{240}$$

ϵ_0 Vacuum permittivity, μ_0 Magnetic vauum permeability, c Speed of light

Poisson equation for electrostatics

$$\triangle\Phi(\vec{r}) = -\frac{\rho(\vec{r})}{\epsilon} \tag{241}$$

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]

$$\vec{S} = \vec{E} \times \vec{H} \tag{242}$$

Electric field

$$\vec{\mathcal{E}} = -\vec{\nabla}\phi - \frac{\partial\vec{A}}{\partial t} \tag{243}$$

$\vec{\mathcal{E}}$ Electric field, ϕ Electric potential, $\vec{A}$ Magnetic vector potential

Hamiltonian of a particle in an electromagnetic field
In the ed:em:gauge:coulomb

$$\hat{H} = \frac{1}{2m}\left[\hat{p} \frac{e\vec{A}}{c}\right]^2 \tag{244}$$

m Mass, $\hat{p}$ Momentum operator, q Charge, $\vec{A}$ Magnetic vector potential, c Speed of light

18.1 Maxwell-Equations

Vacuum
microscopic formulation

$$\vec{\nabla} \cdot \vec{\mathcal{E}} = \frac{\rho_\text{el}}{\epsilon_0} \tag{245}$$

$$\vec{\nabla} \cdot \vec{B} = 0 \tag{246}$$

$$\vec{\nabla} \times \vec{\mathcal{E}} = -\frac{\mathrm{d}\vec{B}}{\mathrm{d}t} \tag{247}$$

$$\vec{\nabla} \times \vec{B} = \mu_0\vec{j} + \frac{1}{c^2}\frac{\mathrm{d}\vec{\mathcal{E}}}{\mathrm{d}t} \tag{248}$$

Matter
Macroscopic formulation

$$\vec{\nabla} \cdot \vec{D} = \rho_\text{el} \tag{249}$$

$$\vec{\nabla} \cdot \vec{B} = 0 \tag{250}$$

$$\vec{\nabla} \times \vec{\mathcal{E}} = -\frac{\mathrm{d}\vec{B}}{\mathrm{d}t} \tag{251}$$

$$\vec{\nabla} \times \vec{H} = \vec{j} + \frac{\mathrm{d}\vec{D}}{\mathrm{d}t} \tag{252}$$

18.1.1 Gauges

Coulomb gauge

$$\vec{\nabla} \cdot \vec{A} = 0 \tag{253}$$

$\vec{A}$ Magnetic vector potential

TODO:Polarization

18.2 Induction

Faraday's law of induction

$$U_\text{ind} = -\frac{\mathrm{d}}{\mathrm{d}t}\Phi_\text{B} = -\frac{\mathrm{d}}{\mathrm{d}t}\iint_A \vec{B} \cdot \mathrm{d}\vec{A} \tag{254}$$

Lenz's law

Change of magnetic flux through a conductor induces a current that counters that change of magnetic flux.

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19 Optics

Properties of light and its interactions with matter

Refraction index

Symbol: $\tilde{n}$ Unit:

$$\tilde{n} = n' + in'' \tag{255}$$

$$n = \sqrt{\epsilon_\text{r}\mu_\text{r}} \tag{256}$$

$$n = \frac{c_0}{c_\text{M}} \tag{257}$$

??? ???:relative permittivity, ??? ???:relative permeability, c Speed of light, c_M speed of light in the medium

---

TODO:what does the complex part of the dielectric function represent?

Real part of the refraction index

Symbol: n' Unit:

Extinction coefficient
Complex part of the refraction index

Symbol: n'' Unit:
sometimes κ

Reflectio

$$R = \left|\frac{\tilde{n} - 1}{\tilde{n} + 1}\right| \tag{258}$$

$\tilde{n}$ Refraction index

Snell's law

$$n_1' \sin\theta_1 = n_2' \sin\theta_2 \tag{259}$$

n_i' Real part of the refraction index, θ_i incidence angle (normal to the surface)

Group velocity
Velocity with which the envelope of a wave propagates through space

$$v_{\mathrm{g}} \equiv \frac{\partial \omega}{\partial k} \tag{260}$$

ω Angular frequency, ??? ???:angular wavenumber

Phase velocity
Velocity with which a wave propagates through a medium

$$v_{\mathrm{p}} = \frac{\omega}{k} = \frac{\lambda}{T} \tag{261}$$

ω Angular frequency, ??? ???:angular wavenumber, ??? ???:wavelength, T Time period

---

Absorption coefficient
Intensity reduction while traversing a medium, not necessarily by energy transfer to the medium

Symbol: α Unit: $1\,\mathrm{cm}^{-1}$

$$\alpha = 2n''\frac{\omega}{c} \tag{262}$$

$$\alpha = \frac{\omega}{nc}\epsilon' \tag{263}$$

TODO:For direct band gaps; from adv. sc: sheet 10 2b). Check wh

n'' Extinction coefficient, c Speed of light, ω Angular frequency

---

Electromagnetic radiation intensity
Surface power density

Symbol: I Unit: $1\,\mathrm{W/m^2} = 1\,/\mathrm{s}^3$

$$I = |\langle S \rangle_t| \tag{264}$$

S ed:poynting

Beer-Lambert law
Intensity in an absorbing medium

$$I(z) = I_0\,\mathrm{e}^{-\kappa z} \tag{265}$$

I Electromagnetic radiation intensity, α Absorption coefficient, z penetration depth

---

20 Hall-Effect

Cyclontron frequency

$$\omega_{\mathrm{c}} = \frac{eB}{m_{\mathrm{e}}} \tag{266}$$

TODO:Move

20.1 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

$$U_{\mathrm{H}} = \frac{IB}{ned} \tag{267}$$

n charge carrier density

Hall coefficient
Sometimes R_{H}

$$A_{\mathrm{H}} := -\frac{E_y}{j_x B_z} \overset{\text{metals}}{\overset{\downarrow}{=}} \frac{1}{ne} = \frac{\rho_{xy}}{B_z} \tag{268}$$

Resistivity

$$\rho_{xx} = \frac{m_\mathrm{e}}{ne^2\tau} \tag{269}$$

$$\rho_{xy} = \frac{B}{ne} \tag{270}$$

20.2 Integer quantum hall effect

Conductivity tensor

$$\sigma = \begin{pmatrix} \sigma_{xy} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \tag{271}$$

Resistivity tensor

$$\rho = \sigma^{-1} \tag{272}$$

Resistivity

$$\rho_{xy} = \frac{2\pi\hbar}{e^2}\frac{1}{\nu} \tag{273}$$

$\nu \in \mathbb{Z}$ filing factor

Fractional quantum hall effect

$$\nu = \frac{1}{3}, \frac{2}{5}, \frac{3}{7}, \frac{2}{3}\dots \tag{274}$$

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

21 Dipole-stuff

Dipole radiation Poynting vector

$$\vec{S} = \left(\frac{\mu_0 p_0^2 \omega^4}{32\pi^2 c}\right)\frac{\sin^2\theta}{r^2}\vec{r} \tag{275}$$

Time-average power

$$P = \frac{\mu_0 \omega^4 p_0^2}{12\pi c} \tag{276}$$

22 misc

Impedance of an ohmic resistor

$$Z_R = R \tag{277}$$

??? ???:resistance

Impedance of a capacitor

$$Z_C = \frac{1}{i\omega C} \tag{278}$$

??? ???:capacity, ??? ???:angular velocity

Impedance of an inductor

$$Z_L = i\omega L \tag{279}$$

??? ???:inductance, ??? ???:angular velocity

TODO:impedance addition for parallel / linear

Part VI

Quantum Mechanics

23 Basics

23.1 Operators

Dirac notation

$$\langle x|\ \text{"Bra" Row vector} \tag{280}$$
$$|x\rangle\ \text{"Ket" Column vector} \tag{281}$$
$$\hat{A}\,|\beta\rangle = |\alpha\rangle \Rightarrow \langle\alpha| = \langle\beta|\,\hat{A}^\dagger \tag{282}$$

Dagger

$$\hat{A}^\dagger = (\hat{A}^*)^\mathrm{T} \tag{283}$$
$$(c\hat{A})^\dagger = c^*\hat{A}^\dagger \tag{284}$$
$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger \tag{285}$$
$$\tag{286}$$

Adjoint operator

$$\langle\alpha|\hat{A}^\dagger|\beta\rangle = \langle\beta|\hat{A}|\alpha\rangle^* \tag{287}$$

Hermitian operator

$$\hat{A} = \hat{A}^\dagger \tag{288}$$

23.1.1 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

$$p(\lambda) = \langle\psi|\hat{P}_\lambda|\psi\rangle \tag{289}$$

State after measurement

$$|\psi\rangle_\text{post} = \frac{1}{\sqrt{p(\lambda)}}\hat{P}_\lambda\,|\psi\rangle \tag{290}$$

23.1.2 Pauli matrices

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |0\rangle\,\langle 1| + |1\rangle\,\langle 0| \tag{291}$$
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -i\,|0\rangle\,\langle 1| + i\,|1\rangle\,\langle 0| \tag{292}$$
$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |0\rangle\,\langle 0| - |1\rangle\,\langle 1| \tag{293}$$

23.2 Probability theory

Continuity equation

$$\frac{\partial \rho(\vec{x},t)}{\partial t} + \nabla \cdot \vec{j}(\vec{x},t) = 0 \tag{294}$$

ρ density of a conserved quantity q, j flux density of q

State probability

$$\textit{TODO} \tag{295}$$

Dispersion

$$\Delta \hat{A} = \hat{A} - \langle \hat{A} \rangle \tag{296}$$

Generalized uncertainty principle

$$\sigma_A \sigma_B \geq \frac{1}{4} \langle [\hat{A}, \hat{B}] \rangle^2 \tag{297}$$

$$\sigma_A \sigma_B \geq \frac{1}{2} \left| \langle [\hat{A}, \hat{B}] \rangle \right| \tag{298}$$

23.3 Commutator

Commutator

$$[A, B] = AB - BA \tag{299}$$

Anticommutator

$$\{A, B\} = AB + BA \tag{300}$$

Commutation relations

$$[A, BC] = [A, B]C - B[A, C] \tag{301}$$

TODO:add some more?

Commutator involving a function

$$[f(A), B] = [A, B] \frac{\partial f}{\partial A} \tag{302}$$

given $[A, [A, B]] = 0$

Jacobi identity

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \tag{303}$$

Hadamard's Lemma

$$\mathrm{e}^A B \,\mathrm{e}^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \ldots \tag{304}$$

Canonical commutation relation

$$[x_i, x_j] = 0 \tag{305}$$

$$[p_i, p_j] = 0 \tag{306}$$

$$[x_i, p_j] = i\hbar\delta_{ij} \tag{307}$$

x, p canonical conjugates

---

24 Schrödinger equation

Energy operator

$$E = i\hbar \frac{\partial}{\partial t} \tag{308}$$

Momentum operator	$\vec{p} = -i\hbar\vec{\nabla}_x$ (309)
Space operator	$\vec{x} = i\hbar\vec{\nabla}_p$ (310)
Stationary Schrödingerequation	$\hat{H}\left\|\psi\right\rangle = E\left\|\psi\right\rangle$ (311)
Schrödinger equation	$i\hbar\frac{\partial}{\partial t}\psi(x,t) = (-\frac{\hbar^2}{2m}\vec{\nabla}^2 + \vec{V}(x))\psi(x)$ (312)
Hellmann-Feynman-Theorem Derivative of the energy to a parameter	$\frac{\mathrm{d}E_\lambda}{\mathrm{d}\lambda} = \int \mathrm{d}^3 r \psi_\lambda^* \frac{\mathrm{d}\hat{H}_\lambda}{\mathrm{d}\lambda}\psi_\lambda = \left\langle \psi(\lambda) \middle\| \frac{\mathrm{d}\hat{H}_\lambda}{\mathrm{d}\lambda} \middle\| \psi(\lambda) \right\rangle$ (313)
Variational principle	If $\hat{H}\psi = E\psi$, then $E_0 \leq E = \left\langle \psi \middle\| \hat{H} \middle\| \psi \right\rangle$. The ground state can thus be found by varying ψ until E is minimized.

24.1 Time evolution

The time evolution of the Hamiltonian is given by:

Time evolution operator	$\left\|\psi(t)\right\rangle = \hat{U}(t,t_0)\left\|\psi(t_0)\right\rangle$ (314) U unitary
Von-Neumann Equation Time evolution of the density operator in the Schrödinger picture. Qm analog to the Liouville equation ??	$\frac{\partial\hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}]$ (315)
Lindblad master equation Generalization of von-Neumann equation for open quantum systems	$\dot{\rho} = \underbrace{-\frac{i}{\hbar}[\hat{H},\rho]}_{\text{reversible}} + \underbrace{\sum_{n.m} h_{nm}\left(\hat{A}_n\rho\hat{A}_{m^\dagger} - \frac{1}{2}\left\{\hat{A}_m^\dagger\hat{A}_n,\rho\right\}\right)}_{\text{irreversible}}$ (316) h positive semidifnite matrix, $\hat{A}$ arbitrary operator

TODO:unitary transformation of time dependent H

24.1.1 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	$\left\|\psi(t)_\mathrm{S}\right\rangle = \hat{U}(t,t_0)\left\|\psi(t_0)\right\rangle$ (317)

Heisenberg time evolution

$$|\psi_{\mathrm{H}}\rangle = |\psi_{\mathrm{S}}(t_0)\rangle \tag{318}$$

$$A_{\mathrm{H}} = U^\dagger(t,t_0)A_{\mathrm{S}}U(t,t_0) \tag{319}$$

$$\frac{\mathrm{d}\hat{A}_{\mathrm{H}}}{\mathrm{d}t} = \frac{1}{i\hbar}[\hat{A}_{\mathrm{H}},\hat{H}_{\mathrm{H}}] + \left(\frac{\partial \hat{A}_{\mathrm{S}}}{\partial t}\right)_{\mathrm{H}} \tag{320}$$

H and S being the Heisenberg and Schrödinger picture, respectively

24.1.2 Ehrenfest theorem

See also **??**

Ehrenfest theorem
applies to both pictures

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle \tag{321}$$

Ehrenfest theorem example
Example for x

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x\rangle = -\langle\nabla V(x)\rangle = \langle F(x)\rangle \tag{322}$$

Correspondence principle

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

25 Pertubation theory

The following holds true if the pertubation $\hat{H}_1$ is sufficently small and the $E_n^{(0)}$ levels are not degenerate.

Hamiltonian

$$\hat{H} = \hat{H}_0 + \lambda\hat{H}_1 \tag{323}$$

Power series

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \tag{324}$$

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle + \dots \tag{325}$$

1. order energy shift

$$E_n^{(1)} = \left\langle\psi_n^{(0)}\middle|\hat{H}_1\middle|\psi_n^{(0)}\right\rangle \tag{326}$$

1. order states

$$|\psi_n^{(1)}\rangle = \sum_{k\neq n}\frac{\left\langle\psi_k^{(0)}\middle|\hat{H}_1\middle|\psi_n^{(0)}\right\rangle}{E_n^{(0)} - E_k^{(0)}}|\psi_k^{(0)}\rangle \tag{327}$$

2. order energy shift

$$E_n^{(2)} = \sum_{k\neq n}\frac{\left|\left\langle\psi_k^{(0)}\middle|\hat{H}_1\middle|\psi_n^{(0)}\right\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}} \tag{328}$$

Fermi's golden rule
Transition rate from initial state $|i\rangle$ under a pertubation H^1 to final state $|f\rangle$

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}\left|\langle f|H^1|i\rangle\right|^2\rho(E_f) \tag{329}$$

26 Harmonic oscillator

Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{330}$$

$$= \frac{1}{2}\hbar\omega + \omega a^\dagger a \tag{331}$$

Energy spectrum

$$E_n = \hbar\omega\left(\frac{1}{2} + n\right) \tag{332}$$

See also 26.1

26.1 Creation and Annihilation operators / Ladder operators

Particle number operator/occupation number operator

$$\hat{N} := a^\dagger a \tag{333}$$

$$\hat{N}\left|n\right\rangle = n\left|N\right\rangle \tag{334}$$

$|n\rangle$ = Fock states, $\hat{a}$ = Annihilation operator, $\hat{a}^\dagger$ = Creation operator

Commutator

$$[\hat{a}, \hat{a}^\dagger] = 1 \tag{335}$$

$$[N, \hat{a}] = -\hat{a} \tag{336}$$

$$[N, \hat{a}^\dagger] = \hat{a}^\dagger \tag{337}$$

Application on states

$$\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle \tag{338}$$

$$\hat{a}^\dagger\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle \tag{339}$$

$$\left|n\right\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\left|0\right\rangle \tag{340}$$

Matrix forms

$$\hat{n} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & N \end{pmatrix} \tag{341}$$

$$\hat{a} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \sqrt{N} \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{342}$$

$$\hat{a}^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 \\ 0 & 0 & \sqrt{N} & 0 \end{pmatrix} \tag{343}$$

26.1.1 Harmonischer Oszillator

Harmonic oscillator

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \tag{344}$$

$$\hat{p} = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^\dagger) \tag{345}$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2} \qquad = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \tag{346}$$

$$a = \frac{1}{\sqrt{2}}(\tilde{X} + i\tilde{P}) \tag{347}$$

$$a^\dagger = \frac{1}{\sqrt{2}}(\tilde{X} - i\tilde{P}) \tag{348}$$

---

27 Angular momentum

27.1 Aharanov-Bohm effect

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

$$\delta = \frac{2e}{\hbar}\oint \vec{A}\cdot \mathrm{d}\vec{s} = \frac{2e}{\hbar}\Phi \tag{349}$$

TODO:replace with loop intergral symbol and add more info

28 Periodic potentials

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

$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \cdot u_{\vec{k}}(\vec{r}) \tag{350}$$

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

Periodicity

$$u_{\vec{k}}(\vec{r} + \vec{R}) = u_{\vec{k}}(\vec{r}) \tag{351}$$

$$\psi_{\vec{k}+\vec{G}}(\vec{r}) = \psi_{\vec{k}}(\vec{r}) \tag{352}$$

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

---

29 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

$$\hat{U}\hat{H}\hat{U}^\dagger = \hat{H} \Leftrightarrow [\hat{U}, \hat{H}] = 0 \tag{353}$$

29.1 Time-reversal symmetry

Time-reversal symmetry

$$T : t \to -t \tag{354}$$

Anti-unitary

$$T^2 = -1 \tag{355}$$

---

30 Two-level systems (TLS)

James-Cummings Hamiltonian
TLS interacting with optical cavity

$$H = \underbrace{\hbar\omega_c \hat{a}^\dagger \hat{a}}_{\text{field}} + \underbrace{\hbar\omega_{\mathrm{a}} \frac{\hat{\sigma}_z}{2}}_{\text{atom}} + \underbrace{\frac{\hbar\Omega}{2} \hat{E}\hat{S}}_{\text{int}} \tag{356}$$

after RWA:

$$\tag{357}$$

$$= \hbar\omega_c \hat{a}^\dagger \hat{a} + \hbar\omega_{\mathrm{a}} \hat{\sigma}^\dagger \hat{\sigma} + \frac{\hbar\Omega}{2} (\hat{a}\sigma\hat{}^\dagger + \hat{a}^\dagger \hat{\sigma}) \tag{358}$$

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

---

31 Other

Rotating Wave Approximation (RWS)
Rapidly oscilating terms are neglected

$$\Delta\omega := |\omega_0 - \omega_{\mathrm{L}}| \ll |\omega_0 + \omega_{\mathrm{L}}| \approx 2\omega_0 \tag{359}$$

ω_{L} light frequency, ω_0 transition frequency

Adiabatic theorem

A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum.

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

$$\Psi(q_1, \dots, q_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_a(q_1) & \phi_a(q_2) & \cdots & \phi_a(q_N) \\ \phi_b(q_1) & \phi_b(q_2) & \cdots & \phi_b(q_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_z(q_1) & \phi_z(q_2) & \cdots & \phi_z(q_N) \end{vmatrix} \tag{360}$$

---

32 Hydrogen Atom

Reduced mass

$$\mu = \frac{m_{\mathrm{e}} m_{\mathrm{K}}}{m_{\mathrm{e}} + m_{\mathrm{K}}} \overset{m_{\mathrm{e}} \ll m_{\mathrm{K}}}{\overset{\downarrow}{\approx}} m_{\mathrm{e}} \tag{361}$$

Coulumb potential
For a single electron atom

$$V(\vec{r}) = \frac{Z e^2}{4\pi\epsilon_0 r} \tag{362}$$

Z atomic number

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2\mu}\vec{\nabla}_{\vec{r}}^2 - V(\vec{r}) \tag{363}$$

$$= \frac{\hat{p}_r^2}{2\mu} + \frac{\hat{L}^2}{2\mu r} + V(r) \tag{364}$$

Wave function

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi) \tag{365}$$

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

Radial part

$$R_{nl} = -\sqrt{\frac{(n-l-1)!(2\kappa)^3}{2n[(n+l)!]^3}}(2\kappa r)^l\, \mathrm{e}^{-\kappa r}\, L_{n+1}^{2l+1}(2\kappa r) \tag{366}$$

with

$$\kappa = \frac{\sqrt{2\mu|E|}}{\hbar} = \frac{Z}{na_{\mathrm{B}}} \tag{367}$$

$L_r^s(x)$ Laguerre-polynomials

Energy eigenvalues

$$E_n = \frac{Z^2\mu e^4}{n^2(4\pi\epsilon_0)^2 2\hbar^2} = -E_{\mathrm{H}}\frac{Z^2}{n^2} \tag{368}$$

Rydberg constant
for heavy atoms

Symbol: R_∞
Experimental value
$10973731.568157(12)\,\mathrm{m}^{-1}$

$$R_\infty = \frac{m_e e^4}{8\epsilon_0^2 h^3 c} \tag{369}$$

m_{e} Electron mass, ??? ???:elementary charge, ??? ???:vacuum permittivity, h Planck Constant, ??? ???:vacuum speed of light

---

Rydberg constant
corrected for nucleus mass M

$$R_{\mathrm{M}} = \frac{\mu}{m_{\mathrm{e}}}R_\infty \tag{370}$$

??? ???:rydberg constant heavy, $\mu = \left(\frac{1}{m_{\mathrm{e}}} + \frac{1}{M}\right)^{-1}$ reduced mass, m_{e} Electron mass

---

Rydberg energy
Energy unit

$$1\,\mathrm{Ry} = hc\,R_\infty \tag{371}$$

R_∞ Rydberg constant, h Planck Constant, ??? ???:vacuum speed of light

---

Bohr radius

Symbol: a_0
Experimental value
$5.29177210544(82)\cdot 10^{-11}\,\mathrm{m}$

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{e^2 m_{\mathrm{e}}} \tag{372}$$

ϵ_0 Vacuum permittivity, m_{e} Electron mass

32.1 Corrections

32.1.1 Darwin term

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

Energy shift

$$\Delta E_{\text{rel}} = -E_n \frac{Z^2\alpha^2}{n}\left(\frac{3}{4n} - \frac{1}{l+\frac{1}{2}}\right) \tag{373}$$

Fine-structure constant
Sommerfeld constant

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137} \tag{374}$$

32.1.2 Spin-orbit coupling (LS-coupling)

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

Energy shift

$$\Delta E_{\text{LS}} = \frac{\mu_0 Z e^2}{8\pi m_\text{e}^2 r^3}\langle \vec{S}\cdot\vec{L}\rangle \tag{375}$$

TODO:name

$$\begin{aligned}\langle \vec{S}\cdot\vec{L}\rangle &= \frac{1}{2}\langle [J^2 - L^2 - S^2]\rangle \\ &= \frac{\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)] \qquad (376)\end{aligned}$$

32.1.3 Fine-structure

The fine-structure combines relativistic corrections 32.1.1 and the spin-orbit coupling 32.1.2.

Energy shift

$$\Delta E_{\text{FS}} = \frac{Z^2\alpha^2}{n}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right) \tag{377}$$

32.1.4 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

$$\langle E_{\text{pot}}\rangle = -\frac{Ze^2}{4\pi\epsilon_0}\left\langle \frac{1}{r+\delta r}\right\rangle \tag{378}$$

δr pertubation of r

32.1.5 Hyperfine structure

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

Nuclear spin

$$\vec{F} = \vec{J} + \vec{I} \tag{379}$$

$$\left|\vec{I}\right| = \sqrt{i(i+1)}\hbar \tag{380}$$

$$I_z = m_i\hbar \tag{381}$$

$$m_i = -i, -i+1, \dots, i-1, i \tag{382}$$

Combined angular momentum

$$\vec{F} = \vec{J} + \vec{I} \tag{383}$$
$$\left|\vec{F}\right| = \sqrt{f(f+1)}\hbar \tag{384}$$
$$F_z = m_f \hbar \tag{385}$$

Selection rule

$$f = j \pm i \tag{386}$$
$$m_f = -f, -f+1, \dots, f-1, f \tag{387}$$

Hyperfine structure constant

$$A = \frac{g_i \mu_\text{K} B_\text{HFS}}{\sqrt{j(j+1)}} \tag{388}$$

B_HFS hyperfine field, μ_K nuclear magneton, g_i nuclear g-factor **??**

Energy shift

$$\Delta H_\text{HFS} = \frac{A}{2}[f(f+1) - j(j+1) - i(i+1)] \tag{389}$$

TODO:landé factor

32.2 Effects in magnetic field

TODO:all
TODO:Hunds rules

32.3 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 TODO:Lattice vibrations, van hove singularities, debye frequency

Density of states (DOS)

$$D(E) = \frac{1}{V} \sum_{i=1}^{N} \delta(E - E(\vec{k}_i)) \tag{390}$$

V Volume, N number of energy levels, ??? ???:energy

Density of states for parabolic dispersion

Applies to Free electron gas

$$D_1(E) = \frac{1}{2\sqrt{c_k(E - E_0)}} \quad \text{(1D)} \tag{391}$$

$$D_2(E) = \frac{\pi}{2c_k} \quad \text{(2D)} \tag{392}$$

$$D_3(E) = \pi \sqrt{\frac{E - E_0}{c_k^3}} \quad \text{(3D)} \tag{393}$$

---

33 Lattice vibrations

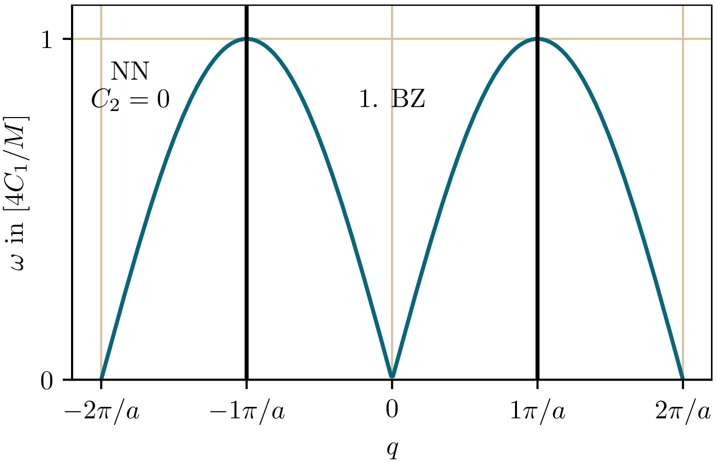
Phonon dispersion of a lattice with a one-atom basis

same as the dispersion of a linear chain

$$\omega^2 = \frac{4C_1}{M} \left[\sin^2\left(\frac{qa}{2}\right) + \frac{C2}{C1} \sin^2(qa)\right] \tag{394}$$

with

$$u_{s+n} = U \, \mathrm{e}^{-i[\omega t - q(s+n)a]} \tag{395}$$



C_n force constants between layer s and $s+n$, M Mass of the reference atom, a Lattice constant, q phonon ???:wavevector, u Ansatz for the atom displacement

---

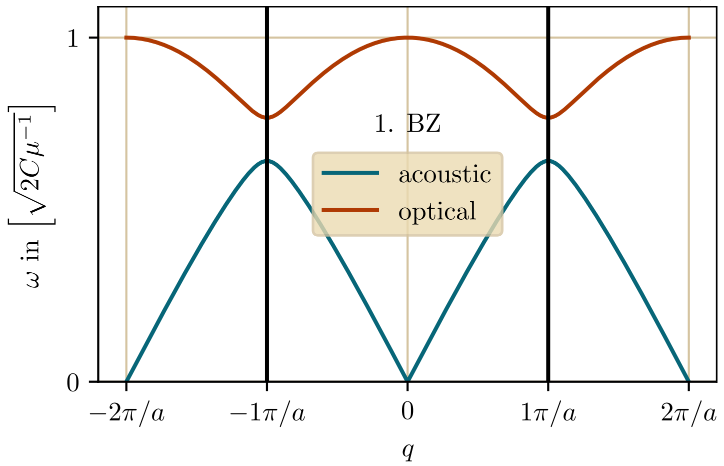
TODO:Plots

Phonon dispersion of a lattice with a two-atom basis

$$\omega_{\text{a,o}}^2 = C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \mp C\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4}{M_1 M_2}\sin^2\left(\frac{qa}{2}\right)} \tag{396}$$

with

$$u_s = U\,\mathrm{e}^{-i(\omega t - qsa)}, \quad v_s = V\,\mathrm{e}^{-i(\omega t - qsa)} \tag{397}$$



C force constant between layers, M_i Mass of the basis atoms, a Lattice constant, q phonon ???:wavevector, u, v Ansatz for the displacement of basis atom 1 and 2, respectively

Vibration branches

Acoustic: 3 modes (1 longitudinal, 2 transversal), the two basis atoms oscillate in phase.
Optical: 3 modes, the two basis atoms oscillate in opposition. A dipole moment is created that can couple to photons.

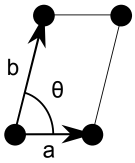
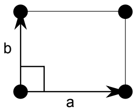
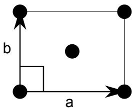
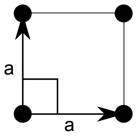
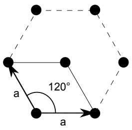
33.1 Debye model

Atoms behave like coupled quantum harmonic oscillators. The finite sample size leads to periodic boundary conditio. The finite sample size leads to periodic boundary conditions for the vibrations.

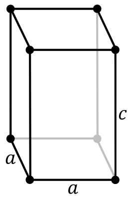
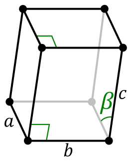
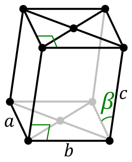
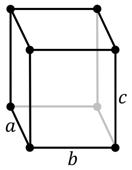
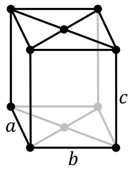
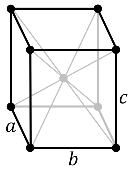
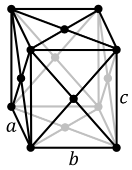
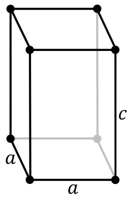
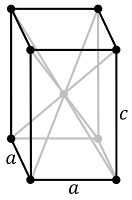
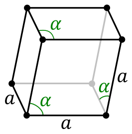
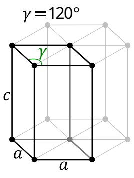
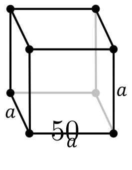
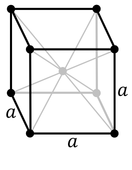
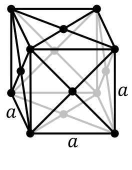
34 Crystals

34.1 Bravais lattice

2D : 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		

3D : 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:

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \tag{398}$$

$n_i \in \mathbb{Z}$

TODO:primitive unit cell: contains one lattice point

Miller index

$$(hkl)\text{plane} \tag{399}$$

$$[hkl]\text{direction} \tag{400}$$

$$\{hkl\}\text{millerFamily} \tag{401}$$

Miller family: planes that are equivalent due to crystal symmetry

34.2 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

$$\vec{b}_1 = \frac{2\pi}{V_c}\vec{a}_2 \times \vec{a}_3 \tag{402}$$

$$\vec{b}_2 = \frac{2\pi}{V_c}\vec{a}_3 \times \vec{a}_1 \tag{403}$$

$$\vec{b}_3 = \frac{2\pi}{V_c}\vec{a}_1 \times \vec{a}_2 \tag{404}$$

a_i real-space lattice vectors, V_c volume of the primitive lattice cell

---

Reciprokal attice vector

Symbol: $\vec{G}$ Unit:

$$\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 \tag{405}$$

$n_i \in \mathbb{Z}$

34.3 Scattering processes

Matthiessen's rule

Approximation, only holds if the processes are independent of each other

$$\frac{1}{\mu} = \sum_{i=\text{Scattering processes}} \frac{1}{\mu_i} \tag{406}$$

$$\frac{1}{\tau} = \sum_{i=\text{Scattering processes}} \frac{1}{\tau_i} \tag{407}$$

μ Electrical mobility, τ Scattering time

34.4 Lattices

Simple cubic (SC)
Reciprocal: Simple cubic

$$\vec{a}_1 = a \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \vec{a}_2 = a \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \vec{a}_3 = a \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{408}$$

a Lattice constant

Body centered cubic (BCC)
Reciprocal: cm:bravais:fcc

$$\vec{a}_1 = \frac{a}{2} \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}, \vec{a}_2 = \frac{a}{2} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \vec{a}_3 = \frac{a}{2} \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} \tag{409}$$

a Lattice constant

Face centered cubic (FCC)
Reciprocal: cm:bravais:bcc

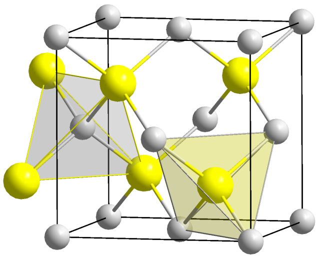
$$\vec{a}_1 = \frac{a}{2} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \vec{a}_2 = \frac{a}{2} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \vec{a}_3 = \frac{a}{2} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \tag{410}$$

a Lattice constant

Diamond lattice

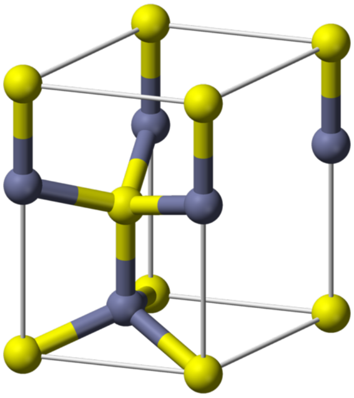
cm:bravais:fcc with basis $\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$ and $\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{pmatrix}$

Zincblende lattice



Like cm:bravais:diamond but with different species on each basis

Wurtzite structure
hP4



Placeholder cm:crystal:lat:wurtzite:desc

35 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)

$$\vec{v}_\text{D} = \vec{v} - \vec{v}_\text{th} \tag{411}$$

v_th thermal velocity

Mean free path

$$\ell = \langle v \rangle \tau \tag{412}$$

Electrical mobility

How quickly a particle moves through a material when moved by an electric field

Symbol: μ Unit: $1\,\mathrm{cm^2/Vs}$

$$\mu = \frac{q\tau}{m} \tag{413}$$

q Charge, m Mass, τ Scattering time

35.1 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

$$\Delta E = \frac{\hbar^2\pi^2}{2m_\mathrm{e}L^2} \tag{414}$$

Energy

$$E_n = \underbrace{\frac{\hbar^2 k_\parallel^2}{2m_\mathrm{e}}}_{x\text{-}y\text{: plain wave}} + \underbrace{\frac{\hbar^2\pi^2}{2m_\mathrm{e}L^2}n^2}_{z} \tag{415}$$

35.2 1D electron gas / quantum wire

Energy

$$E_n = \frac{\hbar^2 k_x^2}{2m_\mathrm{e}} + \frac{\hbar^2\pi^2}{2m_\mathrm{e}L_z^2}n_1^2 + \frac{\hbar^2\pi^2}{2m_\mathrm{e}L_y^2}n_2^2 \tag{416}$$

TODO:conduntance

35.3 0D electron gas / quantum dot

TODO:TODO

36 Charge transport

36.1 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

$$m_\mathrm{e}\frac{\mathrm{d}\vec{v}}{\mathrm{d}t} + \frac{m_\mathrm{e}}{\tau}\vec{v}_\mathrm{D} = -e\vec{\mathcal{E}} \tag{417}$$

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: $1\,\mathrm{A/m^2}$

$$\vec{j} = -ne\vec{v}_\mathrm{D} = ne\mu\vec{\mathcal{E}} \tag{418}$$

n charge particle density

Drude-conductivity

$$\sigma = \frac{\vec{j}}{\vec{\mathcal{E}}} = \frac{e^2\tau n}{m_\mathrm{e}} = ne\mu \tag{419}$$

36.2 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

$$\vec{j} = -en\langle v\rangle = -en\frac{\hbar}{m_\mathrm{e}}\langle\vec{k}\rangle = -e\frac{1}{V}\sum_{\vec{k},\sigma}\frac{\hbar\vec{k}}{m_\mathrm{e}} \tag{420}$$

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

36.3 Boltzmann-transport

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

Boltzmann Transport equation
for charge transport

$$\frac{\partial f(\vec{r},\vec{k},t)}{\partial t} = -\vec{v}\cdot\vec{\nabla}_{\vec{r}}f - \frac{e}{\hbar}(\vec{\mathcal{E}}+\vec{v}\times\vec{B})\cdot\vec{\nabla}_{\vec{k}}f + \left(\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right)_\text{scatter} \tag{421}$$

f ??

36.4 misc

Tsu-Esaki tunneling current
Describes the current $I_{\mathrm{L}\leftrightarrow\mathrm{R}}$ through a barrier

$$I_\mathrm{T} = \frac{2e}{h}\int_{U_\mathrm{L}}^{\infty}\left(f(E,\mu_\mathrm{L}) - f(E,\mu_\mathrm{R})\right)T(E)\,\mathrm{d}E \tag{422}$$

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

$$\frac{\partial\rho}{\partial t} = -\nabla\vec{j} \tag{423}$$

ρ Charge density, $\vec{j}$ Current density

37 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.

37.1 London equations

Quantitative description of the Meißner-Ochsenfeld effect.

First London Equation	$\frac{\partial \vec{j}_\text{s}}{\partial t} = \frac{n_\text{s} q_\text{s}^2}{m_\text{s}} \vec{E} - \mathcal{O}\left(\vec{j}_\text{s}^2\right)$ (424) $\vec{j}$ current density, n_s, m_s, q_s density, mass and charge of superconduticng particles
Second London Equation Describes the Meißner-Ochsenfeld effect	$\vec{\nabla} \times \vec{j}_\text{s} = -\frac{n_\text{s} q_\text{s}^2}{m_\text{s}} \vec{B}$ (425) $\vec{j}$ current density, n_s, m_s, q_s density, mass and charge of superconduticng particles
London penetration depth	$\lambda_\text{L} = \sqrt{\frac{m_\text{s}}{\mu_0 n_\text{s} q_\text{s}^2}}$ (426)

37.2 Ginzburg-Landau Theory (GLAG)

TODO:TODO

Ginzburg-Landau Coherence Length	$\xi_\text{GL} = \frac{\hbar}{\sqrt{2m \lvert\alpha\rvert}}$ (427) $\xi_\text{GL}(T) = \xi_\text{GL}(0) \frac{1}{\sqrt{1 - \frac{T}{T_\text{c}}}}$ (428)
Ginzburg-Landau Penetration Depth / Field screening length	$\lambda_\text{GL} = \sqrt{\frac{m_\text{s} \beta}{\mu_0 \lvert\alpha\rvert q_s^2}}$ (429) $\lambda_\text{GL}(T) = \lambda_\text{GL}(0) \frac{1}{\sqrt{1 - \frac{T}{T_\text{c}}}}$ (430)
First Ginzburg-Landau Equation	$\alpha \Psi + \beta \lvert\Psi\rvert^2 \Psi + \frac{1}{2m} (-i\hbar\vec{\nabla} + 2e\vec{A})^2 \Psi = 0$ (431) ξ_GL Ginzburg-Landau Coherence Length, λ_GL Ginzburg-Landau Penetration Depth / Field screening length
Second Ginzburg-Landau Equation	$\vec{j}_\text{s} = \frac{ie\hbar}{m} (\Psi^* \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^*) - \frac{4e^2}{m} \lvert\Psi\rvert^2 \vec{A}$ (432)

TODO:proximity effect

37.3 Microscopic theory

Isotope effect
Superconducting behaviour depends on atomic mass and thereby of the lattice
⇒Microscopic origin

$$T_\mathrm{c} \propto \frac{1}{\sqrt{M}} \tag{433}$$

$$\omega_\mathrm{ph} \propto \frac{1}{\sqrt{M}} \Rightarrow T_\mathrm{c} \propto \omega_\mathrm{ph} \tag{434}$$

T_c critial temperature, M isotope mass, ω_ph

Cooper pairs

Conduction electrons reduce their energy through an attractive interaction: One electron passing by atoms attracts the these, which creats a positive charge region behind the electron, which in turn attracts another electron.

37.3.1 BCS-Theory

Electron pairs form bosonic quasi-particles called Cooper pairs which can condensate into the ground state. The wave function spans the whole material, which makes it conduct without resistance. The exchange bosons between the electrons are phonons.

BCS Hamiltonian
for N interacting electrons

$$\hat{H}_\mathrm{BCS} = \sum_\sigma \sum_{\vec{k}} \epsilon_{\vec{k}} \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} + \sum_{\vec{k},\vec{k}'} V_{\vec{k},\vec{k}'} \hat{c}^\dagger_{\vec{k}\uparrow} \hat{c}^\dagger_{-\vec{k}\downarrow} \hat{c}_{-\vec{k}'\downarrow} \hat{c}_{\vec{k}',\uparrow} \tag{435}$$

$c_{\vec{k}\sigma}$ creation/annihilation operators create/destroy at $\vec{k}$ with spin σ
First term: non-interacting free electron gas
Second term: interaction energy

Bogoliubov-Valatin transformation
Diagonalization of the BCS Hamiltonian to derive excitation energies

$$\hat{H}_\mathrm{BCS} - N\mu = \sum_{\vec{k}} \left[\xi_{\vec{k}} - E_{\vec{k}} + \Delta_{\vec{k}} g^*_{\vec{k}}\right] + \sum_{\vec{k}} \left[E_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}} + E_{\vec{k}} \beta^\dagger_{-\vec{k}} \beta_{-\vec{k}}\right] \tag{436}$$

BCS-gap equation

$$\Delta^*_{\vec{k}} = -\sum_{\vec{k}}^{+} \prime V_{\vec{k},\vec{k}'} \frac{\Delta_{\vec{k}'}}{2E_{\vec{k}}} \tanh\left(\frac{E_{\vec{k}'}}{2k_\mathrm{B}T}\right) \tag{437}$$

38 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 $\frac{E_\mathrm{c}-E_\mathrm{F}}{k_\mathrm{B}T} > 3.6$ and $\frac{E_\mathrm{F}-E_\mathrm{v}}{k_\mathrm{B}T} > 3.6$

$$n_0 \approx N_\mathrm{c}(T) \exp\left(-\frac{E_\mathrm{c} - E_\mathrm{F}}{k_\mathrm{B}T}\right) \tag{438}$$

$$p_0 \approx N_\mathrm{v}(T) \exp\left(-\frac{E_\mathrm{F} - E_\mathrm{v}}{k_\mathrm{B}T}\right) \tag{439}$$

Intrinsic charge density

$$n_\mathrm{i} \approx \sqrt{n_0 p_0} = \sqrt{N_\mathrm{c}(T) N_\mathrm{v}(T)} \exp\left(-\frac{E_\mathrm{gap}}{2 k_\mathrm{B} T}\right) \tag{440}$$

Mass action law

Charge densities at thermal equilibrium, independent of doping

$$np = n_i^2 \tag{441}$$

Bandgaps of common semiconductors

	$E_\mathrm{gap}(0\,\mathrm{K})[\mathrm{eV}]$	$E_\mathrm{gap}(300\,\mathrm{K})[\mathrm{eV}]$	
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)

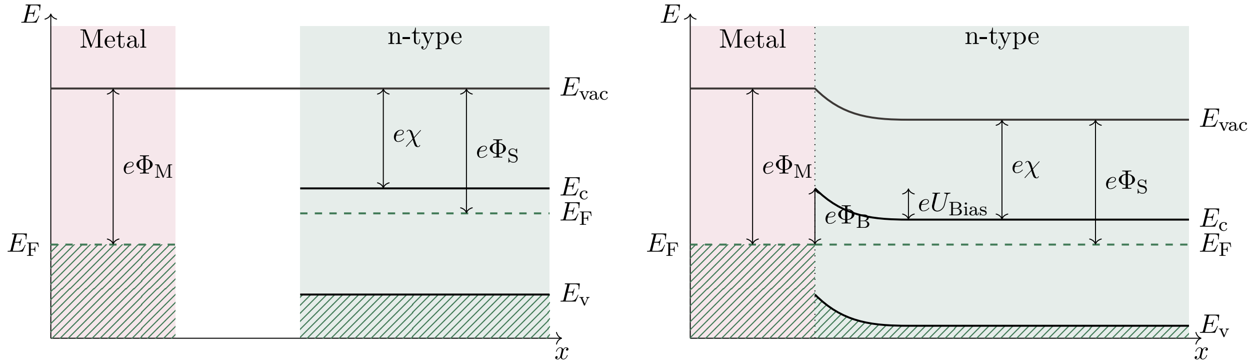
TODO:effective mass approx

38.1 Devices and junctions

Metal-semiconductor junction

☐

Schottky barrier : Rectifying cm:sc:junctions:metal-sc



TODO:Work function electron affinity sind doch Energien und keine Potentiale, warum wird also immer q davor geschrieben?

Schottky-Mott rule

$$\Phi_\mathrm{B} \approx \Phi_\mathrm{M} - \chi_\mathrm{sc} \tag{442}$$

Φ_B barrier potential, Φ_M Metal Work function, χ_sc Electron affinity

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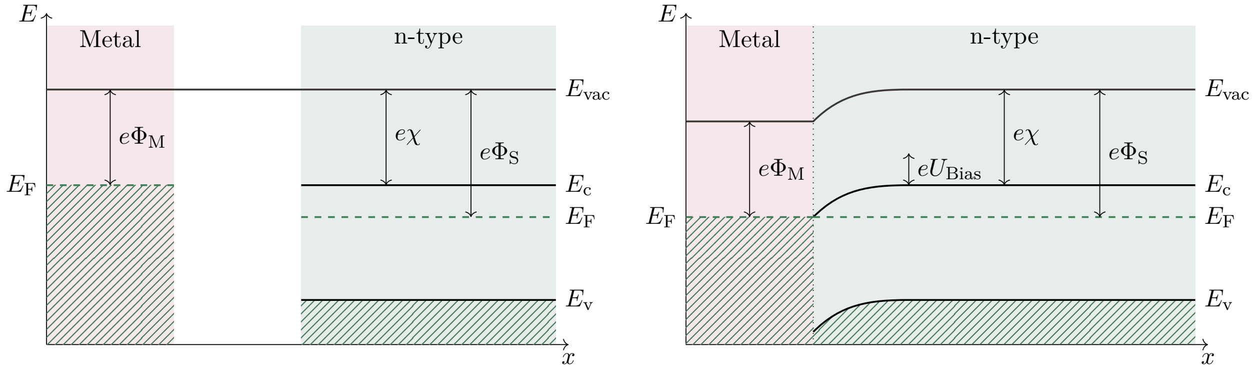
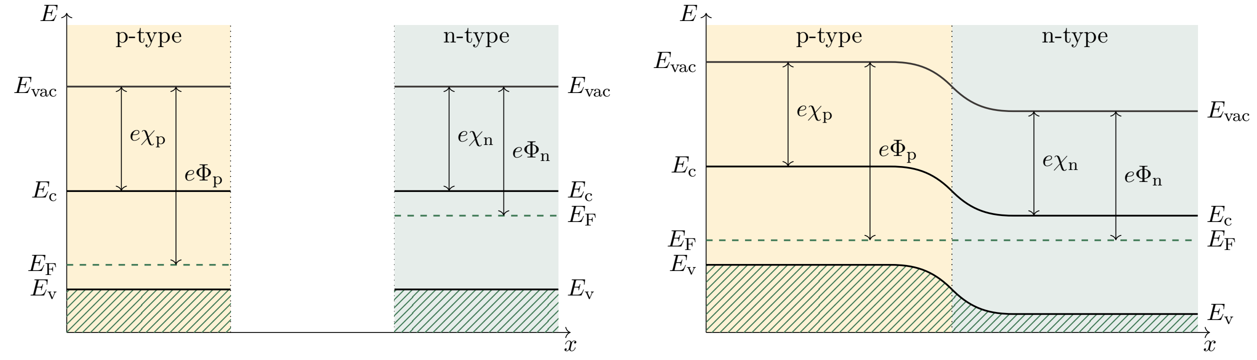
TODO:work function verhältnisse, wann ist es ohmisch wann depleted?

Ohmic contact



p-n junction



38.2 Excitons

Exciton	Quasi particle, excitation in condensed matter as bound electron-hole pair. Free (Wannier) excitons: delocalised over many lattice sites Bound (Frenkel) excitonsi: localised in single unit cell
Exciton Rydberg energy for free Excitons	$E(n) = -\left(\frac{\mu}{m_0 \epsilon_r^2}\right) R_{\mathrm{H}} \frac{1}{n^2}$ (443) R_{H} Rydberg energy
Exciton Bohr radius for free Excitons	$r_n = \left(\frac{m_{\mathrm{e}} \epsilon_r a_{\mathrm{B}}}{mu}\right) n^2$ (444) ??? ???:relative permittivity, a_0 Bohr radius, m_{e} Electron mass, mu reduced mass

39 Band theory

39.1 Hybrid orbitals

Hybrid orbitals are linear combinations of other atomic orbitals.

sp3 Orbital eg CH_4	1s + 3p = sp3  (445)

sp2 Orbital

$$1\mathrm{s} + 2\mathrm{p} = \mathrm{sp2} \tag{446}$$

sp Orbital

$$1\mathrm{s} + 1\mathrm{p} = \mathrm{sp} \tag{447}$$

40 Diffusion

Diffusion coefficient

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

Particle current density
Number of particles through an area

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

Einstein relation
Classical

$$D = \frac{\mu k_\mathrm{B} T}{q} \tag{448}$$

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

Concentration
A quantity per volume

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

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

$$J = -D\frac{c}{x} \tag{449}$$

J Particle current density, D Diffusion coefficient, c Concentration

Fick's second law

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{450}$$

J Particle current density, D Diffusion coefficient, c Concentration

41 misc

Work function
Lowest energy required to remove an electron into the vacuum

Symbol: W Unit: $1\,\mathrm{eV}$

$$W = E_\mathrm{vac} - E_\mathrm{F} \tag{451}$$

Electron affinity
Energy required to remove one electron from an anion with one negative charge.
Energy difference between vacuum level and conduction band

Symbol: χ Unit: $1\,\mathrm{eV}$

$$\chi = (E_\mathrm{vac} - E_\mathrm{c}) \tag{452}$$

Laser Light amplification by stimulated emission of radiation	*Gain medium* is energized *pumping energy* (electric current or light), light of certain wavelength is amplified in the gain medium

42 Measurement techniques

42.1 Raman spectroscopy

Raman spectroscopy

Application	Vibrational modes, Crystal structure, Doping, Band Gaps, Layer thickness in cm:misc:vdw material
how	Monochromatic light (Laser) shines on sample, inelastic scattering because of rotation-, vibration-, phonon and spinflip-processes, plot spectrum as shift of the laser light (in cm^{-1})

Photoluminescence spectroscopy

Application	Crystal structure, Doping, Band Gaps, Layer thickness in cm:misc:vdw material
how	Monochromatic light (Laser) shines on sample, electrons are excited, relax to the conduction band minimum and finally accross the band gap under photon emission

42.2 ARPES

what? in? how? plot

42.3 Scanning probe microscopy SPM

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

Atomic force microscopy (AMF)

Application	Surface stuff
how	With needle

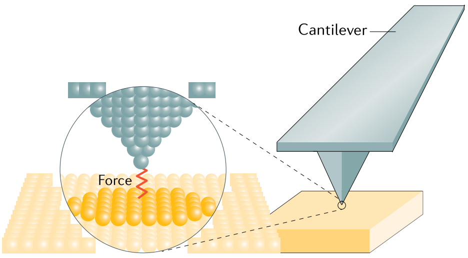


Figure 1: [?]

Scanning tunneling microscopy (STM)

Application	Surface stuff
how	With TUnnel

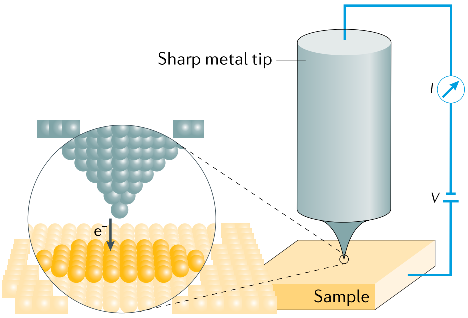


Figure 2: [?]

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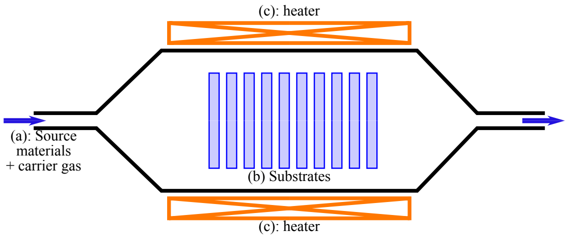
43 Fabrication techniques

Chemical vapor deposition (CVD)

how	A substrate is exposed to volatile precursors, which react and/or decompose on the heated substrate surface to produce the desired deposit. By-products are removed by gas flow through the chamber.
Application	• Polysilicon Si • Silicon dioxide SiO_2 • Graphene • Diamond

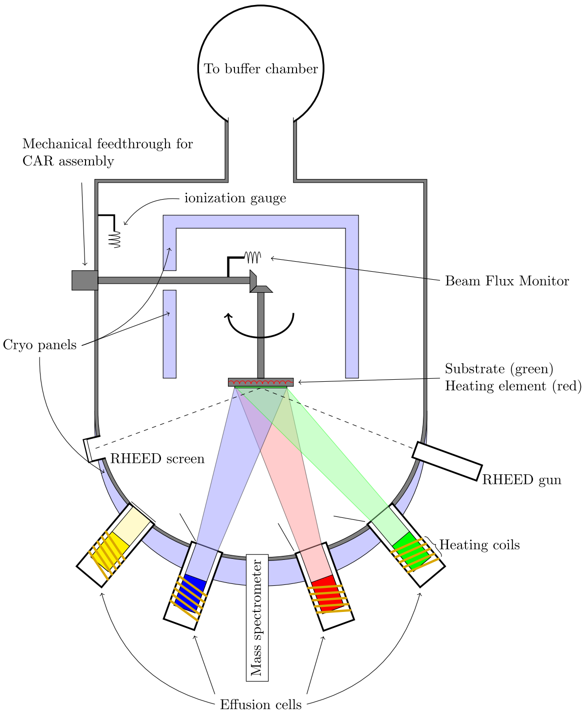


43.1 Epitaxy

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

Molecular Beam Epitaxy (MBE)

how	In a ultra-high vacuum, the elements are heated until they slowly sublime. The gases then condensate on the substrate surface
Application	• Gallium arsenide GaAs TODO:Link to GaAs



44 Topological Materials

44.1 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

$$H(\vec{R}(t))\,|n(\vec{R}(t))\rangle = \epsilon(\vec{R}(t))\,|n(\vec{R}(t))\rangle \tag{453}$$

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

$$|\psi_n(t)\rangle = \underbrace{\mathrm{e}^{i\gamma_n(t)}}_{\text{Berry Phase}}\ \underbrace{\mathrm{e}^{\frac{-i}{\hbar}\int^{r}\epsilon_n(\vec{R}(t'))\,\mathrm{d}t}}_{\text{Dynamical Phase}}|n(\vec{R}(t))\rangle \tag{454}$$

Berry connection

$$A_n(\vec{R}) = i\,\langle\psi|\nabla_R|\psi\rangle \tag{455}$$

Berry curvature
Gauge invariant

$$\vec{\Omega}_n = \vec{\nabla}_R \times A_n(\vec{R}) \tag{456}$$

Berry phase
Gauge invariant up to 2π

$$\gamma_n = \oint_C \mathrm{d}\vec{R}\cdot A_n(\vec{R}) = \int_S \mathrm{d}\vec{S}\cdot\vec{\Omega}_n(\vec{R}) \tag{457}$$

Chern number
Eg. number of Berry curvature monopoles in the Brillouin zone (then $\vec{R} = \vec{k}$)

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.

$$C_n = \frac{1}{2\pi}\oint \mathrm{d}\vec{S}\ \cdot\vec{\Omega}_n(\vec{R}) \tag{458}$$

$\vec{S}$ 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

$$\vec{\sigma}_{xy} = \sum_n \frac{e^2}{h} \int_\text{occupied} \mathrm{d}^2 k \, \frac{\Omega_{xy}^n}{2\pi} = \sum_n C_n \frac{e^2}{h} \tag{459}$$

Topological insulator

A 2D insulator with a non-zero Chern number is called a **topological insulator**.

45 Material physics

Tortuosity

Degree of the winding of a transport path through a porous material.

Multiple definitions exist

Symbol: τ Unit:

$$\tau = \left(\frac{l}{L}\right)^2 \tag{460}$$

$$\tau = \frac{l}{L} \tag{461}$$

l path length, L distance of the end points

Stress

Force per area

Symbol: σ Unit: $1\,\mathrm{N/m^2}$

$$[\sigma]_{ij} = \frac{F_i}{A_j} \tag{462}$$

$\vec{F}$ Force, A Area

Strain

Symbol: ϵ Unit:

$$\epsilon = \frac{\Delta x}{x_0} \tag{463}$$

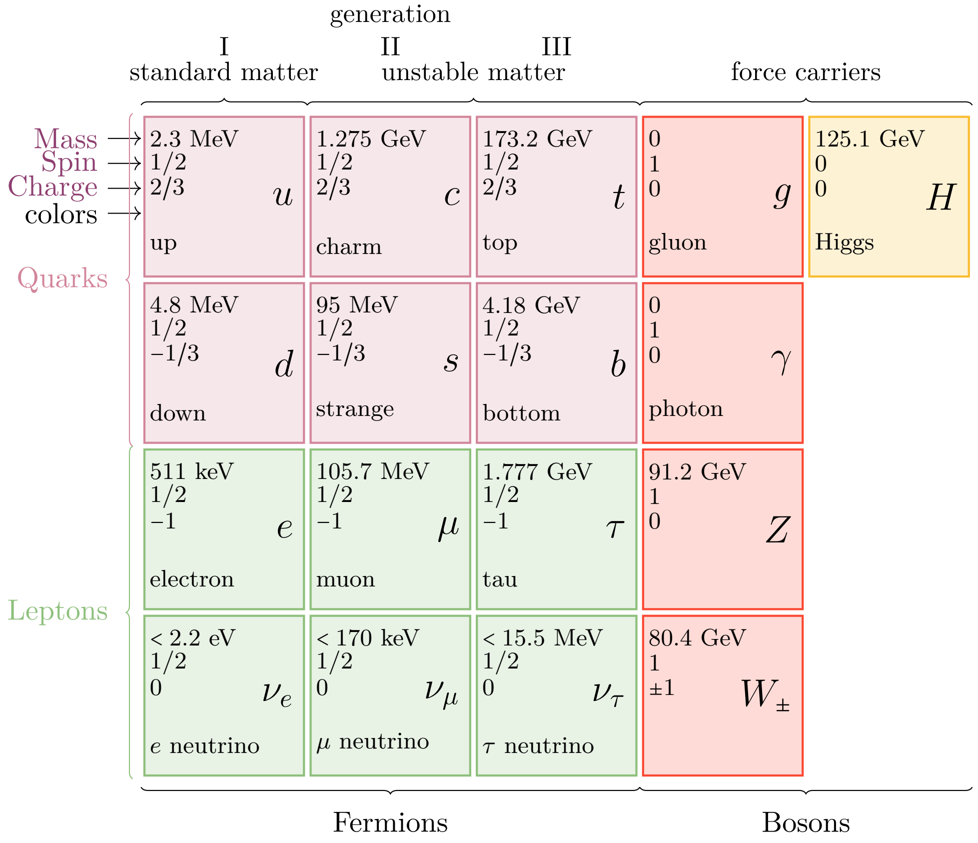
Δx distance from reference position x_0

Part VIII

Particle physics

Electron mass	Symbol: m_e Experimental value $9.1093837139(28) \cdot 10^{-31}$ kg
Spin	Symbol: σ Unit:

Standard model



	I	II	III		
Quarks	2.3 MeV 1/2 2/3 u up	1.275 GeV 1/2 2/3 c charm	173.2 GeV 1/2 2/3 t top	0 1 0 g gluon	125.1 GeV 0 0 H Higgs
	4.8 MeV 1/2 $-1/3$ d down	95 MeV 1/2 $-1/3$ s strange	4.18 GeV 1/2 $-1/3$ b bottom	0 1 0 γ photon	
Leptons	511 keV 1/2 -1 e electron	105.7 MeV 1/2 -1 μ muon	1.777 GeV 1/2 -1 τ tau	91.2 GeV 1 0 Z	
	< 2.2 eV 1/2 0 ν_e e neutrino	< 170 keV 1/2 0 ν_μ μ neutrino	< 15.5 MeV 1/2 0 ν_τ τ neutrino	80.4 GeV 1 ± 1 $W_\pm$	

Part IX

Quantum Computing

46 Qubits

Bloch sphere

$$
\begin{aligned}
|\psi\rangle &= \alpha\,|0\rangle + \beta\,|1\rangle && (464)\\
&= \cos\frac{\theta}{2}\,\mathrm{e}^{i\phi_\alpha}\,|0\rangle + \sin\frac{\theta}{2}\,\mathrm{e}^{i\phi_\beta}\,|1\rangle && (465)\\
&= \mathrm{e}^{i\phi_\alpha}\cos\frac{\theta}{2}\,|0\rangle + \sin\frac{\theta}{2}\,\mathrm{e}^{i\phi}\,|1\rangle && (466)
\end{aligned}
$$

---

47 Gates

Gates

$$\text{Bitflip:} \quad \hat{X} = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{467}$$

$$\text{Bit-Phase flip:} \quad \hat{Y} = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{468}$$

$$\text{Phaseflip:} \quad \hat{Z} = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{469}$$

$$\text{Hadamard:} \quad \hat{H} = \frac{1}{\sqrt{2}}(\hat{X} - \hat{Z}) = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{470}$$

---

48 Superconducting qubits

48.1 Building blocks

48.1.1 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

$$\hat{H}_\mathrm{J} = -\frac{E_\mathrm{J}}{2}\sum_n \left[|n\rangle\langle n+1| + |n+1\rangle\langle n|\right] \tag{471}$$

---

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

$$\hat{I}\,|\delta\rangle = I_\mathrm{C}\sin\delta\,|\delta\rangle \tag{472}$$

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

---

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

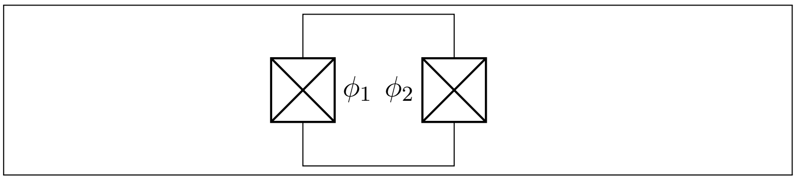
$$\frac{\mathrm{d}\hat{\delta}}{\mathrm{d}t} = \frac{1}{i\hbar}[\hat{H},\hat{\delta}] = -\frac{2eU}{i\hbar}[\hat{n},\hat{\delta}] = \frac{1}{\varphi_0}U \tag{473}$$

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

48.1.2 SQUID

SQUID

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

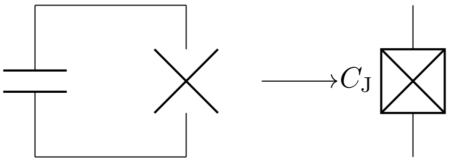


Hamiltonian

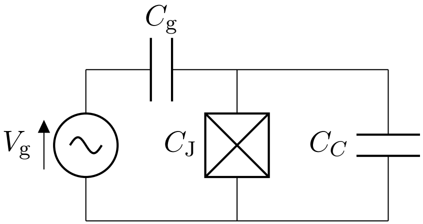
$$\hat{H} = -E_{\mathrm{J}1} \cos \hat{\phi}_1 - E_{\mathrm{J}2} \cos \hat{\phi}_2 \tag{474}$$

$\hat{\phi}$ phase difference across the junction

48.2 Josephson Qubit??



TODO:Include schaltplan



Charging energy / electrostatic energy

$$E_{\mathrm{C}} = \frac{(2e)^2}{C} \tag{475}$$

Josephson energy

$$E_{\mathrm{J}} = \frac{I_0 \phi_0}{2\pi} \tag{476}$$

TODO:Was ist I0

Inductive energy

$$E_{\mathrm{L}} = \frac{\varphi_0^2}{L} \tag{477}$$

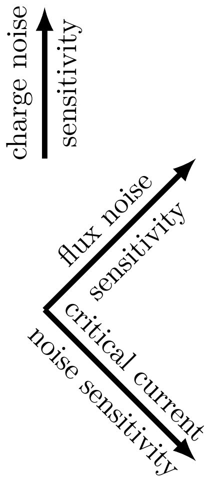
Gate charge or offset charge

$$n_{\mathrm{g}} = \frac{C_g V_{\mathrm{g}}}{2e} \tag{478}$$

Anharmonicity

$$\alpha := \omega_{1\leftrightarrow 2} - \omega_{0\leftrightarrow 1} \tag{479}$$

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

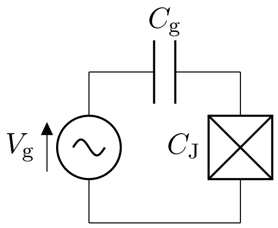


48.3 Cooper Pair Box (CPB) qubit

= voltage bias junction
= charge qubit?

Cooper Pair Box / Charge qubit

- large anharmonicity
- sensitive to charge noise



Hamiltonian

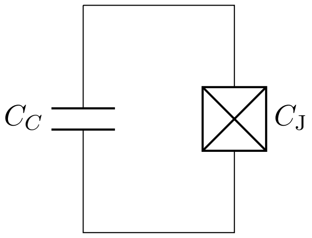
$$\hat{H} = 4E_C(\hat{n} - n_g)^2 - E_J \cos\hat{\phi} \tag{480}$$

$$= \sum_n \left[4E_C(n - n_g)^2 |n\rangle\langle n| - \frac{E_J}{2} |n\rangle\langle n+1| + |n+1\rangle\langle n| \right] \tag{481}$$

48.4 Transmon qubit

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

- charge noise insensitive
- small anharmonicity

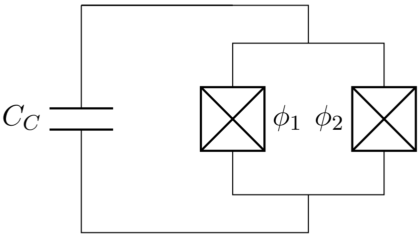


Hamiltonian

$$\hat{H} = 4E_C\hat{n}^2 - E_J \cos\hat{\phi} \tag{482}$$

48.4.1 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

$$E_{\text{J,eff}}(\Phi_{\text{ext}}) = (E_{\text{J1}} + E_{\text{J2}})\sqrt{\cos^2\left(\pi\frac{\Phi_{\text{ext}}}{\Phi_0}\right) + d^2\sin\left(\pi\frac{\Phi_{\text{ext}}}{\Phi_0}\right)} \tag{483}$$

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

Hamiltonian

$$\hat{H} = 4E_C\hat{n}^2 - \frac{1}{2}E_{\text{J,eff}}(\Phi_{\text{ext}})\sum_n\left[|n\rangle\langle n+1| + |n+1\rangle\langle n|\right] \tag{484}$$

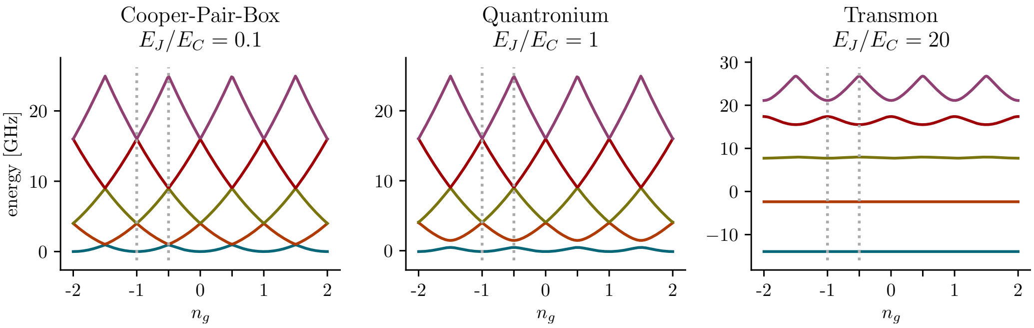
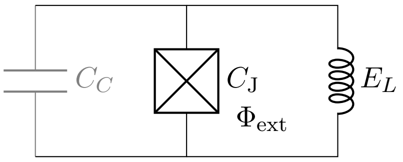


Figure 3: Transmon and so TODO

48.5 Phase qubit

Phase qubit



TODO:Ist beim Fluxonium noch die Voltage source dran?

Hamiltonian

$$\hat{H} = E_C\hat{n}^2 - E_J\cos\hat{\delta} + E_L(\hat{\delta} - \delta_s)^2 \tag{485}$$

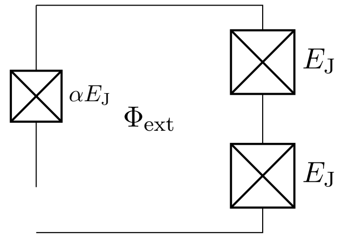
$\delta = \frac{\phi}{\phi_0}$

This is only a test

48.6 Flux qubit

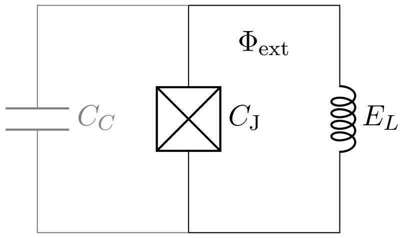
TODO:TODO

Flux qubit / Persistent current qubit



48.7 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

$$\hat{H} = 4E_C\hat{n}^2 - E_J\cos\hat{\delta} + E_L(\hat{\delta} - \delta_s)^2 \tag{486}$$

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

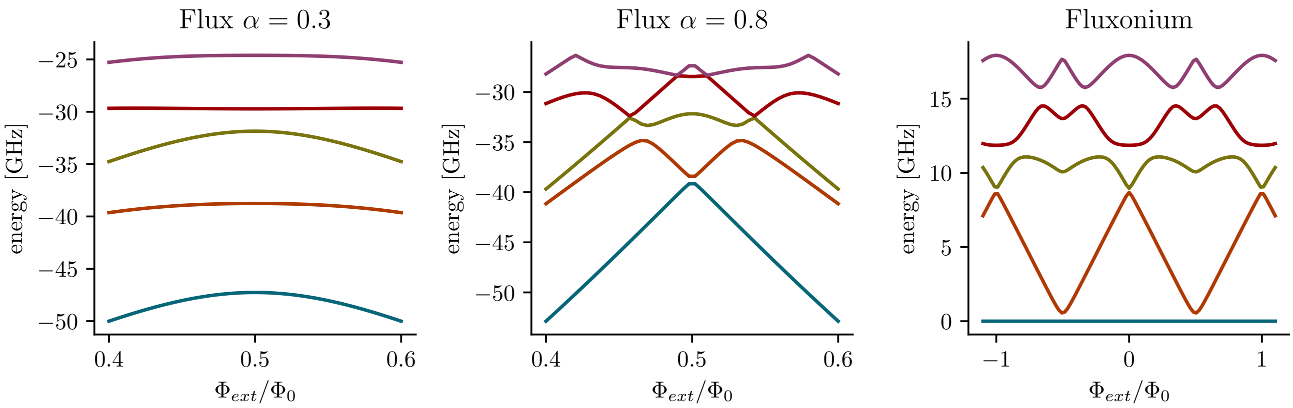


Figure 4: img/

49 Two-level system

Resonance frequency

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} \tag{487}$$

TODO:sollte das nicht 10 sein?

Rabi oscillations

$$\Omega_{\text{TODO:TODO}} \tag{488}$$

ω_{21} resonance frequency of the energy transition, Ω Rabi frequency

49.1 Ramsey interferometry

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

50 Noise and decoherence

Longitudinal relaxation rate
$\Gamma_{1\downarrow}$: $|1\rangle \rightarrow |0\rangle$
$\Gamma_{1\uparrow}$: $|0\rangle \rightarrow |1\rangle$

$$\boxed{\Gamma_1 = \frac{1}{T_1} = \Gamma_{1\uparrow} + \Gamma_{1\downarrow}} \tag{489}$$

$\Gamma_{1\uparrow}$ is supressed at low temperatures because of detailed balance

Pure dephasing rate

$$\boxed{\Gamma_\phi} \tag{490}$$

Transversal relaxation rate

$$\boxed{\Gamma_2 = \frac{1}{T_2} = \frac{\Gamma_1}{2} + \Gamma_\phi} \tag{491}$$

Bloch-Redfield density matrix

2-level System weakly coupled to noise sources with short correlation time

$$\boxed{\rho_{\text{BR}} = \begin{pmatrix} 1 + (|\alpha|^2 - 1)\,\mathrm{e}^{-\Gamma_1 t} & \alpha\beta^*\,\mathrm{e}^{-\Gamma_2 t} \\ \alpha^*\beta\,\mathrm{e}^{-\Gamma_2 t} & |\beta|^2\,\mathrm{e}^{-\Gamma_1 t} \end{pmatrix}} \tag{492}$$

Part X

Computational Physics

51 Quantum many-body physics

51.1 Quantum many-body models

Homogeneous electron gas (HEG) Also "Jellium"	Both positive (nucleus) and negative (electron) charges are distributed uniformly.

51.2 Methods

51.2.1 Quantum Monte-Carlo

TODO:TODO

51.3 Importance sampling

TODO:Monte Carlo

51.4 Matrix product states

52 Electronic structure theory

Kinetic energy of species i	$\hat{T}_i = -\sum_{n=1}^{N_i} \frac{\hbar^2}{2m_i}\vec{\nabla}_n^2$ (493) i = nucleons/electrons, N number of particles, m Mass
Electrostatic potential between species i and j	$\hat{V}_{i\leftrightarrow j} = -\sum_{k,l}\frac{Z_i Z_j e^2}{\lvert\vec{r}_k - \vec{r}_l\rvert}$ (494) i, j = nucleons/electrons, r particle position, Z_i charge of species i, e Unit charge
Electronic structure Hamiltonian	$\hat{H} = \hat{T}_\text{e} + \hat{T}_\text{n} + V_{\text{e}\leftrightarrow\text{e}} + V_{\text{n}\leftrightarrow\text{e}} + V_{\text{n}\leftrightarrow\text{n}}$ (495) $\hat{T}$ Kinetic energy, $\hat{V}$ Electrostatic potential, e electrons, n nucleons
Mean field approximation Replaces 2-particle operator by 1-particle operator	$\frac{1}{2}\sum_{i\neq j}\frac{e^2}{\lvert\vec{r}_i - \vec{r}_j\rvert} \approx \sum_i V_\text{eff}(\vec{r}_i)$ (496) Example for Coulomb interaction between many electrons

52.1 Tight-binding

Assumptions	- Atomic wave functions are localized ⇒Small overlap, interaction cutoff

Tight-binding Hamiltonian in second quantized form	$\hat{H} = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i - \sum_{i,j} t_{i,j} \left(\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i \right) \quad (497)$ $\hat{a}_i^\dagger$, $\hat{a}_i$ Creation / Annihilation operators create/destory an electron on site i, ϵ_i on-site energy, $t_{i,j}$ hopping amplitude, usually ϵ and t are determined from experiments or other methods

52.2 Density functional theory (DFT)

52.2.1 Hartree-Fock

Description	• Assumes wave functions are Slater determinant ⇒Approximation • Mean field approximation theory obeying the Pauli principle • Self-interaction free: Self interaction is cancelled out by the Fock-term
Hartree-Fock equation	$\left(\hat{T} + \hat{V}_\text{en} + \hat{V}_\text{HF}^\xi \right) \varphi_\xi(x) = \epsilon_\xi \varphi_\xi(x) \quad (498)$ 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, $x = \vec{r}, \sigma$ position and spin
Hartree-Fock potential	$V_\text{HF}^\xi(\vec{r}) = \sum_\vartheta \int \text{d}x' \frac{e^2}{\lvert \vec{r} - \vec{r}' \rvert} \left(\underbrace{\lvert \varphi_\xi(x') \rvert^2}_\text{Hartree-Term} - \underbrace{\frac{\varphi_\vartheta^*(x') \varphi_\xi(x') \varphi_\vartheta(x)}{\varphi_\xi(x)}}_\text{Fock-Term} \right) \quad (499)$
Self-consistent field cycle	1. Initial guess for φ 2. Solve SG for each particle 3. Make new guess for φ

52.2.2 Hohenberg-Kohn Theorems

Hohenberg-Kohn theorem (HK1)	For any system of interacting electrons, the ground state electron density $n(\vec{r})$ determines $\hat{V}_\text{ext}$ uniquely up to a trivial constant.
Hohenberg-Kohn theorem (HK2)	Given the energy functional $E[n(\vec{r})]$, the ground state density and energy can be obtained variationally. The density that minimizes the total energy is the exact ground state density.
Ground state electron density	$n(\vec{r}) = \left\langle \psi_0 \middle\vert \sum_{i=1}^N \delta(\vec{r} - \vec{r}_i) \middle\vert \psi_0 \right\rangle \quad (500)$

52.2.3 Kohn-Sham DFT

Kohn-Sham map	Maps fully interacting system of electrons to a system of non-interacting electrons with the same ground state density $n'(\vec{r}) = n(\vec{r})$ $$n(\vec{r}) = \sum_{i=1}^{N} \lvert \phi_i(\vec{r}) \rvert^2 \tag{501}$$
Kohn-Sham functional	$$E_\text{KS}[n(\vec{r})] = T_\text{KS}[n(\vec{r})] + V_\text{ext}[n(\vec{r})] + E_\text{H}[n(\vec{r})] + E_\text{XC}[n(\vec{r})] \tag{502}$$ T_KS kinetic enery, V_ext external potential, E_H Hartree term, E_XC Exchange-Correlation functional
Kohn-Sham equation Exact single particle SE (though often exact E_XC is not known) Solving it uses up a large portion of supercomputer resources	$$\left\{ -\frac{\hbar^2 \nabla^2}{2m} + v_\text{ext}(\vec{r}) + e^2 \int \mathrm{d}^3\vec{r}\,' \frac{n(\vec{r}\,')}{\lvert \vec{r} - \vec{r}\,' \rvert} + \frac{\partial E_\text{X}[n(\vec{r})]}{\partial n(\vec{r})} + \frac{\partial E_\text{C}[n(\vec{r})]}{\partial n(\vec{r})} \right\} \phi_i^\text{KS}(\vec{r}) = \epsilon_i^\text{KS} \phi_i^\text{KS}(\vec{r}) \tag{503}$$ ϕ_i^KS KS orbitals, $\int \mathrm{d}^3 r v_\text{ext}(\vec{r}) n(\vec{r}) = V_\text{ext}[n(\vec{r})]$
Self-consistent field cycle for Kohn-Sham	1. Initial guess for $n(\vec{r})$ 2. Calculate effective potential V_eff 3. Solve Kohn-Sham equation 4. Calculate density $n(\vec{r})$ 5. Repeat 2-4 until self consistent

52.2.4 Exchange-Correlation functionals

Exchange-Correlation functional	$$E_\text{XC}[n(\vec{r})] = \langle \hat{T} \rangle - T_\text{KS}[n(\vec{r})] + \langle \hat{V}_\text{int} \rangle - E_\text{H}[n(\vec{r})] \tag{504}$$ Accounts for: - Kinetic energy difference between interaction and non-interacting system - Exchange energy due to Pauli principle - Correlation energy due to many-body Coulomb interaction (not accounted for in mean field Hartree term E_H)
Local density approximation (LDA) Simplest DFT functionals	$$E_\text{XC}^\text{LDA}[n(\vec{r})] = \int \mathrm{d}^3 r\, n(r) \Big[\epsilon_\text{X}[n(\vec{r})] + \epsilon_\text{C}[n(\vec{r})] \Big] \tag{505}$$ ϵ_X calculated exchange energy from HEG model, ϵ_C correlation energy calculated with Quantum Monte-Carlo

Generalized gradient approximation (GGA)

$$E_{\mathrm{XC}}^{\mathrm{GGA}}[n(\vec{r})] = \int \mathrm{d}^3r\, n(r)\epsilon_{\mathrm{X}}[n(\vec{r})]\, F_{\mathrm{XC}}[n(\vec{r}), \vec{\nabla}n(\vec{r})] \tag{506}$$

ϵ_{X} calculated exchange energy from HEG model, F_{XC} function containing exchange-correlation energy dependency on n and $\vec{\nabla}n$

TODO:PBE

Hybrid functionals

$$\alpha E_{\mathrm{X}}^{\mathrm{HF}} + (1-\alpha)E_{\mathrm{X}}^{\mathrm{GGA}} + E_{\mathrm{C}}^{\mathrm{GGA}} \tag{507}$$

Include Fock term (exact exchange) in other functional, like GGA . Computationally expensive

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Range separated hyrid functionals (RSH)
Here HSE as example

$$\frac{1}{r} = \frac{\mathrm{erf}(\omega r)}{r} + \frac{\mathrm{erfc}\,\omega r}{r} \tag{508}$$

$$E_{\mathrm{XC}}^{\mathrm{HSE}} = \alpha E_{\mathrm{X,SR}}^{\mathrm{HF}}(\omega) + (1-\alpha)E_{\mathrm{X,SR}}^{\mathrm{GGA}}(\omega) + E_{\mathrm{X,LR}}^{\mathrm{GGA}}(\omega) + E_{\mathrm{C}}^{\mathrm{GGA}} \tag{509}$$

Use GGA and Fock exchange for short ranges (SR) and only GGA??? for long ranges (LR). GGA??? correlation is always used. Useful when dielectric screening reduces long range interactions, saves computational cost.

α mixing paramter, E_{X} exchange energy, E_{C} correlation energy

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Comparison of DFT functionals

TODO:HFtotal energy: upper boundary for GS density n

52.2.5 Basis sets

Plane wave basis
Plane wave ansatz in Kohn-Sham equation
Good for periodic structures, allows computation parallelization over a sample points in the brillouin zone???

$$\sum_{\vec{G}'}\left[\frac{\hbar^2\left|\vec{G}+\vec{k}\right|^2}{2m}\delta_{\vec{G},\vec{G}'} + V_{\mathrm{eff}}(\vec{G}-\vec{G}')\right]c_{i,\vec{k},\vec{G}'} = \epsilon_{i,\vec{k}}c_{i,\vec{k},\vec{G}} \tag{510}$$

Plane wave cutoff
Number of plane waves included in the calculation must be finite

$$E_{\mathrm{cutoff}} = \frac{\hbar^2\left|\vec{k}+\vec{G}\right|^2}{2m} \tag{511}$$

52.2.6 Pseudo-Potential method

Ansatz

Core electrons are absorbed into the potential since they do not contribute much to interesting properties.

53 Atomic dynamics

Electron Hamiltonian

$$\hat{H}_\text{e} = \hat{T}_\text{e} + V_{\text{e}\leftrightarrow\text{e}} + V_{\text{n}\leftrightarrow\text{e}} \tag{512}$$

$\hat{T}$ Kinetic energy, $\hat{V}$ Electrostatic potential, e electrons, n nucleons

---

Wave function ansatz

$$\psi_\text{en}^n\big(\{\vec{r},\sigma\},\{\vec{R}\}\big) = \sum_i c^{ni}\big(\{\vec{R}\}\big)\,\psi_\text{e}^i\big(\{\vec{r},\sigma\},\{\vec{R}\}\big) \tag{513}$$

ψ_en^n eigenstate n of Electronic structure Hamiltonian, ψ_e^i eigenstate i of comp:ad:bo:hamiltonian, $\vec{r}, \vec{R}$ electron/nucleus positions, σ electron spin, c^{ni} coefficients

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Equation

$$\Big[E_\text{e}^j\big(\{\vec{R}\}\big) + \hat{T}_\text{n} + V_{\text{n}\leftrightarrow\text{n}} - E^n\Big]\,c^{nj} = -\sum_i \Lambda_{ij} c^{ni}\big(\{\vec{R}\}\big) \tag{514}$$

Exact nonadiabtic coupling operator
Electron-phonon couplings / electron-vibrational couplings

$$\Lambda_{ij} = \int \mathrm{d}^3r\,(\psi_\text{e}^j)^*\left(-\sum_I \frac{\hbar^2\nabla^2_{\vec{R}_I}}{2M_I}\right)\psi_\text{e}^i + \sum_I \frac{1}{M_I}\int \mathrm{d}^3r\left[(\psi_\text{e}^j)^*(-i\hbar\nabla_{\vec{R}_I})\psi_\text{e}^i\right](-i\hbar\nabla_{\vec{R}_I}) \tag{515}$$

ψ_e^i electronic states, $\vec{R}$ nucleus position, M nucleus Mass

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53.1 Born-Oppenheimer Approximation

Adiabatic approximation
Electronic configuration remains the same when atoms move (Adiabatic theorem)

$$\Lambda_{ij} = 0 \quad \text{for } i \neq j \tag{516}$$

Λ_{ij} Exact nonadiabtic coupling operator

Born-Oppenheimer approximation
Electrons are not influenced by the movement of the atoms

$$\Lambda_{ij} = 0 \tag{517}$$

comp:ad:bo:equation $\Rightarrow$

$$\Big[E_e^i\big(\{\vec{R}\}\big) + \hat{T}_\text{n} - E^n\Big]\,c^{ni}\big(\{\vec{R}\}\big) = 0 \tag{518}$$

see Equation, $V_{\text{n}\leftrightarrow\text{n}} = \text{const}$ absorbed into E_e^j

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Born-Oppenheimer surface
Potential energy surface (PES)
The nuclei follow Newtons equations of motion on the BO surface if the system is in the electronic ground state

$$V_\text{BO}\big(\{\vec{R}\}\big) = E_\text{e}^0\big(\{\vec{R}\}\big) \tag{519}$$

$$M_I\ddot{\vec{R}}_I(t) = -\vec{\nabla}_{\vec{R}_I} V_\text{BO}\big(\{\vec{R}(t)\}\big) \tag{520}$$

$E_\text{e}^0, \psi_\text{e}^0$ lowest eigenvalue/eigenstate of comp:ad:bo:hamiltonian

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Ansatz for Born-Oppenheimer approximation
Product of single electronic and single nuclear state

$$\psi_\text{BO} = c^{n0}\big(\{\vec{R}\}\big)\,\psi_\text{e}^0\big(\{\vec{r},\sigma\},\{\vec{R}\}\big) \tag{521}$$

Limitations

- Nuclei velocities must be small and electron energy state differences large
- Nuclei need spin for effects like spin-orbit coupling
- Nonadiabitc effects in photochemistry, proteins

Valid when Massey parameter $\xi \gg 1$

$$\xi = \frac{\tau_{\text{n}}}{\tau_{\text{e}}} = \frac{L \Delta E}{\hbar \left|\dot{\vec{R}}\right|} \tag{522}$$

τ passage of time for electrons/nuclei, L characteristic length scale of atomic dynamics, $\dot{\vec{R}}$ nuclear velocity, ΔE difference between two electronic states

53.2 Structure optimization

Forces

$$\vec{F}_I = -\vec{\nabla}_{\vec{R}_I} E \overset{\text{Hellmann-Feynman-Theorem}}{\overset{\downarrow}{=}} -\left\langle \psi(\vec{R}_I) \middle| \left(\vec{\nabla}_{\vec{R}_I} \hat{H}(\vec{R}_I)\right) \middle| \psi(\vec{R}) \right\rangle \tag{523}$$

Ionic cycle
Self-consistent field cycle for Kohn-Sham for geometry optimization

1. Initial guess for $n(\vec{r})$
   (a) Calculate effective potential V_{eff}
   (b) Solve Kohn-Sham equation
   (c) Calculate density $n(\vec{r})$
   (d) Repeat b-d until self consistent
2. Calculate Forces
3. If $F \neq 0$, get new geometry by interpolating R and restart

Transformation of atomic positions under stress

$$R_\alpha([\epsilon]_{\alpha\beta}) = \sum_\beta \left(\delta_{\alpha\beta} + [\epsilon]_{\alpha\beta}\right) R_\beta(0) \tag{524}$$

$\alpha, \beta = 1, 2, 3$ position components, R position, $R(0)$ zero-strain position, $[\epsilon]$ Strain tensor

Stress tensor

$$[\sigma]_{\alpha,\beta} = \frac{1}{\Omega} \left(\frac{\partial E_{\text{total}}}{\partial [\epsilon]_{\alpha\beta}}\right)_{[\epsilon]=0} \tag{525}$$

Ω unit cell volume, $[\epsilon]$ Strain tensor

Pulay stress

$$N_{\text{PW}} \propto E_{\text{cut}}^{\frac{3}{2}} \propto \left|\vec{G}_{\text{max}}\right|^3 \tag{526}$$

Number of plane waves N_{PW} depends on E_{cut}. If G changes during optimization, N_{PW} may change, thus the basis set can change. This typically leads to too small volumes.

53.3 Lattice vibrations

Force constant matrix

$$\Phi_{IJ}^{\mu\nu} = \left(\frac{\partial^2 V(\{\vec{R}\})}{\partial R_I^\mu \, \partial R_J^\nu}\right)_{\{\vec{R}_I\}=\{\vec{R}_I^0\}} \tag{527}$$

Harmonic approximation

Hessian matrix, 2nd order Taylor expansion of the Born-Oppenheimer surface around every nucleus position $\vec{R}_I^0$

$$V^{\text{BO}}(\{\vec{R}_I\}) \approx V^{\text{BO}}(\{\vec{R}_I^0\}) + \frac{1}{2}\sum_{I,J}^{N}\sum_{\mu,\nu}^{3} s_I^\mu s_J^\nu \Phi_{IJ}^{\mu\nu} \tag{528}$$

$\Phi_{IJ}^{\mu\nu}$ Force constant matrix, s displacement

53.3.1 Finite difference method

Approximation

Assume forces in equilibrium structure vanish

$$\Phi_{IJ}^{\mu\nu} \approx \frac{\vec{F}_I^\mu(\vec{R}_1^0, \dots, \vec{R}_J^0 + \Delta s_J^\nu, \dots, \vec{R}_N^0)}{\Delta s_J^\nu} \tag{529}$$

Δs displacement of atom J

Dynamical matrix

Mass reduced fourier transform of the Force constant matrix

$$D_{\alpha\beta}^{\mu\nu} = \frac{1}{\sqrt{M_\alpha M_\beta}} \sum_{n'} \Phi_{\alpha\beta}^{\mu\nu}(n - n')\, \text{e}^{i\vec{q}(\vec{L}_n - \vec{L}_{n'})} \tag{530}$$

$\vec{L}$ vector from origin to unit cell n, α/β atom index in th unit cell, $\vec{q}$???:wave vector, Φ Force constant matrix, M Mass

Eigenvalue equation

For a periodic crystal, reduces number of equations from $3N_p \times N$ to $3N_p$. Eigenvalues represent phonon band structure.

$$\omega^2 \vec{c}(\vec{q}) = \underline{D}(\vec{q}) \vec{c}(\vec{q}) \tag{531}$$

N_p number of atoms per unit cell, $\vec{c}$ displacement amplitudes, $\vec{q}$???:wave vector, $\underline{D}$ Dynamical matrix

53.3.2 Anharmonic approaches

Quasi-harmonic approximation

Include thermal expansion by assuming Born-Oppenheimer surface is volume dependant.

Pertubative approaches

Expand Force constant matrix to third order.

53.4 Molecular Dynamics

Description

- Exact (within previous approximations) approach to treat anharmonic effects in materials.
- Computes time-dependant observables.
- Assumes fully classical nuclei.
- Macroscropical observables from statistical ensembles
- System evolves in time (ehrenfest). Number of points to consider does NOT scale with system size.
- Exact because time dependance is studied explicitly, not via harmonic approx.

TODO:cleanup

MD simulation procedure

1. Initialize with optimized geometry, interaction potential, ensemble, integration scheme, temperature/pressure control
2. Equilibrate to desired temperature/pressure (eg with statistical starting velocities)
3. Production run, run MD long enough to calculate desired observables

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53.4.1 Ab-initio molecular dynamics

Born-Oppenheimer MD (BOMD)

1. Calculate electronic ground state of current nucleui configuration $\{\vec{R}(t)\}$ with KS-DFT
2. Calculate forces from the Born-Oppenheimer surface
3. Update positions and velocities

- ”ab-inito” - no empirical information required
- Many expensive DFT calculations

Car-Parrinello MD (CPMD)

Evolve electronic wave function φ (adiabatically) along with the nuclei ⇒only one full KS-DFT

$$M_I \frac{\mathrm{d}^2 \vec{R}_I}{\mathrm{d}t^2} = -\vec{\nabla}_{\vec{R}_I} E[\{\varphi_i\}, \{\vec{R}_I\}] \tag{532}$$

$$\mu \frac{\mathrm{d}^2 \varphi_i(\vec{r}, t)}{\mathrm{d}t^2} = -\frac{\partial}{\partial \varphi_i^*(\vec{r}, t)} E[\{\varphi_i\}, \{\vec{R}_I\}] + \sum_j \lambda_{ij} \varphi_j(\vec{r}, t) \tag{533}$$

μ electron orbital mass, φ_i KS-DFT eigenststate, λ_{ij} Lagrange multiplier

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53.4.2 Force-field MD

Force field MD (FFMD)

- Use empirical interaction potential instead of electronic structure
- Force fields need to be fitted for specific material ⇒not transferable
- Faster than BOMD
- Example: Lennard-Jones

53.4.3 Integration schemes

Procedures for updating positions and velocities to obey the equations of motion.

Euler method

First-order procedure for solving ode??? s with a given initial value.

Taylor expansion of $\vec{R}/\vec{v}(t + \Delta t)$

$$\vec{R}(t + \Delta t) = \vec{R}(t) + \vec{v}(t)\Delta t + \mathcal{O}\left(\Delta t^2\right) \tag{534}$$

$$\vec{v}(t + \Delta t) = \vec{v}(t) + \vec{a}(t)\Delta t + \mathcal{O}\left(\Delta t^2\right) \tag{535}$$

Cumulative error scales linearly $\mathcal{O}(\Delta t)$. Not time reversible.

Verlet integration
Preverses time reversibility, does not require velocity updates. Integration in 2nd order

$$\vec{R}(t+\Delta t) = 2\vec{R}(t) - \vec{R}(t-\Delta t) + \vec{a}(t)\Delta t^2 + \mathcal{O}\left(\Delta t^4\right) \tag{536}$$

Velocity-Verlet integration

$$\vec{R}(t+\Delta t) = \vec{R}(t) + \vec{v}(t)\Delta t + \frac{1}{2}\vec{a}(t)\Delta t^2 + \mathcal{O}\left(\Delta t^4\right) \tag{537}$$

$$\vec{v}(t+\Delta t) = \vec{v}(t) + \frac{\vec{a}(t)+\vec{a}(t+\Delta t)}{2}\Delta t + \mathcal{O}\left(\Delta t^4\right) \tag{538}$$

Leapfrog
Integration in 2nd order

$$x_{i+1} = x_i + v_{i+1/2}\Delta t_i \tag{539}$$

$$v_{i+1/2} = v_{i-1/2} + a_i\Delta t_i \tag{540}$$

53.4.4 Thermostats and barostats

Velocity rescaling
Thermostat, keep temperature at T_0 by rescaling velocities. Does not allow temperature fluctuations and thus does not obey the Canonical ensemble

$$\Delta T(t) = T_0 - T(t) \tag{541}$$

$$= \sum_I^N \frac{M_I\,(\lambda\vec{v}_I(t))^2}{f k_\mathrm{B}} - \sum_I^N \frac{M_I\,\vec{v}_I(t)^2}{f k_\mathrm{B}} \tag{542}$$

$$= (\lambda^2 - 1)T(t) \tag{543}$$

$$\lambda = \sqrt{\frac{T_0}{T(t)}} \tag{544}$$

T target Temperature, M Mass of nucleon I, $\vec{v}$ Velocity, f number of degrees of freedom, λ velocity scaling parameter, k_B Boltzmann constant

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Berendsen thermostat
Does not obey Canonical ensemble but efficiently brings system to target temperature

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{T_0 - T}{\tau} \tag{545}$$

Nosé-Hoover thermostat
Control the temperature with by time stretching with an associated mass.
Compliant with Canonical ensemble

$$\mathrm{d}\tilde{t} = \tilde{s}\,\mathrm{d}t \tag{546}$$

$$\mathcal{L} = \sum_{I=1}^N \frac{1}{2}M_I\tilde{s}^2v_i^2 - V(\tilde{\vec{R}}_1,\dots,\tilde{\vec{R}}_I,\dots,\tilde{\vec{R}}_N) + \frac{1}{2}Q\dot{\tilde{s}}^2 - gk_\mathrm{B}T_0\ln\tilde{s} \tag{547}$$

s scaling factor, Q associated ”mass”, $\mathcal{L}$ Lagrange function , g degrees of freedom

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53.4.5 Calculating observables

Spectral density
Wiener-Khinchin theorem
Fourier transform of Autocorrelation

$$S(\omega) = \int_{-\infty}^{\infty}\mathrm{d}\tau C(\tau)\,\mathrm{e}^{-i\omega t} \tag{548}$$

C Autocorrelation

Vibrational density of states (VDOS)

$$g(\omega) \sim \sum_{I=1}^{N} M_I S_{v_I}(\omega) \tag{549}$$

S_{v_i} velocity Spectral density of particle I

54 Machine-Learning

54.1 Performance metrics

Accuracy

$$a = \frac{\text{correct predictions}}{\text{false predictions} + \text{correct predictions}} \tag{550}$$

Number of data points Anzahl der Datenpunkte

Mean absolute error (MAE)

$$\mathrm{MAE} = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i| \tag{551}$$

y ground truth, $\hat{y}$ prediction, n comp:ml:performance:n desc

Mean squared error (MSE)

$$\mathrm{MSE} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \tag{552}$$

y ground truth, $\hat{y}$ prediction, n comp:ml:performance:n desc

Root mean squared error (RMSE)

$$\mathrm{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2} \tag{553}$$

y ground truth, $\hat{y}$ prediction, n comp:ml:performance:n desc

54.2 Regression

54.2.1 Linear Regression

Linear regression
Fits the data under the assumption of normally distributed errors

$$\underline{y} = \underline{\epsilon} + \underline{x} \cdot \vec{\beta} \tag{554}$$

$\underline{x} \in \mathbb{R}^{N \times M}$ input data, $\underline{y} \in \mathbb{R}^{N \times L}$ output data, $\underline{b}$ bias, $\vec{\beta}$ weights, N samples, M features, L output variables

Design matrix
Stack column of ones to the feature vector
Useful when ϵ is scalar

$$\underline{X} = \begin{pmatrix} 1 & x_{11} & \dots & x_{1M} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{N1} & \dots & x_{NM} \end{pmatrix} \tag{555}$$

x_{ij} feature j of sample i

Linear regression with scalar bias
Using the design matrix, the scalar is absorbed into the weight vector

$$\underline{y} = \underline{X} \cdot \vec{\beta} \tag{556}$$

$\underline{y}$ output data, $\underline{X}$ comp:ml:reg:design matrix, $\vec{\beta}$ weights

Normal equation Solves Linear regression with scalar bias with comp:ml:performance:mse	$\vec{\beta} = \left(\underline{X}^\mathrm{T}\underline{X}\right)^{-1}\underline{X}^T\underline{y}$ (557) $\underline{y}$ output data, $\underline{X}$ Design matrix, $\vec{\beta}$ weights

54.2.2 Kernel method

Kernel trick	Useful when transforming the input data x into a much higher dimensional space $(M_2 \gg M_1)$ $\Phi : \mathbb{R}^{M_1} \mapsto \mathbb{R}^{M_2}, \quad \vec{x} \to \Phi(\vec{x})$ and only the dot product of this transformed data $\Phi(x)^\mathrm{T}\Phi(x)$ is required. Then the dot product can be replaced by a suitable kernel function κ. $k(\vec{x}_i, \vec{x}_j) \equiv \Phi(\vec{x}_i)^\mathrm{T}\Phi(\vec{x}_j)$ (558) $\vec{x}_i \in \mathbb{R}^{M_1}$ input vectors, M_1 dimension of data vector space, M_2 dimension of feature space
Common kernels	Linear, Polynomial, Sigmoid, Laplacian, radial basis funciton (RBF)
Radial basis function kernel (RBF) RBF = Real function of which the value only depends on the distance of the input	$k(\vec{x}_i, \vec{x}_j) = \exp\left(-\frac{\lVert\vec{x}_i - \vec{x}_j\rVert_2^2}{\sigma}\right)$ (559)

54.2.3 Bayesian regression

Bayesian linear regression	Assume a Prior distribution distribution over the weights. Offers uncertainties in addition to the predictions.
Ridge regression Regularization method	Applies a L2 norm penalty on the weights. This ensures unimportant features are less regarded and do not encode noise. Corresponds to assuming a Prior distribution Multivariate normal distribution with $\vec{\mu} = 0$ and independent components ($\underline{\Sigma}$) for the weights.
Optimal weights for ridge regression	$\vec{\beta} = \left(\underline{X}^\mathrm{T}\underline{X} + \lambda\right)^{-1}\underline{X}^\mathrm{T}\vec{y}$ (560) TODO:Does this only work for gaussian data? $\lambda = \frac{\sigma^2}{\xi^2}$ shrinkage parameter, ξ Variance of the gaussian Prior distribution, σ Variance of the gaussian likelihood of the data
Lasso regression Least absolute shrinkage and selection operator Regularization method	Applies a L1 norm penalty on the weights, which means features can be disregarded entirely. Corresponds to assuming a Laplace-distribution for the weights as Prior distribution.

Gaussian process regression (GPR)	Gaussian process: A distribtuion over functions that produce jointly gaussian distribution. Multivariate normal distribution like comp:ml:reg:bayes:bayesian, except that $\vec{\mu}$ and $\underline{\Sigma}$ are functions. GPR: non-parametric Bayesion regressor, does not assume fixed functional form for the underlying data, instead, the data determines the functional shape, with predictions governed by the covariance structure defined by the kernel (often RBF). Offers uncertainties in addition to the predictions. TODO:cleanup

TODO:soap

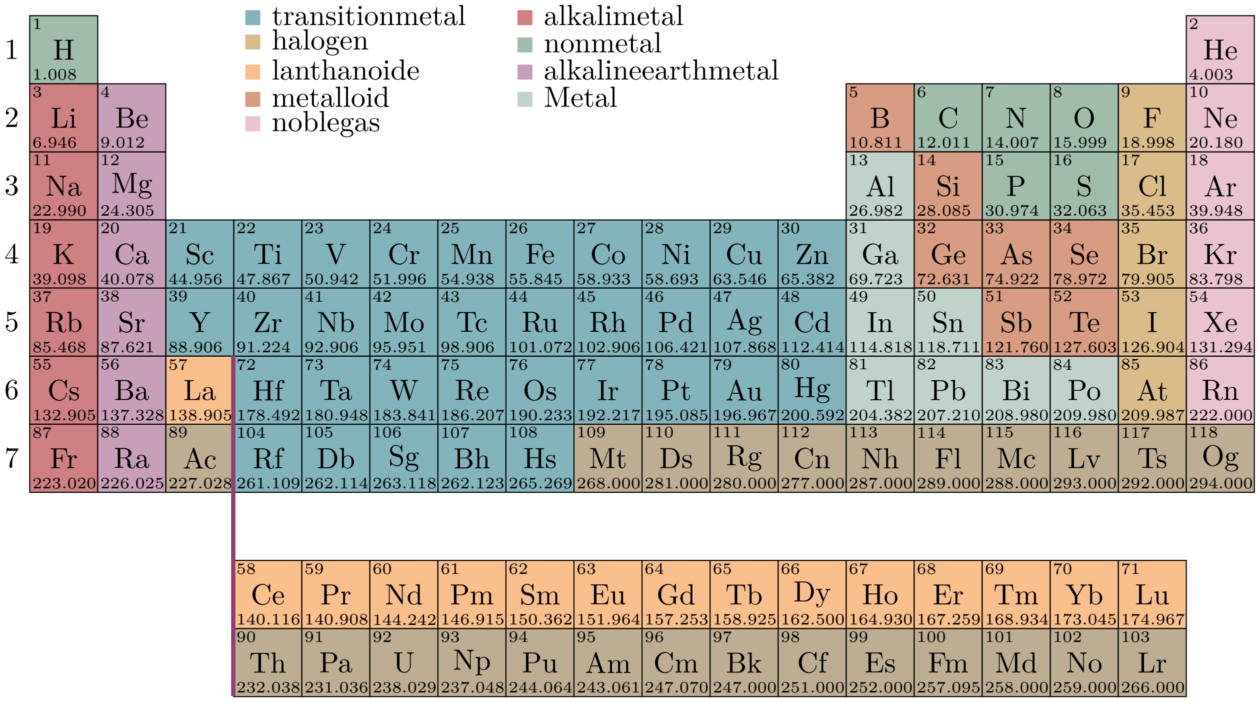
54.3 Gradient descent

TODO:in lecture 30 CMP

Part XI

Chemistry

55 Periodic table



■ transitionmetal
■ halogen
■ lanthanoide
■ metalloid
■ noblegas
■ alkalimetal
■ nonmetal
■ alkalineearthmetal
■ Metal

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	

56 Electrochemistry

Chemical potential
of species i
Energy involved when the
particle number changes

Symbol: μ Unit: 1 J/mol; J

$$\mu_i \equiv \left(\frac{\partial G}{\partial n_i}\right)_{n_j \neq n_i, p, T} \tag{561}$$

??? ???:gibbs free energy, n Amount of substance

Standard chemical potential
In equilibrium

$$\mu_i = \mu_i^\theta + RT \ln(a_i) \tag{562}$$

μ Chemical potential, R Universal gas constant, T Temperature, a Activity

Chemical equilibrium

$$\sum_{\text{products}} \nu_i \mu_i = \sum_{\text{educts}} \nu_i \mu_i \tag{563}$$

μ Chemical potential, ν Stoichiometric coefficient

Activity
relative activity

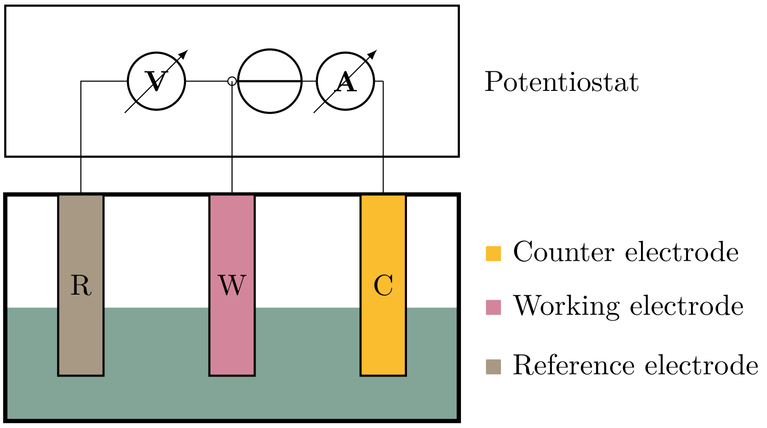
Symbol: a Unit:

$$a_i = \exp\left(\frac{\mu_i - \mu_i^\theta}{RT}\right) \tag{564}$$

μ Chemical potential, ??? ???:standard chemical potential, R Universal gas constant, T Temperature

Electrochemical potential Chemical potential with electrostatic contributions	Symbol: $\overline{\mu}$ Unit: $1\,\mathrm{J/mol; J}$ $\overline{\mu}_i \equiv \mu_i + z_i F \phi \qquad (565)$ μ Chemical potential, z valency (charge), F Faraday constant, ϕ Electric potential (Galvani Potential)

56.1 Electrochemical cell

Schematic	
Electrochemical cell types	- Electrolytic cell: Uses electrical energy to force a chemical reaction - Galvanic cell: Produces electrical energy through a chemical reaction
Faradaic process	Charge transfers between the electrode bulk and the electrolyte.
Non-Faradaic (capacitive) process	Charge is stored at the electrode-electrolyte interface.
Electrode potential	Symbol: E Unit: $1\,\mathrm{V}$
Standard cell potential	$E^{\theta}_{\mathrm{rev}} = \frac{-\Delta_{\mathrm{R}} G^{\theta}}{nF} \qquad (566)$ $\Delta_{\mathrm{R}} G^{\theta}$ standard ???:gibbs free energy of reaction, n number of electrons, F Faraday constant
Nernst equation Electrode potential for a half-cell reaction	$E = E^{\theta} + \frac{RT}{zF} \ln \left(\frac{\left(\prod_i (a_i)^{\lvert\nu_i\rvert}\right)_{\text{oxidized}}}{\left(\prod_i (a_i)^{\lvert\nu_i\rvert}\right)_{\text{reduced}}} \right) \qquad (567)$ E Electrode potential, E^{θ} Standard cell potential, R Universal gas constant, ??? ???:temperature, z Charge number, F Faraday constant, a Activity, ν Stoichiometric coefficient

Thermodynamic cell efficiency

$$\eta_{\text{cell}} = \frac{P_{\text{obtained}}}{P_{\text{maximum}}} = \frac{E_{\text{cell}}}{E_{\text{cell,rev}}} \qquad \text{galvanic} \tag{568}$$

$$\eta_{\text{cell}} = \frac{P_{\text{minimum}}}{P_{\text{applied}}} = \frac{E_{\text{cell,rev}}}{E_{\text{cell}}} \qquad \text{electrolytic} \tag{569}$$

P Electric power

56.2 Ionic conduction in electrolytes

Diffusion
caused by concentration gradients

$$i_{\text{diff}} = \sum_i -z_i F D_i \left(\frac{\mathrm{d}c_i}{\mathrm{d}x}\right) \tag{570}$$

z_i Charge number of ion i, F Faraday constant, ??? ???:diffusion constant of ion i, c Concentration of ion i

---

Migration
caused by potential gradients

$$i_{\text{mig}} = \sum_i -z_i^2 F^2 c_i \, \mu_i \, \nabla \Phi_{\text{s}} \tag{571}$$

z_i Charge number of ion i, F Faraday constant, c Concentration of ion i, μ Electrical mobility of ion i, $\nabla \phi_{\text{s}}$ potential gradient in the solution

---

Convection
caused by pressure gradients

$$i_{\text{conv}} = \sum_i -z_i F \, c_i \, v_i^{\text{flow}} \tag{572}$$

z_i Charge number of ion i, F Faraday constant, c Concentration of ion i, v_i^{flow} Velocity of ion i in flowing electrolyte

---

Ionic mobility

Symbol: $u_\pm$ Unit: $1\,\text{cm}^2\text{mol/Js}$

$$u_\pm = -\frac{v_\pm}{\nabla \phi \, z_\pm F} = \frac{e}{6\pi F \eta_{\text{dyn}} r_\pm} \tag{573}$$

$v_\pm$ steady state drift Velocity, ϕ Electric potential, z Charge number, F Faraday constant, e Unit charge, η, μ Dynamic viscosity, $r_\pm$ ion radius

---

Stokes's law
Frictional force exerted on spherical objects moving in a viscous fluid at low Reynolds numbers

$$F_{\text{R}} = 6\pi \, r \eta v \tag{574}$$

r particle radius, η, μ Dynamic viscosity, v particle Velocity

---

Ionic conductivity

Symbol: κ Unit: $1\,\Omega^{-1}\,\text{cm} = 1\,\text{S}\,\text{cm}^{-1}$

$$\kappa = F^2 \left(z_+^2 \, c_+ \, u_+ + z_-^2 \, c_- \, u_-\right) \tag{575}$$

F Faraday constant, z_i, c_i, u_i charge number, Concentration and Ionic mobility of the positive (+) and negative (-) ions

---

Ohmic resistance of ionic current flow

$$R_\Omega = \frac{L}{A\,\kappa} \tag{576}$$

L Length, A Area, κ Ionic conductivity

Transference number
Ion transport number
Fraction of the current carried by positive / negative ions

$$t_{+/-} = \frac{i_{+/-}}{i_+ + i_-} \tag{577}$$

$i_{+/-}$ current through positive/negative charges

Molar conductivity

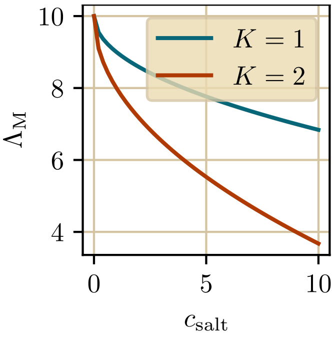
Symbol: Λ_M Unit: $1\,\text{S}\text{cm}^2/\text{mol} = 1\,\text{A}\text{cm}^2/\text{V}\text{mol}$

$$\Lambda_\text{M} = \frac{\kappa}{c_\text{salt}} \tag{578}$$

κ Ionic conductivity, c_salt Concentration des Elektrolyts

Kohlrausch's law
For strong electrolytes

$$\Lambda_\text{M} = \Lambda_\text{M}^0 - K\sqrt{c_\text{salt}} \tag{579}$$



Λ_M^0 Molar conductivity at infinite dilution, c_salt Concentration des Elektrolyts, K constant

---

Molality
Amount per mass

Symbol: b Unit: $1\,\text{mol}\,\text{kg}^{-1}$

$$b = \frac{n}{m} \tag{580}$$

n Amount of substance of the solute, m Mass of the solvent

Molarity
Amount per volume
Concentration

Symbol: c Unit: $1\,\text{mol}\,\text{L}^{-1}$

$$c = \frac{n}{V} \tag{581}$$

n Amount of substance of the solute, V Volume of the solvent

Ionic strength
Measure of the electric field in a solution through solved ions

Symbol: I Unit: $1\,\text{mol/kg; mol/L}$

$$I_b = \frac{1}{2}\sum_i b_i z_i^2 \tag{582}$$

$$I_c = \frac{1}{2}\sum_i c_i z_i^2 \tag{583}$$

b Molality, c Molarity, z Charge number

Debye screening length

$$\lambda_\mathrm{D} = \sqrt{\frac{\epsilon k_\mathrm{B} T}{2 N_\mathrm{A} e^2 I_C}} \tag{584}$$

N_A Avogadro constant, e Unit charge, I Ionic strength, ϵ Permittivity, k_B Boltzmann constant, T Temperature

---

Mean ionic activity coefficient

Accounts for decreased reactivity because ions must divest themselves of their ion cloud before reacting

Symbol: γ Unit:

$$\gamma_\pm = \left(\gamma_+^{\nu_+} \gamma_-^{\nu_-}\right)^{\frac{1}{\nu_+ + \nu_-}} \tag{585}$$

$$a_i \equiv \gamma_i \frac{m_i}{m^0} \tag{586}$$

a Activity, m_i Molality, $m_0 = 1\,\mathrm{mol\,kg^{-1}}$

Debye-Hückel limiting law
For an infinitely dilute solution

$$\ln\left(\gamma_\pm\right) = -A\,|z_+ z_-|\sqrt{I_b} \tag{587}$$

γ Mean ionic activity coefficient, A solvent dependant constant, z Charge number, I Ionic strength in $[\mathrm{mol\,kg^{-1}}]$

56.3 Kinetics

Transfer coefficient

$$\alpha_\mathrm{A} = \alpha \tag{588}$$

$$\alpha_\mathrm{C} = 1 - \alpha \tag{589}$$

Overpotential

Potential deviation from the equilibrium cell potential

Activation verpotential

$$\eta_\mathrm{act} = E_\mathrm{electrode} - E_\mathrm{ref} \tag{590}$$

$E_\mathrm{electrode}$ potential at which the reaction starts E_ref thermodynamic potential of the reaction

56.3.1 Mass transport

Concentration overpotential
Due to concentration gradient near the electrode, the ions need to diffuse to the electrode before reacting

$$\eta_\mathrm{conc,anodic} = -\frac{RT}{\alpha\,zF}\ln\left(\frac{c_\mathrm{red}^0}{c_\mathrm{red}^\mathrm{S}}\right) \tag{591}$$

$$\eta_\mathrm{conc,cathodic} = -\frac{RT}{(1-\alpha)zF}\ln\left(\frac{c_\mathrm{ox}^0}{c_\mathrm{ox}^\mathrm{S}}\right) \tag{592}$$

R Universal gas constant, T Temperature, 0/S ion concentration in the electrolyte / at the double layer, z Charge number, F Faraday constant

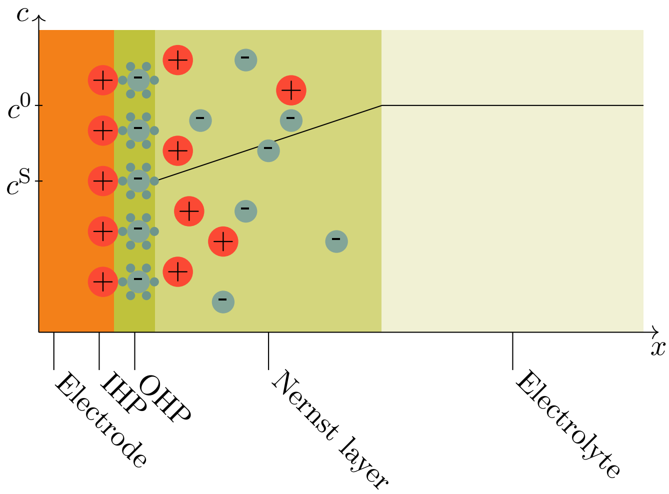
---

Diffusion overpotential
Due to mass transport limitations

$$\eta_\mathrm{diff} = \frac{RT}{nF}\ln\left(\frac{j_\infty}{j_\infty - j_\mathrm{meas}}\right) \tag{593}$$

j_∞ (Limiting) current density, j_meas measured Current density, R Universal gas constant, T Temperature, n Charge number, F Faraday constant

Cell layers



IHP/OHP inner/outer Helmholtz-plane, c^0 bulk Concentration, c^{S} surface Concentration

---

Nerst Diffusion layer thickness

$$\delta_{\mathrm{N}} = \frac{c^0 - c^{\mathrm{S}}}{\left.\frac{\mathrm{d}c}{\mathrm{d}x}\right|_{x=0}} \tag{594}$$

c^0 bulk Concentration, c^{S} surface Concentration

(Limiting) current density

$$|j| = nFD\frac{c^0 - c^{\mathrm{S}}}{\delta_{\mathrm{diff}}} \tag{595}$$

for $c^{\mathrm{S}} \to 0$

$$|j_\infty| = nFD\frac{c^0}{\delta_{\mathrm{diff}}} \tag{596}$$

n Z Charge number, F Faraday constant, c^0 bulk Concentration, D Diffusion coefficient, δ_{diff} Nerst Diffusion layer thickness

---

Current - concentration relation

$$\frac{j}{j_\infty} = 1 - \frac{c^{\mathrm{S}}}{c^0} \tag{597}$$

c^0 bulk Concentration, c^{S} surface Concentration, j (Limiting) current density

---

Kinetic current density

$$j_{\mathrm{kin}} = \frac{j_{\mathrm{meas}} j_\infty}{j_\infty - j_{\mathrm{meas}}} \tag{598}$$

j_{meas} measured Current density, j_∞ (Limiting) current density

---

Roughness factor
Surface area related to electrode geometry

$$\mathrm{rf} \tag{599}$$

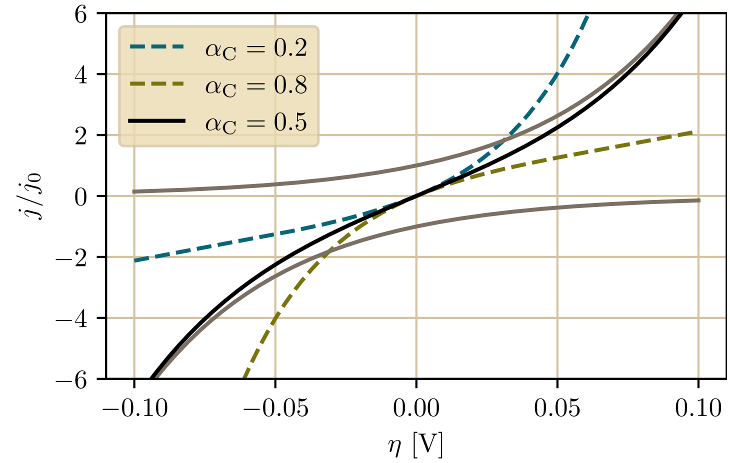
Butler-Volmer equation

Reaction kinetics near the equilibrium potentential

$$j = j_0\,\mathrm{rf}\left[\exp\left(\frac{(1-\alpha_{\mathrm{C}})zF\eta}{RT}\right) - \exp\left(-\frac{\alpha_{\mathrm{C}}zF\eta}{RT}\right)\right] \tag{600}$$

with

$$\alpha_{\mathrm{A}} = 1 - \alpha_{\mathrm{C}} \tag{601}$$



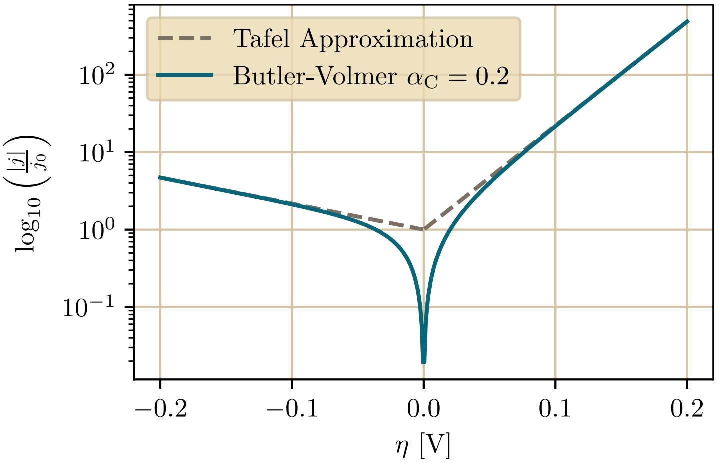
j Current density, j_0 exchange current density, η Overpotential, T Temperature, z Charge number, F Faraday constant, R Universal gas constant, $\alpha_{\mathrm{C/A}}$ cathodic/anodic charge transfer coefficient, rf Roughness factor

Tafel approximation

For slow kinetics: $|\eta| > 0{,}1\,\mathrm{V}$

$$\log(j) \approx \log(j_0) + \frac{\alpha_{\mathrm{C}}zF\eta}{RT\ln(10)} \qquad \eta \gg 0{,}1\,\mathrm{V} \tag{602}$$

$$\log(|j|) \approx \log(j_0) - \frac{(1-\alpha_{\mathrm{C}})zF\eta}{RT\ln(10)} \qquad \eta \ll -0{,}1\,\mathrm{V} \tag{603}$$



56.4 Techniques

56.4.1 Reference electrodes

Defined as reference for measuring half-cell potentententials

Standard hydrogen elektrode (SHE)

Potential of the reaction: $2\,\mathrm{H}^+ + 2\,\mathrm{e}^- \rightleftharpoons \mathrm{H}_2$

$p = 10^5\,\mathrm{Pa},\ a_{\mathrm{H}^+} = 1\,\mathrm{mol\,L^{-1}}\ (\Rightarrow \mathrm{pH} = 0)$

Reversible hydrogen electrode (RHE)
RHE Potential does not change with the pH value

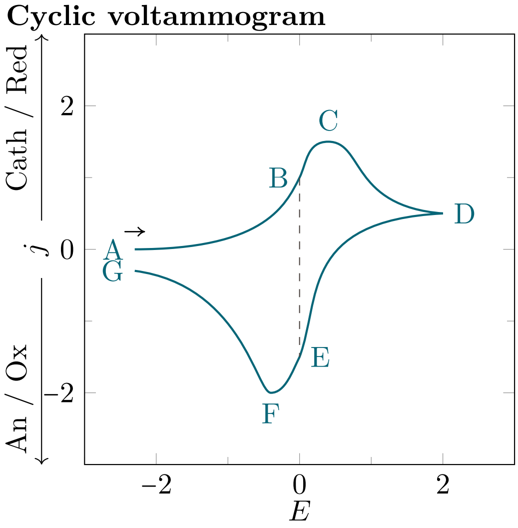
$$E_{\mathrm{RHE}} = E^0 + \frac{RT}{F} \ln\left(\frac{a_{\mathrm{H}^+}}{p_{\mathrm{H}_2}}\right) \tag{604}$$

$E^0 \equiv 0\,\mathrm{V}$, a Activity, p Pressure, see Nernst equation

---

56.4.2 Cyclic voltammetry

Cyclic voltammogram



- A-D: Diffusion layer growth →decreased current after peak
- D: Switching potential
- B,E: Equal concentrations of reactants
- C,F: Formal potential of redox pair: $E \approx \frac{E_\mathrm{C}-E_\mathrm{F}}{2}$
- C,F: Peak separation for reverisble processes: $\Delta E_{\mathrm{rev}} = E_\mathrm{C} - E_\mathrm{F} = n\,59\,\mathrm{mV}$
- Information about surface chemistry
- Double-layer capacity (horizontal lines): $I = Cv$

Charge
Area under the curve

$$q = \frac{1}{v} \int_{E_1}^{E_2} j\,\mathrm{d}E \tag{605}$$

v Scan rate

Randles-Sevcik equation
For reversible faradaic reaction.
Peak current depends on square root of the scan rate

$$i_{\mathrm{peak}} = 0.446\,nFAc^0 \sqrt{\frac{nFvD_{\mathrm{ox}}}{RT}} \tag{606}$$

n Charge number, F Faraday constant, A electrode surface area, c^0 bulk Concentration, v Scan rate, D_{ox} Diffusion coefficient of oxidized analyte, R Universal gas constant, T Temperature

---

Underpotential deposition (UPD)

Reversible deposition of metal onto a foreign metal electrode at potentials positive of the Nernst potential TODO:clarify ch:el:tech:cv:upd:desc

56.4.3 Rotating disk electrodes

Dynamic viscosity

Symbol: η, μ Unit: $1\,\mathrm{Pa\,s} = 1\,\mathrm{Ns/m^2} = 1\,\mathrm{kg\,m^{-1}\,s}$

Kinematic viscosity
Dynamic viscosity related to density of a fluid

Symbol: ν Unit: $1\,\mathrm{cm^2/s}$

$$\nu = \frac{\eta}{\rho} \tag{607}$$

η, μ Dynamic viscosity, ??? ???:density

Diffusion layer thickness
TODO:Where does 1.61 come from

$$\delta_\text{diff} = 1.61 D^{\frac{1}{3}} \nu^{\frac{1}{6}} \omega^{-\frac{1}{2}} \tag{608}$$

D Diffusion coefficient, ν Kinematic viscosity, ω Angular frequency

---

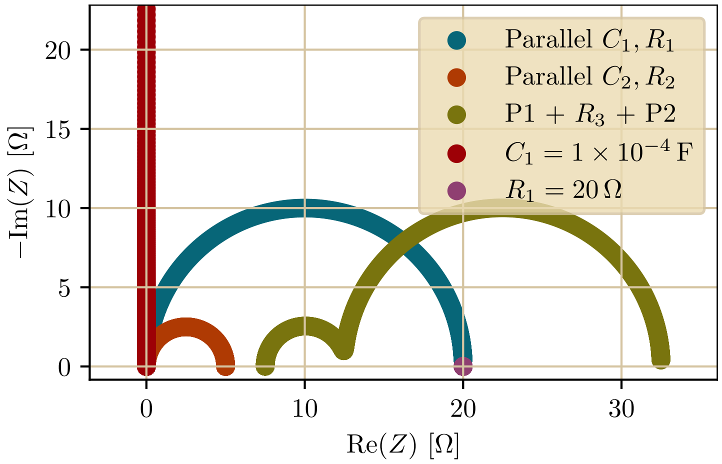
Limiting current density for a RDE

$$j_\infty = nFD\frac{c^0}{\delta_\text{diff}} = \frac{1}{1.61} nFD^{\frac{2}{3}} v^{\frac{-1}{6}} c^0 \sqrt{\omega} \tag{609}$$

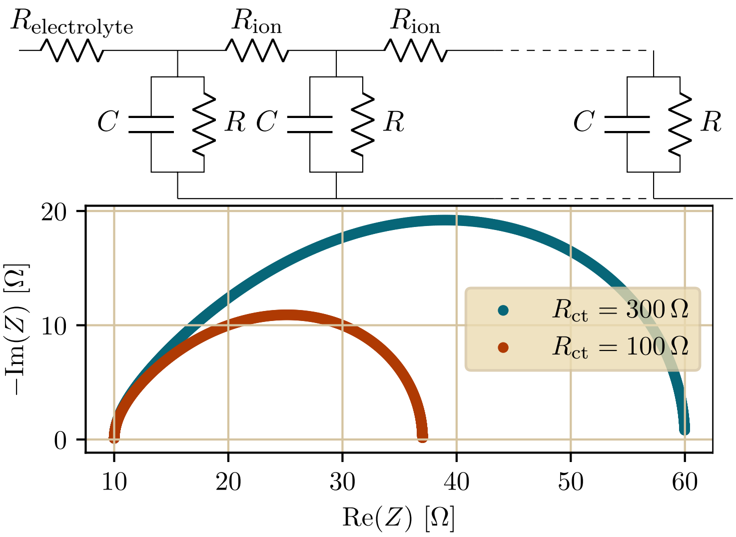
n Z Charge number, F Faraday constant, c^0 bulk Concentration, D Diffusion coefficient, δ_diff Diffusion layer thickness, ν Kinematic viscosity, ω Angular frequency

56.4.4 AC-Impedance

Nyquist diagram
Real and imaginary parts of ???:impedance while varying the frequency



Transmission line model
Model of porous electrodes as many slices



R_ion ion conduction resistance in electrode slice, R / C resistance / capacitance of electode slice

57 Thermoelectricity

Seebeck coefficient
Thermopower

Symbol: S Unit: $1\,\mu\mathrm{V}\,\mathrm{K}^{-1}$

$$S = -\frac{\Delta V}{\Delta T} \tag{610}$$

V voltage, T Temperature

Seebeck effect
Elecromotive force across two points of a material with a temperature difference

$$\vec{j} = \sigma(-\vec{\nabla} V - S\vec{\nabla} T) \tag{611}$$

σ Conductivity, V local voltage, S Seebeck coefficient, T Temperature

---

Thermal conductivity
Conduction of heat, without mass transport

Symbol: κ, λ, k Unit: $1\,\mathrm{W}\,\mathrm{m}^{-1}\,\mathrm{K} = 1\,\mathrm{kgm/s^3K}$

$$\kappa = \frac{\dot{Q} l}{A\,\Delta T} \tag{612}$$

$$\kappa_\text{tot} = \kappa_\text{lattice} + \kappa_\text{electric} \tag{613}$$

??? ???:heat, l Length, A Area, T Temperature

Wiedemann-Franz law

$$\kappa = L\sigma T \tag{614}$$

κ Electric Thermal conductivity, L in $\mathrm{W}\,\Omega\,\mathrm{K}^{-1}$ Lorentz number, σ Conductivity

---

Thermoelectric figure of merit

Dimensionless quantity for comparing different materials

$$zT = \frac{S^2\sigma}{\kappa} T \tag{615}$$

S Seebeck coefficient, σ Conductivity, κ Thermal conductivity, T Temperature

58 misc

Stoichiometric coefficient

Symbol: ν Unit:

Standard temperature and pressure

$$T = 273{,}15\,\mathrm{K} = 0\,^\circ\mathrm{C} \tag{616}$$

$$p = 100\,000\,\mathrm{Pa} = 1{,}000\,\mathrm{bar} \tag{617}$$

---

pH definition

$$\mathrm{pH} = -\log_{10}(a_{\mathrm{H}^+}) \tag{618}$$

a_{H^+} hyrdrogen ion Activity

---

pH
At room temperature 25 °C

$$\mathrm{pH} > 7 \quad \text{basic} \tag{619}$$

$$\mathrm{pH} < 7 \quad \text{acidic} \tag{620}$$

$$\mathrm{pH} = 7 \quad \text{neutral} \tag{621}$$

<table>
<tr><td>Covalent bond</td><td>Bonds that involve sharing of electrons to form electron pairs between atoms.</td></tr>
<tr><td>Grotthuß-mechanism</td><td>The mobility of protons in aqueous solutions is much higher than that of other ions because they can ”move” by breaking and reforming covalent bonds of water molecules.</td></tr>
<tr><td>Common chemicals</td><td>
<table>
<tr><th>Name</th><th>formula</th></tr>
<tr><td>Cyanide</td><td>CN</td></tr>
<tr><td>Ammonia</td><td>NH_3</td></tr>
<tr><td>Hydrogen Peroxide</td><td>H_2O_2</td></tr>
<tr><td>Sulfuric Acid</td><td>H_2SO_4</td></tr>
<tr><td>Ethanol</td><td>C_2H_5OH</td></tr>
<tr><td>Acetic Acid</td><td>CH_3COOH</td></tr>
<tr><td>Methane</td><td>CH_4</td></tr>
<tr><td>Hydrochloric Acid</td><td>HCl</td></tr>
<tr><td>Sodium Hydroxide</td><td>NaOH</td></tr>
<tr><td>Nitric Acid</td><td>HNO_3</td></tr>
<tr><td>Calcium Carbonate</td><td>$CaCO_3$</td></tr>
<tr><td>Glucose</td><td>$C_6H_{12}O_6$</td></tr>
<tr><td>Benzene</td><td>C_6H_6</td></tr>
<tr><td>Acetone</td><td>C_3H_6O</td></tr>
<tr><td>Ethylene</td><td>C_2H_4</td></tr>
<tr><td>Potassium Permanganate</td><td>$KMnO_4$</td></tr>
</table>
</td></tr>
</table>

Part XII

Appendix

World formula

$$\boxed{E = mc^2 + \mathrm{AI} \qquad (622)}$$

59 Physical quantities

59.1 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: $1\,\mathrm{cd}$

59.2 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: $1\,\mathrm{N\,m} = 1\,\mathrm{kgm^2/s^2}$
Pressure	Symbol: p	Unit: $1\,\mathrm{N/m^2}$

59.3 Thermodynamics

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

59.4 Electrodynamics

Charge	Symbol: q Unit: $1\,\mathrm{C} = 1\,\mathrm{A\,s}$
Charge number	Symbol: Z Unit:
Charge density	Symbol: ρ Unit: $1\,\mathrm{C/m^3}$
Frequency	Symbol: f Unit: $1\,\mathrm{Hz} = 1\,\mathrm{s^{-1}}$
Angular frequency	Symbol: ω Unit: $1\,\mathrm{rad\,s^{-1}}$ $\omega = \frac{2\pi/T}{2\pi f}$ (623) T Time period, f Frequency
Time period	Symbol: T Unit: $1\,\mathrm{s}$ $T = \frac{1}{f}$ (624) f Frequency
Conductivity	Symbol: σ Unit: $1\,\Omega^{-1}\,\mathrm{m}$

59.5 Others

Area	Symbol: A Unit: $1\,\mathrm{m^2}$

60 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 $9.64853321233100184 \cdot 10^{4}\,\mathrm{C\,mol^{-1}}$ $N_\mathrm{A}\, e$ N_A Avogadro constant, k_B Boltzmann constant
Unit charge	Symbol: e Defined value $1.602176634 \cdot 10^{-19}\,\mathrm{C}$
Atomic mass unit	Symbol: u Experimental value $1.66053906892(52) \cdot 10^{-27}\,\mathrm{kg}$

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Hydrogen colorless gas (H2)	Symbol: H Number: 1 Crystal structure: hex Electronic configuration: 1s[1] magnetic ordering: diamagnetic atomic mass: 1.0081 set: nonmetal
Helium colorless gas, exhibiting a gray, cloudy glow	Symbol: He Number: 2 Crystal structure: hcp Electronic configuration: 1s[1] magnetic ordering: diamagnetic atomic mass: 4.0026022 set: noblegas
Lithium silvery-white	Symbol: Li Number: 3 Crystal structure: bcc Electronic configuration: He 2s[1] magnetic ordering: paramagnetic atomic mass: 6.946 set: alkalimetal

Beryllium white-gray metallic	Symbol: Be Number: 4 Crystal structure: hcp Electronic configuration: He 2s[2] magnetic ordering: diamagnetic atomic mass: 9.01218315 set: alkalineearthmetal
Boron black-brown	Symbol: B Number: 5 Crystal structure: rho Electronic configuration: He 2s[2] 2p[1] magnetic ordering: diamagnetic atomic mass: 10.811 set: metalloid
Carbon black, metallic-looking (graphite); clear (diamond)	Symbol: C Number: 6 Crystal structure: hex Electronic configuration: He 2s[2] 2p[2] magnetic ordering: diamagnetic atomic mass: 12.01112 set: nonmetal
Nitrogen colorless gas, liquid or solid	Symbol: N Number: 7 Crystal structure: hex Electronic configuration: He 2s[2] 2p[3] magnetic ordering: diamagnetic atomic mass: 14.006714 set: nonmetal
Oxygen colorless (gas); pale blue (liquid and solid)	Symbol: O Number: 8 Crystal structure: sc Electronic configuration: He 2s[2] 2p[4] magnetic ordering: paramagnetic atomic mass: 15.99915 set: nonmetal
Fluorine very pale yellow (gas); bright yellow (liquid); alpha is opaque, beta is transparent (solid)	Symbol: F Number: 9 Crystal structure: sc refractive index: 1.000195 magnetic ordering: diamagnetic atomic mass: 18.9984031636 Electronic configuration: He 2s[2] 2p[5] set: halogen

Neon colorless gas exhibiting an orange-red glow when placed in an electric field	Symbol: Ne Number: 10 Crystal structure: fcc refractive index: 1.000067 magnetic ordering: diamagnetic atomic mass: 20.17976 Electronic configuration: He 2s[2] 2p[6] set: noblegas
Sodium silvery white metallic	Symbol: Na Number: 11 Crystal structure: bcc Electronic configuration: Ne 3s[1] magnetic ordering: paramagnetic atomic mass: 22.989769282 set: alkalimetal
Magnesium shiny grey solid	Symbol: Mg Number: 12 Crystal structure: hcp Electronic configuration: Ne 3s[2] magnetic ordering: paramagnetic atomic mass: 24.30524 set: alkalineearthmetal
Aluminum silvery gray metallic	Symbol: Al Number: 13 Crystal structure: fcc Electronic configuration: Ne 3s[2] 3p[1] magnetic ordering: paramagnetic atomic mass: 26.98153857 set: metal
Silicon crystalline, reflective with bluish-tinged faces	Symbol: Si Number: 14 Crystal structure: dc Electronic configuration: Ne 3s[2] 3p[2] magnetic ordering: diamagnetic atomic mass: 28.08528 set: metalloid
Phosphorus white, red and violet are waxy, black is metallic-looking	Symbol: P Number: 15 Crystal structure: orth refractive index: 1.001212 magnetic ordering: diamagnetic atomic mass: 30.9737619985 Electronic configuration: Ne 3s[2] 3p[3] set: nonmetal

Sulfur yellow sintered microcrystals	Symbol: S Number: 16 Crystal structure: orth refractive index: 1.001111 magnetic ordering: diamagnetic atomic mass: 32.0632 Electronic configuration: Ne 3s[2] 3p[4] set: nonmetal
Chlorine pale yellow-green gas	Symbol: Cl Number: 17 Crystal structure: orth refractive index: 1.000773 magnetic ordering: diamagnetic atomic mass: 35.4535 Electronic configuration: Ne 3s[2] 3p[5] set: halogen
Argon colorless gas exhibiting a lilac/violet glow when placed in an electric field	Symbol: Ar Number: 18 Crystal structure: fcc refractive index: 1.000281 magnetic ordering: diamagnetic atomic mass: 39.9481 Electronic configuration: Ne 3s[2] 3p[6] set: noblegas
Potassium silvery white, faint bluish-purple hue when exposed to air	Symbol: K Number: 19 Crystal structure: bcc Electronic configuration: Ar 4s[1] magnetic ordering: paramagnetic atomic mass: 39.09831 set: alkalimetal
Calcium dull gray, silver; with a pale yellow tint	Symbol: Ca Number: 20 Crystal structure: fcc Electronic configuration: Ar 4s[2] magnetic ordering: diamagnetic atomic mass: 40.0784 set: alkalineearthmetal
Scandium silvery white	Symbol: Sc Number: 21 Crystal structure: hcp Electronic configuration: Ar 3d[1] 4s[2] magnetic ordering: paramagnetic atomic mass: 44.9559085 set: transitionmetal

Titanium silvery grey-white metallic	Symbol: Ti Number: 22 Crystal structure: hcp Electronic configuration: Ar 3d[2] 4s[2] magnetic ordering: paramagnetic atomic mass: 47.8671 set: transitionmetal
Vanadium blue-silver-grey metal	Symbol: V Number: 23 Crystal structure: bcc Electronic configuration: Ar 3d[3] 4s[2] magnetic ordering: paramagnetic atomic mass: 50.94151 set: transitionmetal
Chromium silvery metallic	Symbol: Cr Number: 24 Crystal structure: bcc Electronic configuration: Ar 3d[5] 4s[1] magnetic ordering: antiferromagnetic atomic mass: 51.99616 set: transitionmetal
Manganese silvery metallic	Symbol: Mn Number: 25 Crystal structure: bcc Electronic configuration: Ar 3d[5] 4s[2] magnetic ordering: antiferromagnetic atomic mass: 54.9380443 set: transitionmetal
Iron lustrous metallic with a grayish tinge	Symbol: Fe Number: 26 Crystal structure: bcc Electronic configuration: Ar 3d[6] 4s[2] magnetic ordering: ferromagnetic atomic mass: 55.8452 set: transitionmetal
Cobalt hard lustrous bluish gray metal	Symbol: Co Number: 27 Crystal structure: hcp Electronic configuration: Ar 3d[7] 4s[2] magnetic ordering: ferromagnetic atomic mass: 58.9331944 set: transitionmetal

Nickel glänzend, metallisch, silbrig	Symbol: Ni Number: 28 Crystal structure: fcc Electronic configuration: Ar 3d[8] 4s[2] magnetic ordering: ferromagnetic atomic mass: 58.69344 set: transitionmetal
Copper red-orange metallic luster	Symbol: Cu Number: 29 Crystal structure: fcc Electronic configuration: Ar 3d[10] 4s[1] magnetic ordering: diamagnetic atomic mass: 63.5463 set: transitionmetal
Zinc silver-gray	Symbol: Zn Number: 30 Crystal structure: hcp refractive index: 1.00205 magnetic ordering: diamagnetic atomic mass: 65.382 Electronic configuration: Ar 3d[10] 4s[2] set: transitionmetal
Gallium silvery blue	Symbol: Ga Number: 31 Crystal structure: orth Electronic configuration: Ar 3d[10] 4s[2] 4p[1] magnetic ordering: diamagnetic atomic mass: 69.7231 set: metal
Germanium grayish-white	Symbol: Ge Number: 32 Crystal structure: dc Electronic configuration: Ar 3d[10] 4s[2] 4p[2] magnetic ordering: diamagnetic atomic mass: 72.6308 set: metalloid
Arsenic metallic grey	Symbol: As Number: 33 Crystal structure: rho refractive index: 1.001552 magnetic ordering: diamagnetic atomic mass: 74.9215956 Electronic configuration: Ar 3d[10] 4s[2] 4p[3] set: metalloid

Selenium grey metallic-looking, red, and vitreous black allotropes	Symbol: Se Number: 34 Crystal structure: hex refractive index: 1.000895 magnetic ordering: diamagnetic atomic mass: 78.9718 Electronic configuration: Ar 3d[10] 4s[2] 4p[4] set: metalloid
Bromine reddish-brown	Symbol: Br Number: 35 Crystal structure: orth refractive index: 1.001132 magnetic ordering: diamagnetic atomic mass: 79.90479 Electronic configuration: Ar 3d[10] 4s[2] 4p[5] set: halogen
Krypton colorless gas, exhibiting a whitish glow in an electric field	Symbol: Kr Number: 36 Crystal structure: fcc refractive index: 1.000427 magnetic ordering: diamagnetic atomic mass: 83.7982 Electronic configuration: Ar 3d[10] 4s[2] 4p[6] set: noblegas
Rubidium grey white	Symbol: Rb Number: 37 Crystal structure: bcc Electronic configuration: Kr 5s[1] magnetic ordering: paramagnetic atomic mass: 85.46783 set: alkalimetal
Strontium silvery white metallic; with a pale yellow tint	Symbol: Sr Number: 38 Crystal structure: fcc Electronic configuration: Kr 5s[2] magnetic ordering: paramagnetic atomic mass: 87.621 set: alkalineearthmetal
Yttrium silvery white	Symbol: Y Number: 39 Crystal structure: hcp Electronic configuration: Kr 4d[1] 5s[2] magnetic ordering: paramagnetic atomic mass: 88.905842 set: transitionmetal

Zirconium silvery white	Symbol: Zr Number: 40 Crystal structure: hcp Electronic configuration: Kr 4d[2] 5s[2] magnetic ordering: paramagnetic atomic mass: 91.2242 set: transitionmetal
Niobium gray metallic, bluish when oxidized	Symbol: Nb Number: 41 Crystal structure: bcc Electronic configuration: Kr 4d[4] 5s[1] magnetic ordering: paramagnetic atomic mass: 92.906372 set: transitionmetal
Molybdenum gray metallic	Symbol: Mo Number: 42 Crystal structure: bcc Electronic configuration: Kr 4d[5] 5s[1] magnetic ordering: paramagnetic atomic mass: 95.951 set: transitionmetal
Technetium shiny gray metal	Symbol: Tc Number: 43 Crystal structure: hcp Electronic configuration: Kr 4d[5] 5s[2] magnetic ordering: paramagnetic atomic mass: 98.9063 set: transitionmetal
Ruthenium silvery white metallic	Symbol: Ru Number: 44 Crystal structure: hcp Electronic configuration: Kr 4d[7] 5s[1] magnetic ordering: paramagnetic atomic mass: 101.072 set: transitionmetal
Rhodium silvery white metallic	Symbol: Rh Number: 45 Crystal structure: fcc Electronic configuration: Kr 4d[8] 5s[1] magnetic ordering: paramagnetic atomic mass: 102.905502 set: transitionmetal

Palladium silvery white	Symbol: Pd Number: 46 Crystal structure: fcc Electronic configuration: Kr 4d[10] magnetic ordering: paramagnetic atomic mass: 106.421 set: transitionmetal
Silver lustrous white metal	Symbol: Ag Number: 47 Crystal structure: fcc Electronic configuration: Kr 4d[10] 5s[1] magnetic ordering: diamagnetic atomic mass: 107.86822 set: transitionmetal
Cadmium silvery bluish-gray metallic	Symbol: Cd Number: 48 Crystal structure: hcp Electronic configuration: Kr 4d[10] 5s[2] magnetic ordering: diamagnetic atomic mass: 112.4144 set: transitionmetal
Indium silvery lustrous gray	Symbol: In Number: 49 Crystal structure: tetr Electronic configuration: Kr 4d[10] 5s[2] 5p[1] magnetic ordering: diamagnetic atomic mass: 114.8181 set: metal
Tin silvery-white (beta); gray (alpha)	Symbol: Sn Number: 50 Crystal structure: tetr Electronic configuration: Kr 4d[10] 5s[2] 5p[2] magnetic ordering: paramagnetic atomic mass: 118.7107 set: metal
Antimony silvery lustrous gray	Symbol: Sb Number: 51 Crystal structure: rho Electronic configuration: Kr 4d[10] 5s[2] 5p[3] magnetic ordering: diamagnetic atomic mass: 121.7601 set: metalloid

Tellurium
silvery lustrous gray (crystalline); brown-black powder (amorphous)

Symbol: Te
Number: 52
Crystal structure: hex
refractive index: 1.000991
magnetic ordering: diamagnetic
atomic mass: 127.603
Electronic configuration: Kr 4d[10] 5s[2] 5p[4]
set: metalloid

Iodine
lustrous metallic gray (solid); black/violet (liquid); violet (gas)

Symbol: I
Number: 53
Crystal structure: orth
Electronic configuration: Kr 4d[10] 5s[2] 5p[5]
magnetic ordering: diamagnetic
atomic mass: 126.904473
set: halogen

Xenon
colorless gas, exhibiting a blue glow when placed in an electric field

Symbol: Xe
Number: 54
Crystal structure: fcc
refractive index: 1.000702
magnetic ordering: diamagnetic
atomic mass: 131.2936
Electronic configuration: Kr 4d[10] 5s[2] 5p[6]
set: noblegas

Caesium
pale gold

Symbol: Cs
Number: 55
Crystal structure: bcc
Electronic configuration: Xe 6s[1]
magnetic ordering: paramagnetic
atomic mass: 132.905451966
set: alkalimetal

Barium
silvery gray; with a pale yellow tint

Symbol: Ba
Number: 56
Crystal structure: bcc
Electronic configuration: Xe 6s[2]
magnetic ordering: paramagnetic
atomic mass: 137.3277
set: alkalineearthmetal

Lanthanum
silvery white

Symbol: La
Number: 57
Crystal structure: dhcp
Electronic configuration: Xe 5d[1] 6s[2]
magnetic ordering: paramagnetic
atomic mass: 138.905477
set: lanthanoide

Cerium silvery white	Symbol: Ce Number: 58 Crystal structure: dhcp Electronic configuration: Xe 4f[1] 5d[1] 6s[2] magnetic ordering: paramagnetic atomic mass: 140.1161 set: lanthanoide
Praseodymium grayish white	Symbol: Pr Number: 59 Crystal structure: dhcp Electronic configuration: Xe 4f[3] 6s[2] magnetic ordering: paramagnetic atomic mass: 140.907662 set: lanthanoide
Neodymium silvery white	Symbol: Nd Number: 60 Crystal structure: dhcp Electronic configuration: Xe 4f[4] 6s[2] magnetic ordering: paramagnetic atomic mass: 144.2423 set: lanthanoide
Promethium metallic	Symbol: Pm Number: 61 Crystal structure: dhcp Electronic configuration: Xe 4f[5] 6s[2] magnetic ordering: paramagnetic atomic mass: 146.9151 set: lanthanoide
Samarium silvery white	Symbol: Sm Number: 62 Crystal structure: rho Electronic configuration: Xe 4f[6] 6s[2] magnetic ordering: paramagnetic atomic mass: 150.362 set: lanthanoide
Europium silvery white, with a pale yellow tint; but rarely seen without oxide discoloration	Symbol: Eu Number: 63 Crystal structure: bcc Electronic configuration: Xe 4f[7] 6s[2] magnetic ordering: paramagnetic atomic mass: 151.9641 set: lanthanoide

Gadolinium silvery white	Symbol: Gd Number: 64 Crystal structure: hcp Electronic configuration: Xe 4f[7] 5d[1] 6s[2] magnetic ordering: ferromagnetic atomic mass: 157.253 set: lanthanoide
Terbium silvery white	Symbol: Tb Number: 65 Crystal structure: hcp Electronic configuration: Xe 4f[9] 6s[2] magnetic ordering: paramagnetic atomic mass: 158.925352 set: lanthanoide
Dysprosium silbrig weiß	Symbol: Dy Number: 66 Crystal structure: hcp Electronic configuration: Xe 4f[10] 6s[2] magnetic ordering: paramagnetic atomic mass: 162.5001 set: lanthanoide
Holmium silvery white	Symbol: Ho Number: 67 Crystal structure: hcp Electronic configuration: Xe 4f[11] 6s[2] magnetic ordering: paramagnetic atomic mass: 164.930332 set: lanthanoide
Erbium silvery white	Symbol: Er Number: 68 Crystal structure: hcp Electronic configuration: Xe 4f[12] 6s[2] magnetic ordering: paramagnetic atomic mass: 167.2593 set: lanthanoide
Thulium silvery gray	Symbol: Tm Number: 69 Crystal structure: hcp Electronic configuration: Xe 4f[13] 6s[2] magnetic ordering: paramagnetic atomic mass: 168.934222 set: lanthanoide

Ytterbium silvery white; with a pale yellow tint	Symbol: Yb Number: 70 Crystal structure: fcc Electronic configuration: Xe 4f[14] 6s[2] magnetic ordering: paramagnetic atomic mass: 173.0451 set: lanthanoide
Lutetium silvery white	Symbol: Lu Number: 71 Crystal structure: hcp Electronic configuration: Xe 4f[14] 5d[1] 6s[2] magnetic ordering: paramagnetic atomic mass: 174.96681 set: lanthanoide
Hafnium steel gray	Symbol: Hf Number: 72 Crystal structure: hcp Electronic configuration: Xe 4f[14] 5d[2] 6s[2] magnetic ordering: paramagnetic atomic mass: 178.492 set: transitionmetal
Tantalum gray blue	Symbol: Ta Number: 73 Crystal structure: bcc Electronic configuration: Xe 4f[14] 5d[3] 6s[2] magnetic ordering: paramagnetic atomic mass: 180.947882 set: transitionmetal
Tungsten grayish white, lustrous	Symbol: W Number: 74 Crystal structure: bcc Electronic configuration: Xe 4f[14] 5d[4] 6s[2] magnetic ordering: paramagnetic atomic mass: 183.841 set: transitionmetal
Rhenium silvery-grayish	Symbol: Re Number: 75 Crystal structure: hcp Electronic configuration: Xe 4f[14] 5d[5] 6s[2] magnetic ordering: paramagnetic atomic mass: 186.2071 set: transitionmetal

Osmium silvery, blue cast	Symbol: Os Number: 76 Crystal structure: hcp Electronic configuration: Xe 4f[14] 5d[6] 6s[2] magnetic ordering: paramagnetic atomic mass: 190.233 set: transitionmetal
Iridium silvery white	Symbol: Ir Number: 77 Crystal structure: fcc Electronic configuration: Xe 4f[14] 5d[7] 6s[2] magnetic ordering: paramagnetic atomic mass: 192.2173 set: transitionmetal
Platinum silvery white	Symbol: Pt Number: 78 Crystal structure: fcc Electronic configuration: Xe 4f[14] 5d[9] 6s[1] magnetic ordering: paramagnetic atomic mass: 195.0849 set: transitionmetal
Gold metallic yellow	Symbol: Au Number: 79 Crystal structure: fcc Electronic configuration: Xe 4f[14] 5d[10] 6s[1] magnetic ordering: diamagnetic atomic mass: 196.9665695 set: transitionmetal
Mercury shiny, silvery liquid	Symbol: Hg Number: 80 Crystal structure: rho refractive index: 1.000933 magnetic ordering: diamagnetic atomic mass: 200.5923 Electronic configuration: Xe 4f[14] 5d[10] 6s[2] set: transitionmetal
Thallium silvery white	Symbol: Tl Number: 81 Crystal structure: hcp Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[1] magnetic ordering: diamagnetic atomic mass: 204.38204 set: metal

Lead metallic gray	Symbol: Pb Number: 82 Crystal structure: fcc Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[2] magnetic ordering: diamagnetic atomic mass: 207.21 set: metal
Bismuth lustrous brownish silver	Symbol: Bi Number: 83 Crystal structure: rho Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[3] magnetic ordering: diamagnetic atomic mass: 208.980401 set: metal
Polonium silvery	Symbol: Po Number: 84 Crystal structure: sc Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[4] magnetic ordering: nonmagnetic atomic mass: 209.98 set: metal
Astatine unknown, probably metallic	Symbol: At Number: 85 set: halogen Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[5] Crystal structure: fcc atomic mass: 209.9871
Radon colorless gas	Symbol: Rn Number: 86 Crystal structure: fcc Electronic configuration: Xe 4f[14] 5d[10] 6s[2] 6p[6] magnetic ordering: nonmagnetic atomic mass: 222 set: noblegas
Francium	Symbol: Fr Number: 87 Crystal structure: bcc Electronic configuration: Rn 7s[1] magnetic ordering: paramagnetic atomic mass: 223.0197 set: alkalimetal

Radium silvery white metallic	Symbol: Ra Number: 88 Crystal structure: bcc Electronic configuration: Rn 7s[2] magnetic ordering: nonmagnetic atomic mass: 226.0254 set: alkalineearthmetal
Actinium silvery-white, glowing with an eerie blue light; sometimes with a golden cast	Symbol: Ac Number: 89 set: actinoide Electronic configuration: Rn 6d[1] 7s[2] Crystal structure: fcc atomic mass: 227.0278
Thorium silvery	Symbol: Th Number: 90 Crystal structure: fcc Electronic configuration: Rn 6d[2] 7s[2] magnetic ordering: paramagnetic atomic mass: 232.03774 set: actinoide
Protactinium bright, silvery metallic luster	Symbol: Pa Number: 91 Crystal structure: tetr Electronic configuration: Rn 5f[2] 6d[1] 7s[2] magnetic ordering: paramagnetic atomic mass: 231.035882 set: actinoide
Uranium silvery gray metallic; corrodes to a spalling black oxide coat in air	Symbol: U Number: 92 Crystal structure: orth Electronic configuration: Rn 5f[3] 6d[1] 7s[2] magnetic ordering: paramagnetic atomic mass: 238.028913 set: actinoide
Neptunium silvery metallic	Symbol: Np Number: 93 Crystal structure: orth Electronic configuration: Rn 5f[4] 6d[1] 7s[2] magnetic ordering: paramagnetic atomic mass: 237.0482 set: actinoide

Plutonium
silvery white, tarnishing to dark gray in air

Symbol: Pu
Number: 94
Crystal structure: mon
Electronic configuration: Rn 5f[6] 7s[2]
magnetic ordering: paramagnetic
atomic mass: 244.0642
set: actinoide

Americium
silvery white

Symbol: Am
Number: 95
Crystal structure: dhcp
Electronic configuration: Rn 5f[7] 7s[2]
magnetic ordering: paramagnetic
atomic mass: 243.061375
set: actinoide

Curium
silvery metallic, glows purple in the dark

Symbol: Cm
Number: 96
Crystal structure: dhcp
Electronic configuration: Rn 5f[7] 6d[1] 7s[2]
magnetic ordering: antiferromagnetic
atomic mass: 247.0703
set: actinoide

Berkelium
silvery

Symbol: Bk
Number: 97
Crystal structure: dhcp
Electronic configuration: Rn 5f[9] 7s[2]
magnetic ordering: paramagnetic
atomic mass: 247
set: actinoide

Californium
silvery

Symbol: Cf
Number: 98
set: actinoide
Electronic configuration: Rn 5f[10] 7s[2]
Crystal structure: dhcp
atomic mass: 251

Einsteinium
silvery; glows blue in the dark

Symbol: Es
Number: 99
Crystal structure: fcc
Electronic configuration: Rn 5f[11] 7s[2]
magnetic ordering: paramagnetic
atomic mass: 252
set: actinoide

Fermium

Symbol: Fm
Number: 100
set: actinoide
Electronic configuration: Rn 5f[12] 7s[2]
Crystal structure: fcc
atomic mass: 257.0951

Mendelevium	Symbol: Md Number: 101 set: actinoide Electronic configuration: Rn 5f[13] 7s[2] Crystal structure: fcc atomic mass: 258
Nobelium	Symbol: No Number: 102 set: actinoide Electronic configuration: Rn 5f[14] 7s[2] Crystal structure: fcc atomic mass: 259
Lawrencium	Symbol: Lr Number: 103 set: actinoide Electronic configuration: Rn 5f[14] 7s[2] 7p[1] Crystal structure: hcp atomic mass: 266
Rutherfordium	Symbol: Rf Number: 104 set: transitionmetal Electronic configuration: Rn 5f[14] 6d[2] 7s[2] Crystal structure: hcp atomic mass: 261.1087
Dubnium	Symbol: Db Number: 105 set: transitionmetal Electronic configuration: Rn 5f[14] 6d[3] 7s[2] Crystal structure: bcc atomic mass: 262.1138
Seaborgium	Symbol: Sg Number: 106 set: transitionmetal Electronic configuration: Rn 5f[14] 6d[4] 7s[2] Crystal structure: bcc atomic mass: 263.1182
Bohrium	Symbol: Bh Number: 107 set: transitionmetal Electronic configuration: Rn 5f[14] 6d[5] 7s[2] Crystal structure: hcp atomic mass: 262.1229

Hassium	Symbol: Hs Number: 108 set: transitionmetal Electronic configuration: Rn 5f[14] 6d[6] 7s[2] Crystal structure: hcp atomic mass: 265.269
Meitnerium	Symbol: Mt Number: 109 Crystal structure: fcc Electronic configuration: Rn 5f[14] 6d[7] 7s[2] magnetic ordering: paramagnetic atomic mass: 268 set: unknown
Darmstadtium	Symbol: Ds Number: 110 set: unknown Electronic configuration: Rn 5f[14] 6d[8] 7s[2] Crystal structure: bcc atomic mass: 281
Roentgenium	Symbol: Rg Number: 111 set: unknown Electronic configuration: Rn 5f[14] 6d[9] 7s[2] Crystal structure: bcc atomic mass: 280
Copernicium	Symbol: Cn Number: 112 set: unknown Electronic configuration: Rn 5f[14] 6d[10] 7s[2] Crystal structure: bcc atomic mass: 277
Nihonium	Symbol: Nh Number: 113 set: unknown Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[1] Crystal structure: hcp atomic mass: 287
Flerovium	Symbol: Fl Number: 114 set: unknown Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[2] Crystal structure: fcc atomic mass: 289

Moscovium	Symbol: Mc Number: 115 set: unknown Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[3] atomic mass: 288
Livermorium	Symbol: Lv Number: 116 set: unknown Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[4] atomic mass: 293
Tennessine semimetallic (predicted)	Symbol: Ts Number: 117 set: unknown Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[5] atomic mass: 292
Oganesson metallic (predicted)	Symbol: Og Number: 118 set: unknown Electronic configuration: Rn 5f[14] 6d[10] 7s[2] 7p[6] Crystal structure: fcc atomic mass: 294