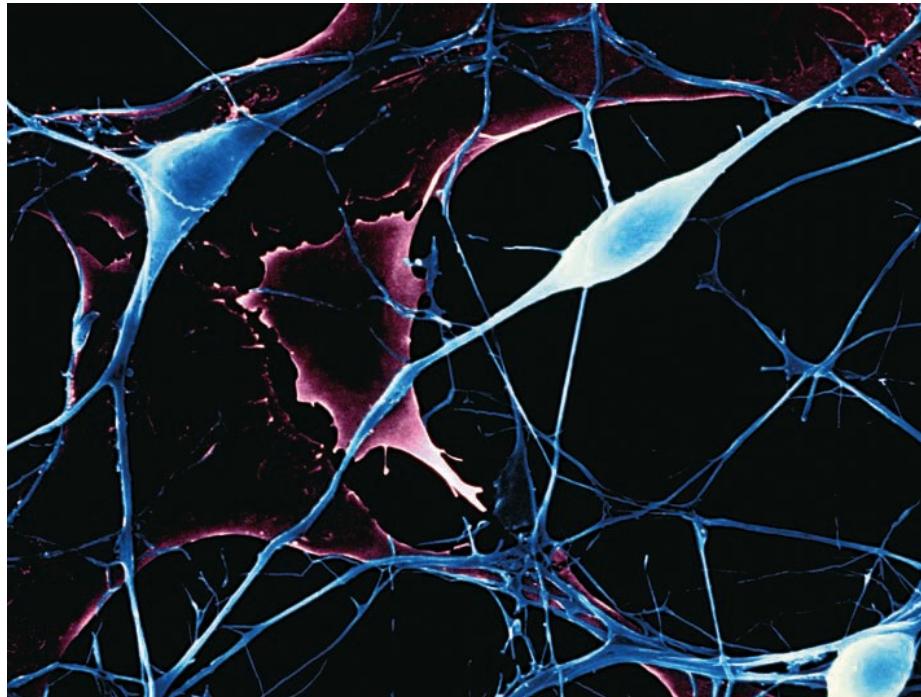


PK Chemie

Elektronen in Atomen

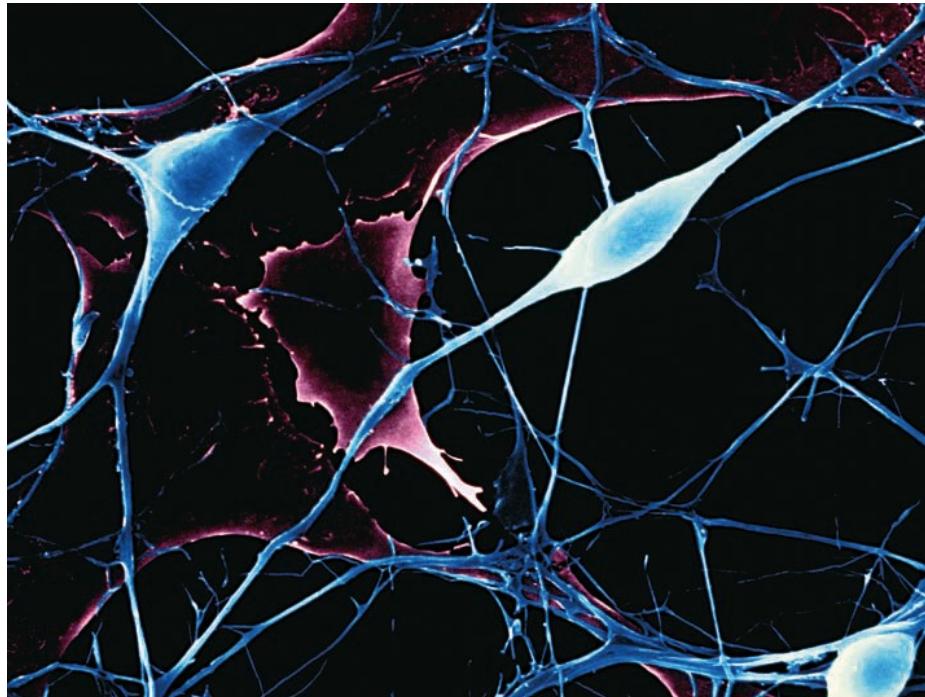
Chemische Verbindungen



INHALTE

- 1 Elektromagnetische Strahlung
- 2 Atomspektren
- 3 Quantentheorie
- 4 Das Bohr-Atom
- 5 Zwei Ideen die zur Quantenmechanik führten
- 6 Quantenzahlen
- 7 Orbitale des Wasserstoff-Atoms

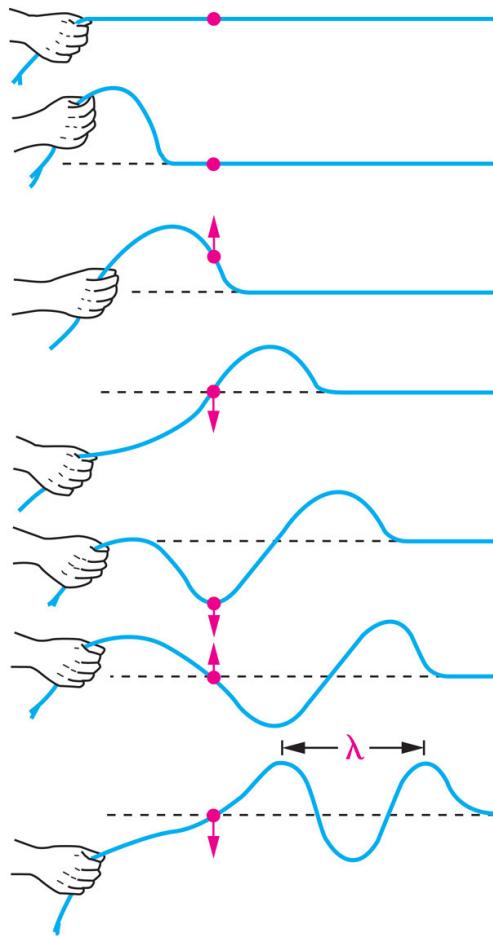
Chemical Compounds



INHALTE

- 8 Elektron-Spin
- 9 Atome mit mehreren Elektronen
- 10 Elektronenkonfigurationen
- 11 Elektronenkonfigurationen und das PSE

Elektromagnetische Strahlung

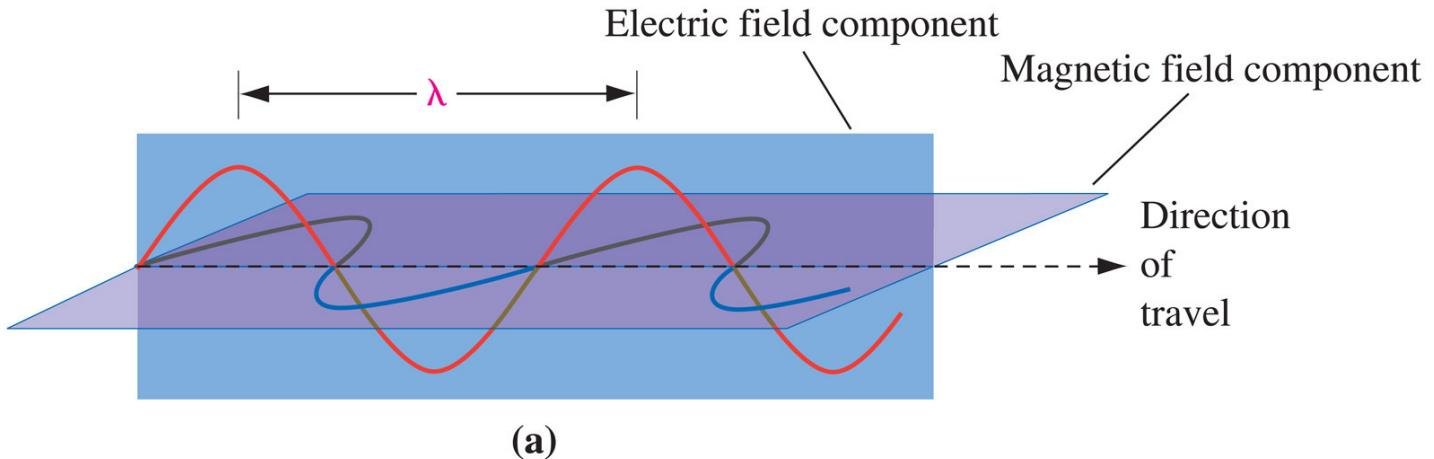


Elektrische und magnetische Felder bewegen sich wie Wellen durch den Raum.
Eine Welle übermittelt Energie.



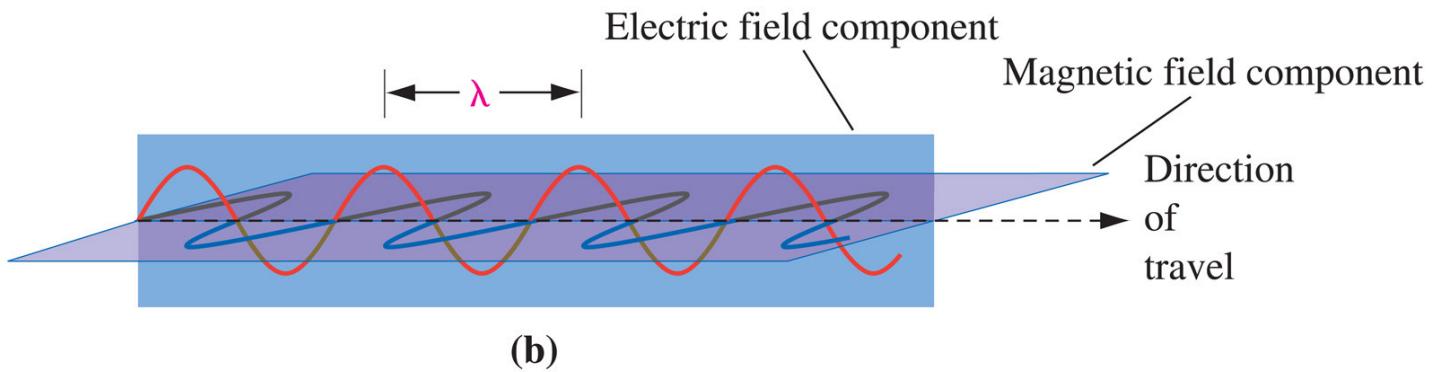
Wellenbewegung eines Seiles

Kleines ν



(a)

Grosses ν



(b)



Elektromagnetische Wellen

Frequenz, Wellenlänge und Geschwindigkeit der elektromagnetischen Strahlung

Frequenz (ν) in Hertz—Hz oder s^{-1} .

Wellenlänge (λ) in Meter—m.

cm

(10^{-2} m)

μm

(10^{-6} m)

nm

(10^{-9} m)

\AA

(10^{-10} m)

p

(10^{-12} m)

Licht-Geschwindigkeit: (c)— $2.997925 \times 10^8 \text{ m s}^{-1}$.

$$c = \lambda \nu$$

$$\lambda = c / \nu$$

$$\nu = c / \lambda$$

Frequency, s^{-1}

10^{24} 10^{22} 10^{20} 10^{18} 10^{16} 10^{14} 10^{12} 10^{10} 10^8 10^6 10^4

γ rays

Radio

X rays

Micro-
wave

Ultra-
violet

Infra-
red

10^{-16} 10^{-14} 10^{-12} 10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2} 10^0 10^2 10^4

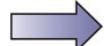
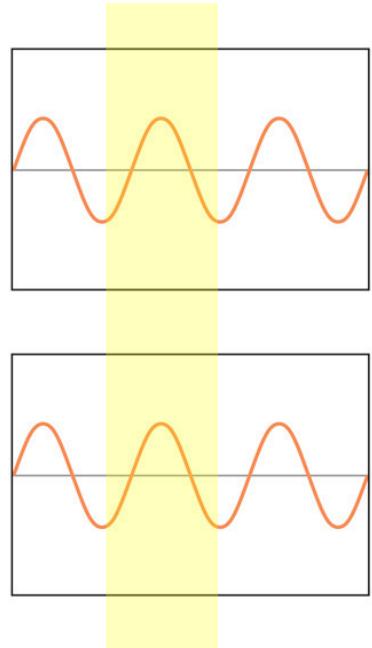
Wavelength, m

Visible

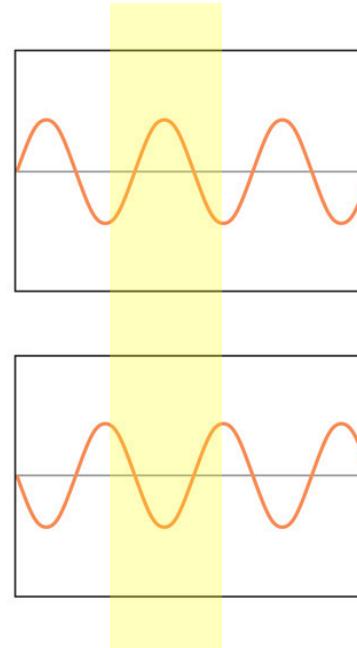
$\lambda = 390$ 450 500 550 600 650 700 760 nm



Elektromagnetisches Spektrum



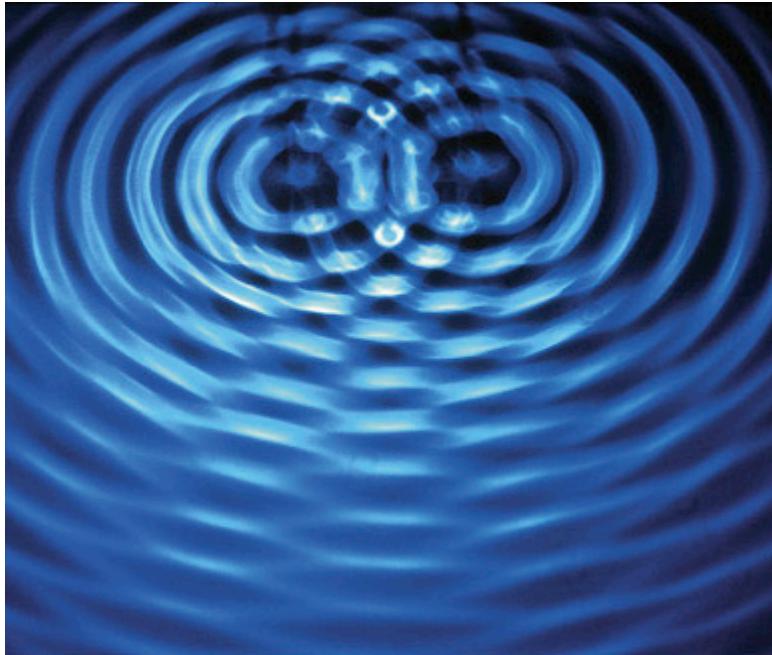
(a)



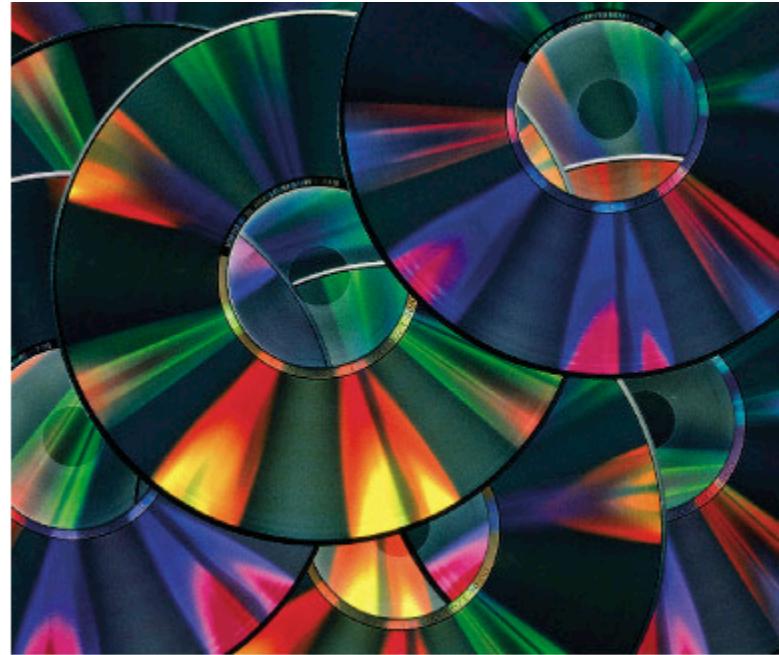
(b)



Interferenz zweier überlappender Wellen



(a)



(b)



Interferenz-Beispiele

Schreibtischlampe



s

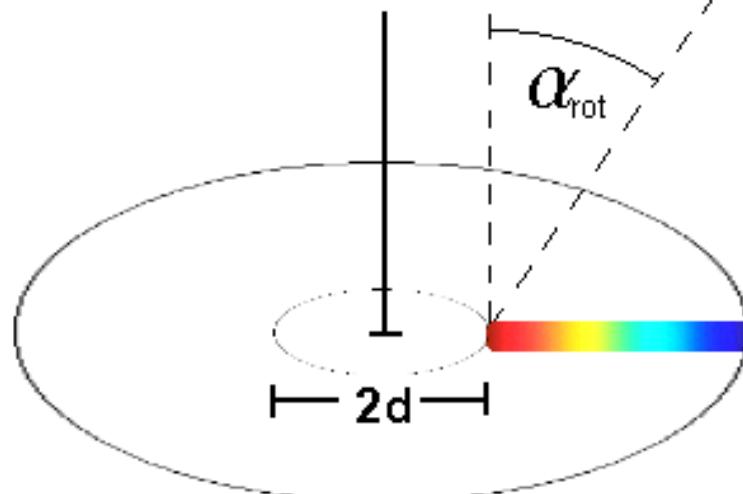


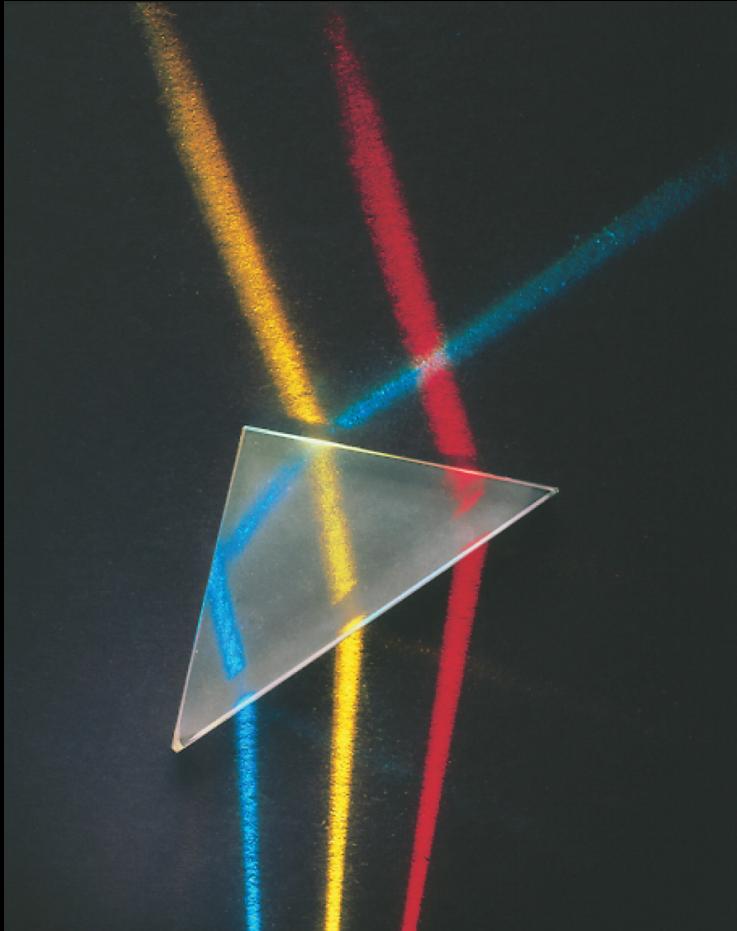
Augenposition

Höhe h

α_{rot}

— 2d —

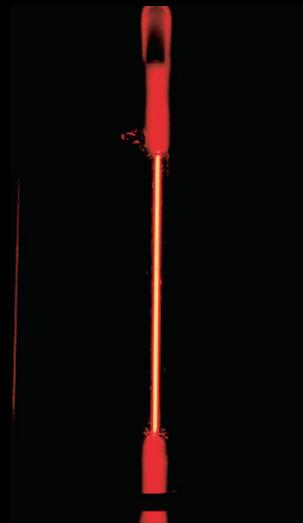




Licht-Brechung



(a)



(b)



(c)



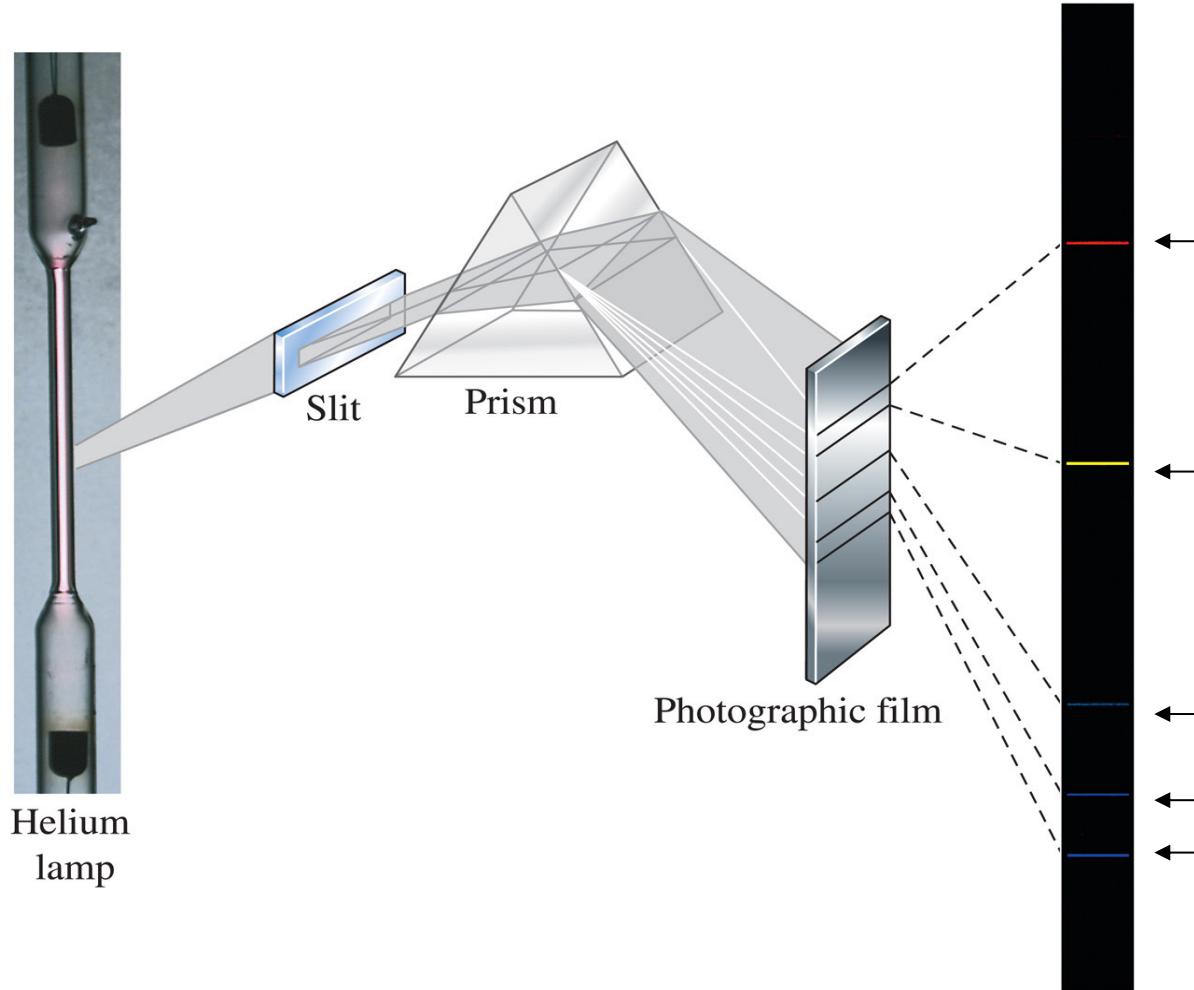
(d)



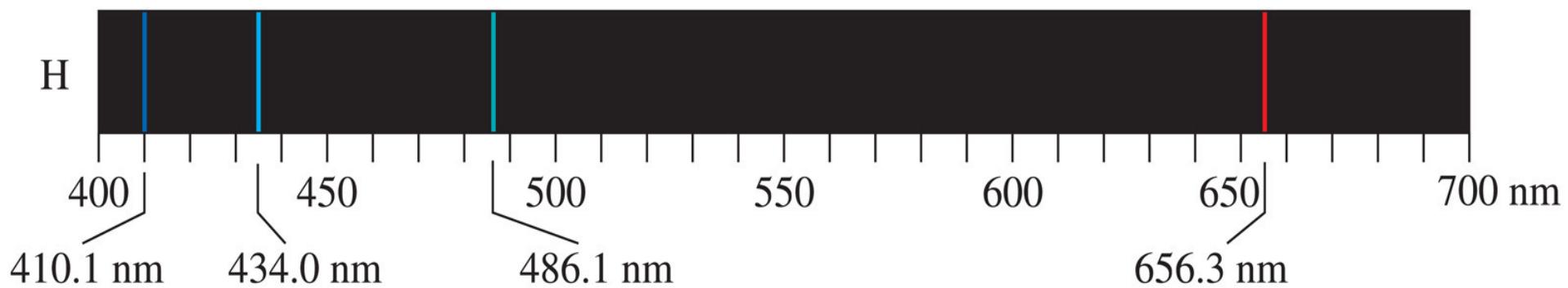
(e)



Quellen für Lichtemission

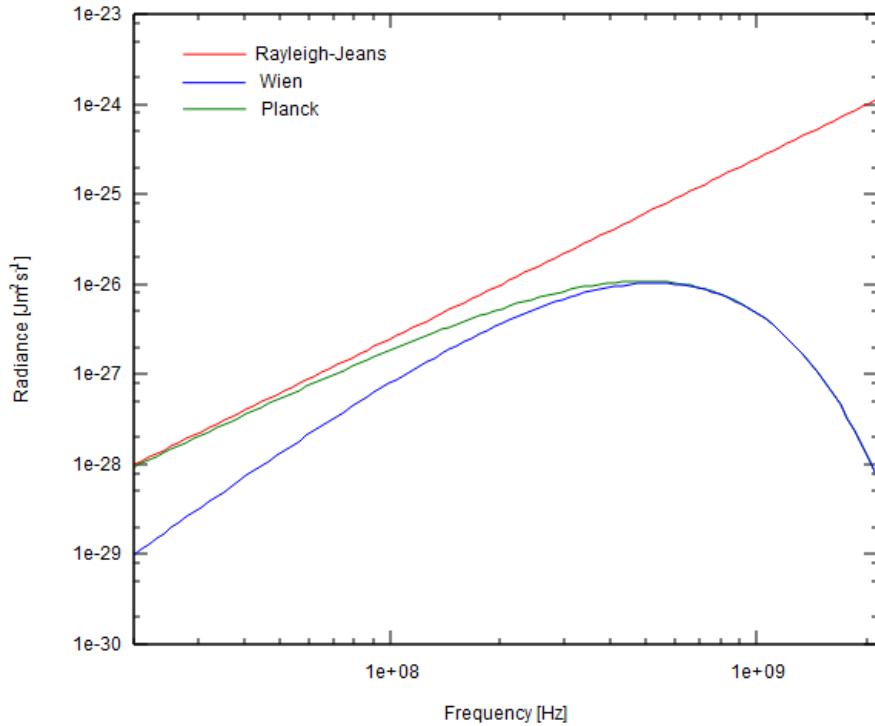


Linienspektrum von Helium

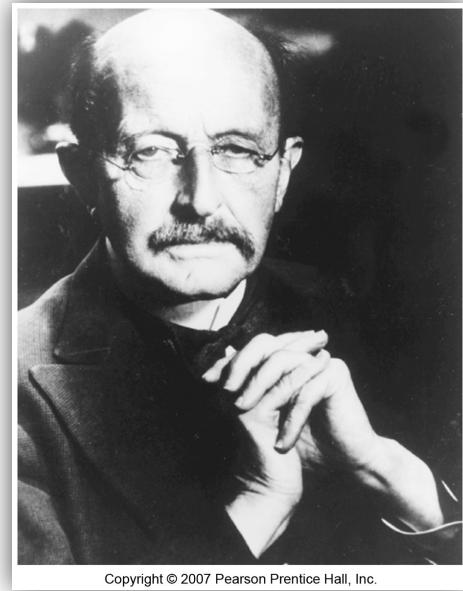


Balmer-Serie für Wasserstoff-Atome - Linienspektrum

Quantentheorie



Strahlungsspektrum eines erhitzten Gegenstandes



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Max Planck, 1900

*Energie ist wie Materie
diskontinuierlich*

$$E = h\nu$$



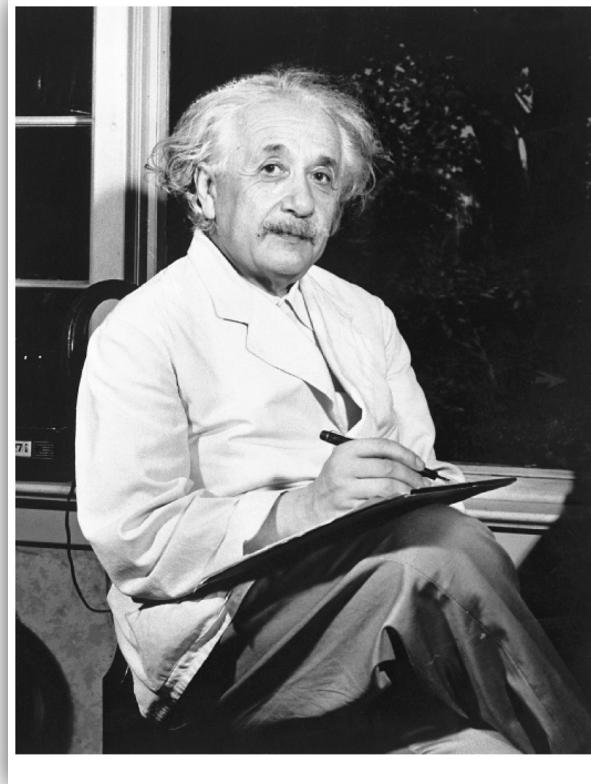
▲ Lichtemission von geschmolzenem Eisen

Der Photoelektrische Effekt

Heinrich Hertz, 1888

Licht, das auf eine metallische Oberfläche trifft, führt zur Freisetzung von Elektronen.

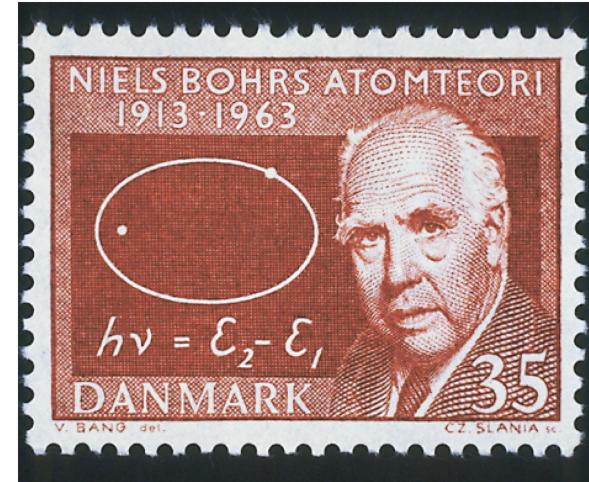
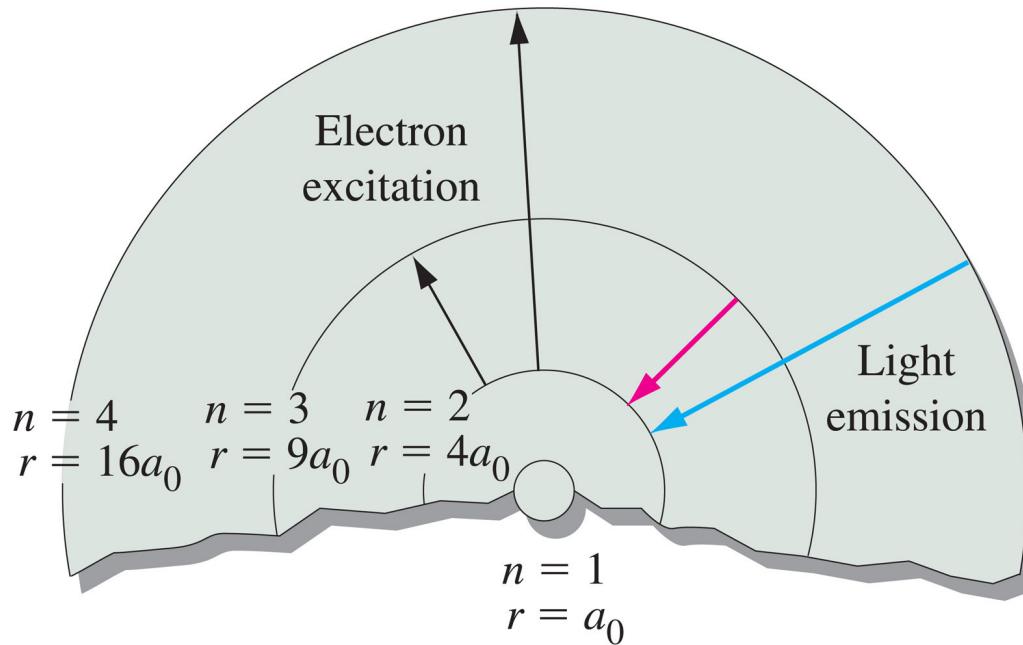
$$\nu > \nu_0$$



Albert Einstein 1905

Das Bohr-Atommodell

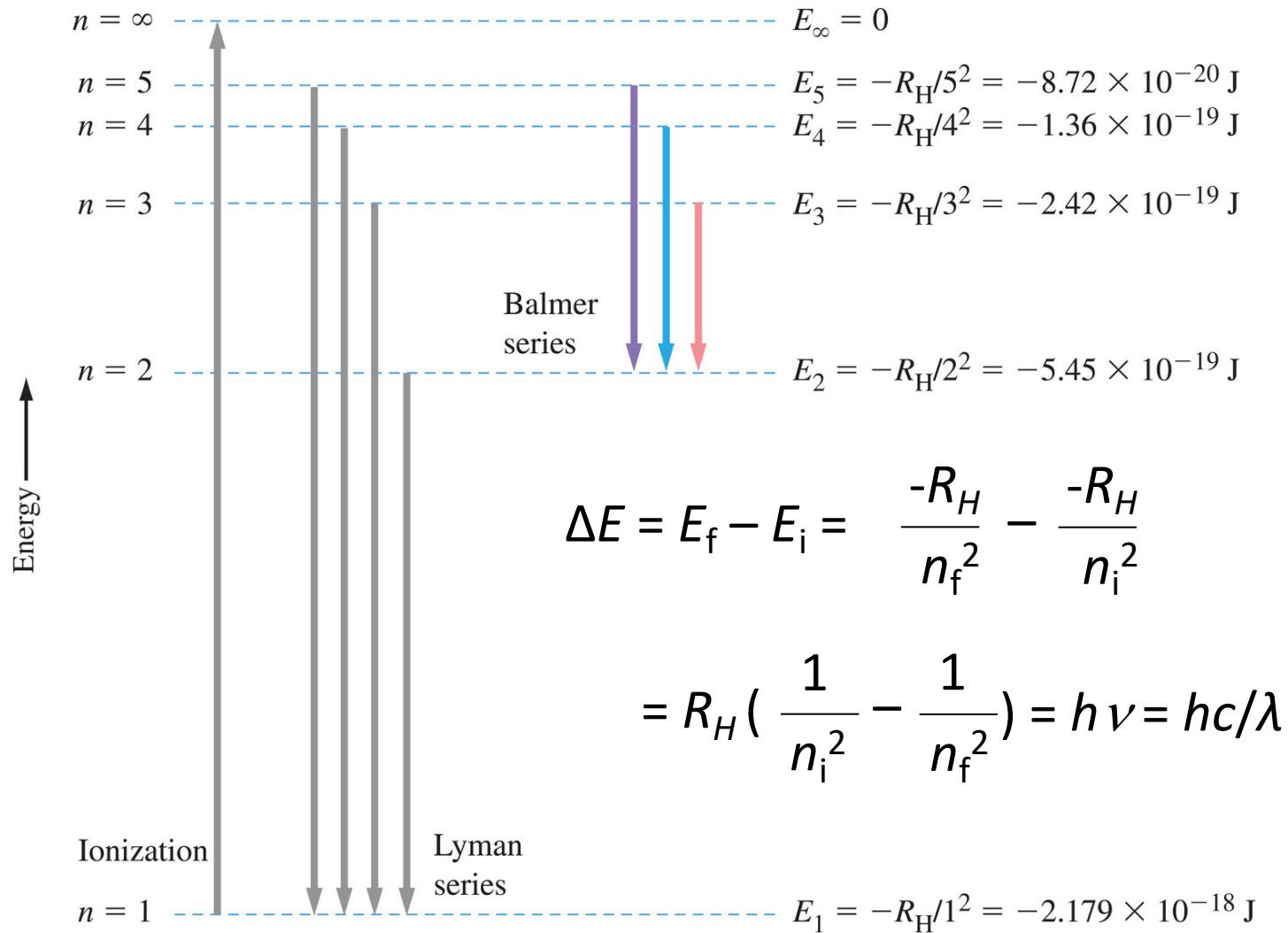
$$E = -\frac{R_H}{n^2}$$



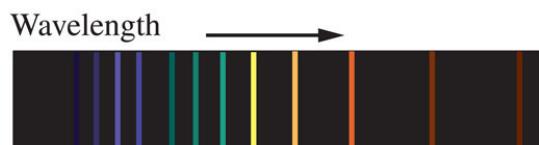
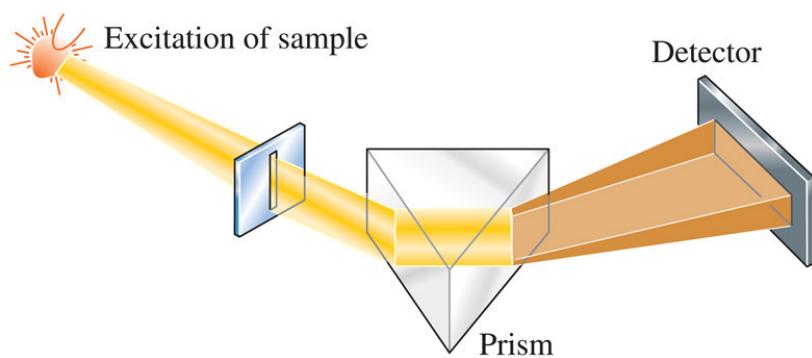
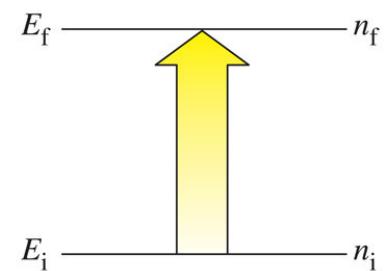
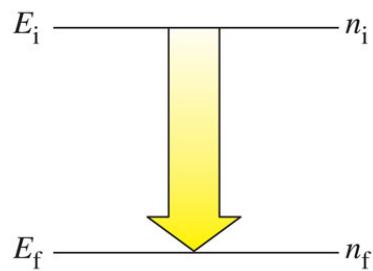
$$R_H = 2.179 \times 10^{-18} \text{ J}$$



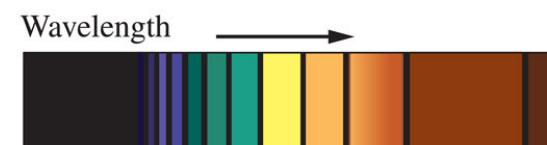
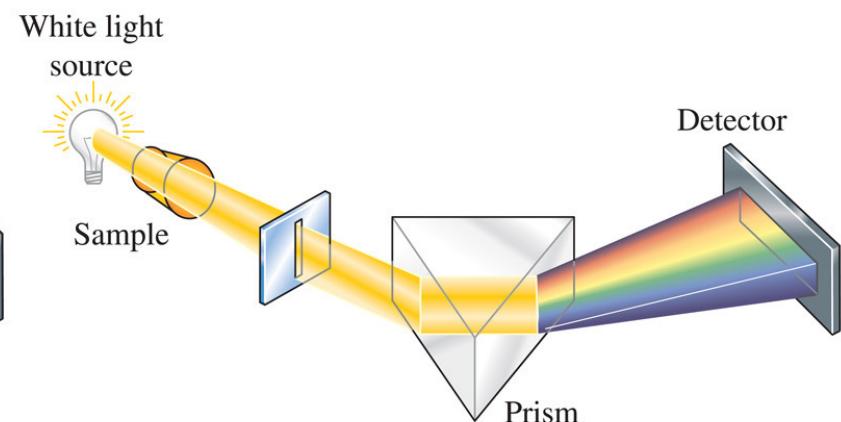
Bohr-Modell des Wasserstoff-Atoms



Energie-Diagramm für das Wasserstoff-Atom



Emission



Absorption



Emissions- und Absorptions-Spektrum

Zwei Ideen die zur Quantenmechanik führten

Wellen-Teilchen-Dualismus

Einstein schlug vor, dass Teilchen-Eigenschaften den photoelektrischen Effekt erklären könnten.

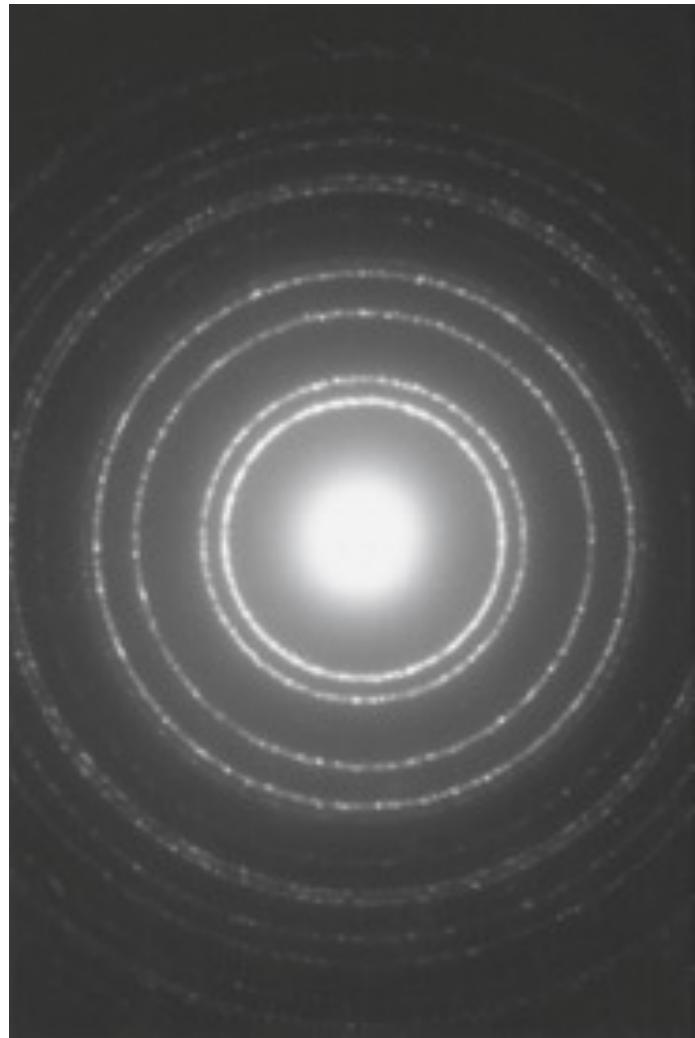
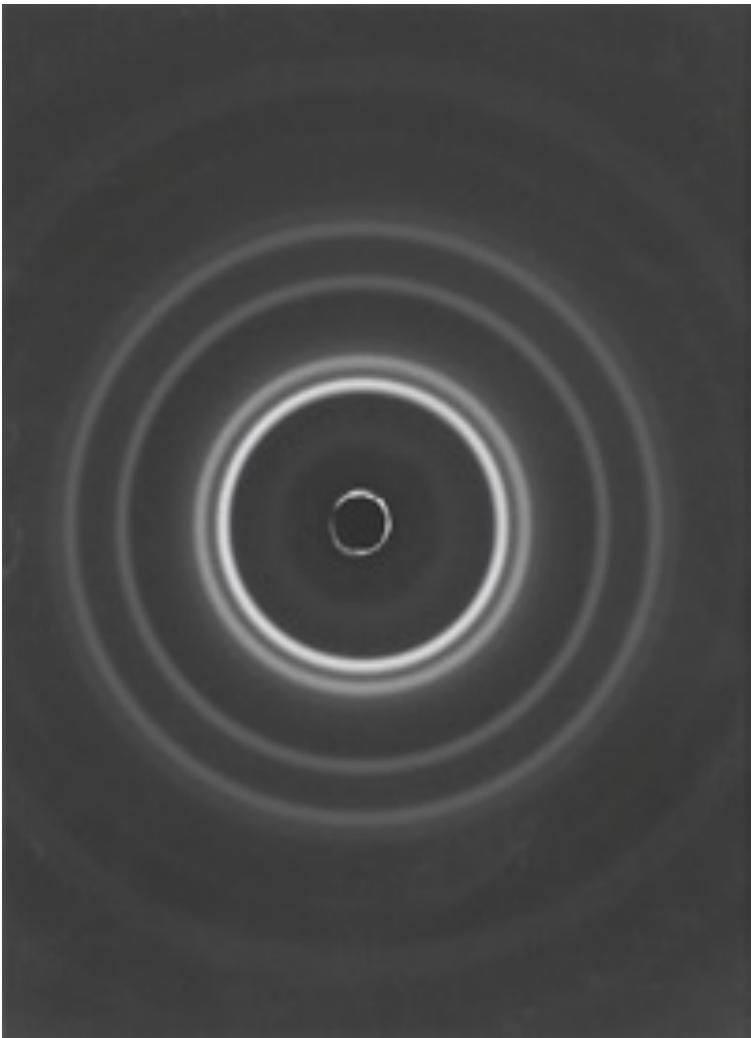
Beugungsmuster deuten auf wellenähnlichen Charakter von Photonen hin.

deBroglie, 1924

Kleine Teilchen können wellenähnliche Eigenschaften zeigen.

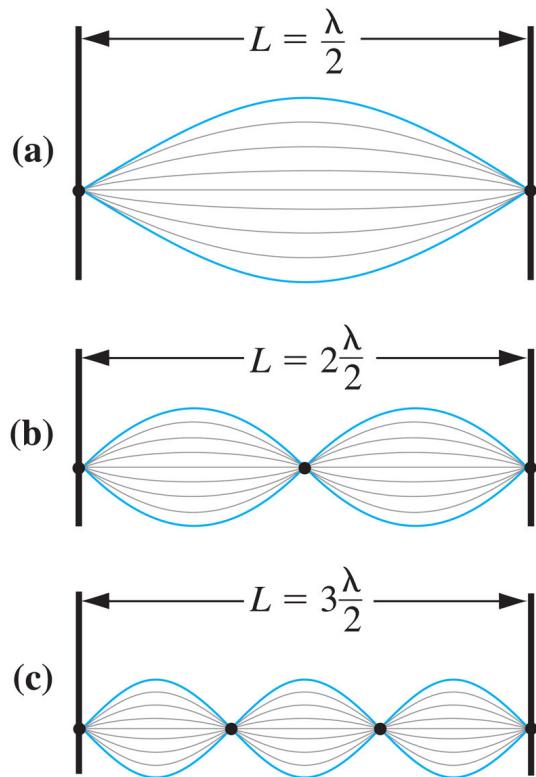


Louis de Broglie
Nobelpreis 1918



Welleneigenschaften von Elektronen experimentell

Wellenmechanik



Stehende Wellen

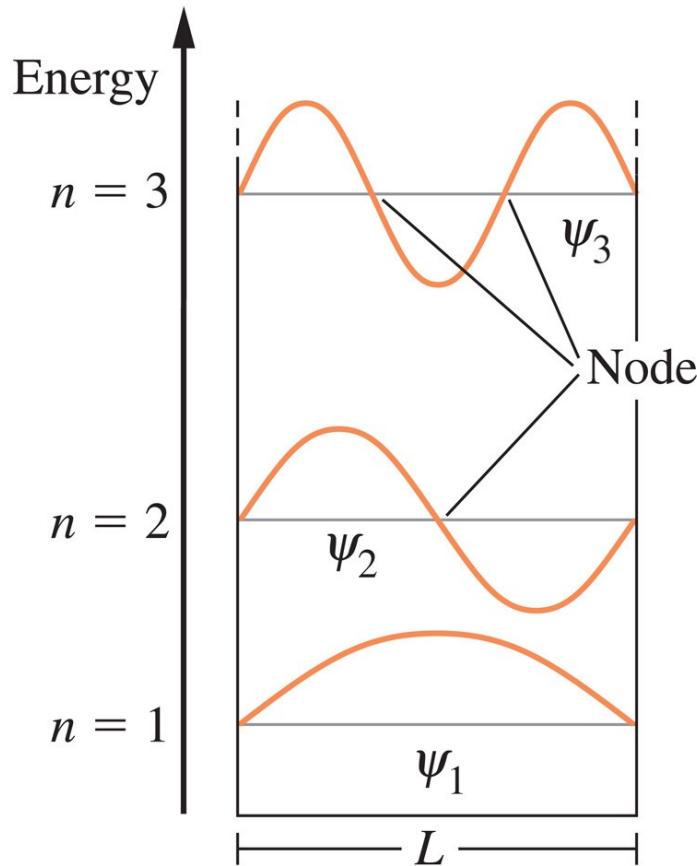
Knoten werden nicht verschoben.

$$\lambda = \frac{2L}{n}, n = 1, 2, 3\dots$$



Stehende Wellen

Teilchen in einer Box: Stehende Wellen, Quantenteilchen und Wellenfunktionen

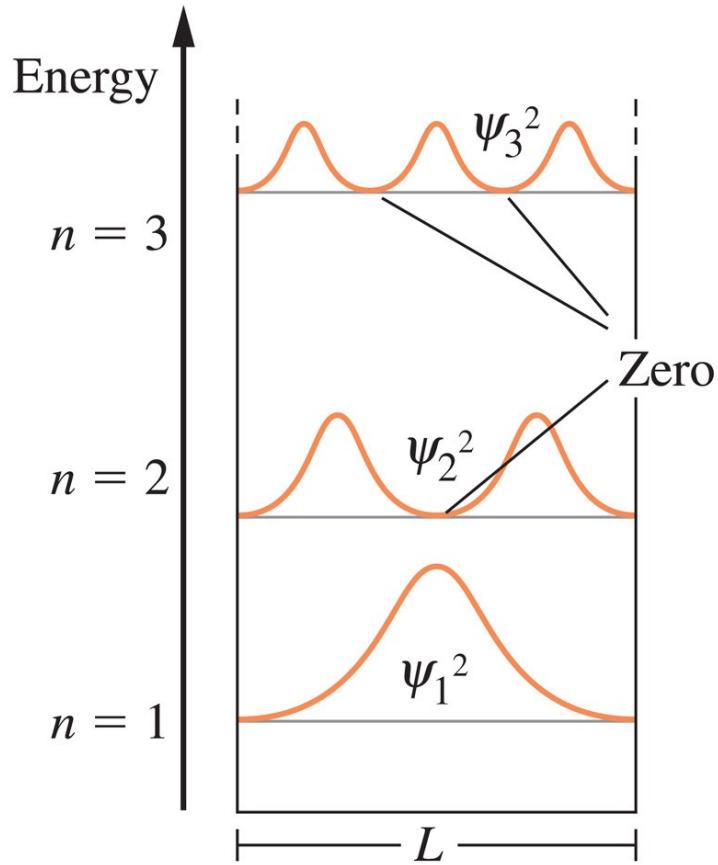


ψ , psi, die Wellenfunktion.
Teilchen in einer Box.

$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right)$$



Stehende Wellen eines Teilchens in einer Box.



$$\psi_n^2(x) = \frac{2}{L} \sin^2\left(\frac{n\pi}{L}x\right)$$



Wahrscheinlichkeiten

Quantenzahlen und Elektronenzahl

Hauptquantenzahl, $n = 1, 2, 3\dots$

Nebenquantenzahl,

$\ell = 0, s$

$\ell = 1, p$

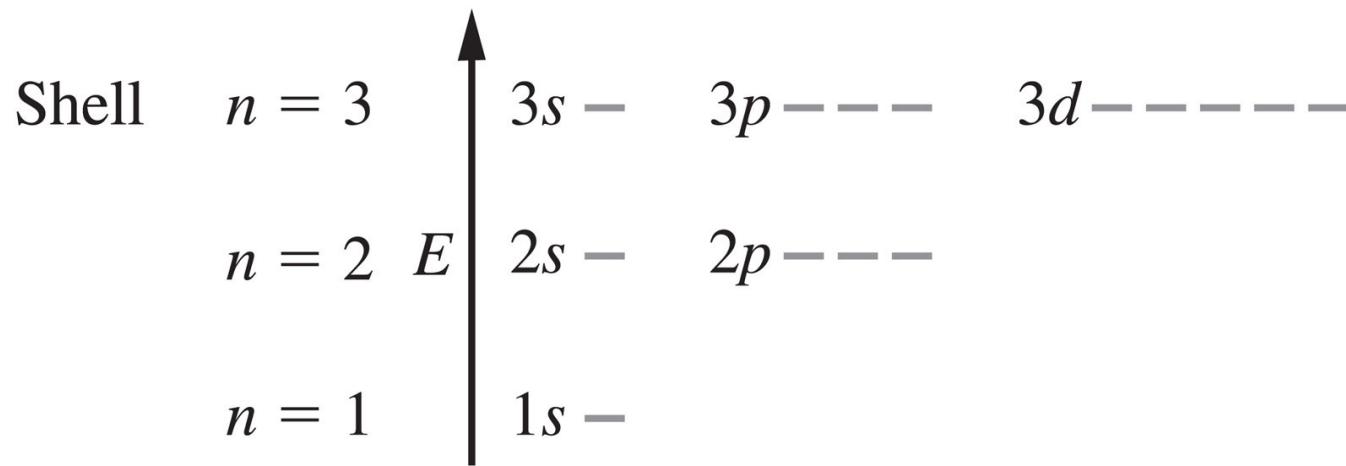
$\ell = 2, d$

$\ell = 3, f$

Magnetquantenzahl,

$m_l = -3, -2, -1, 0, 1, 2, 3$

Haupt- und Unterenergieniveaus



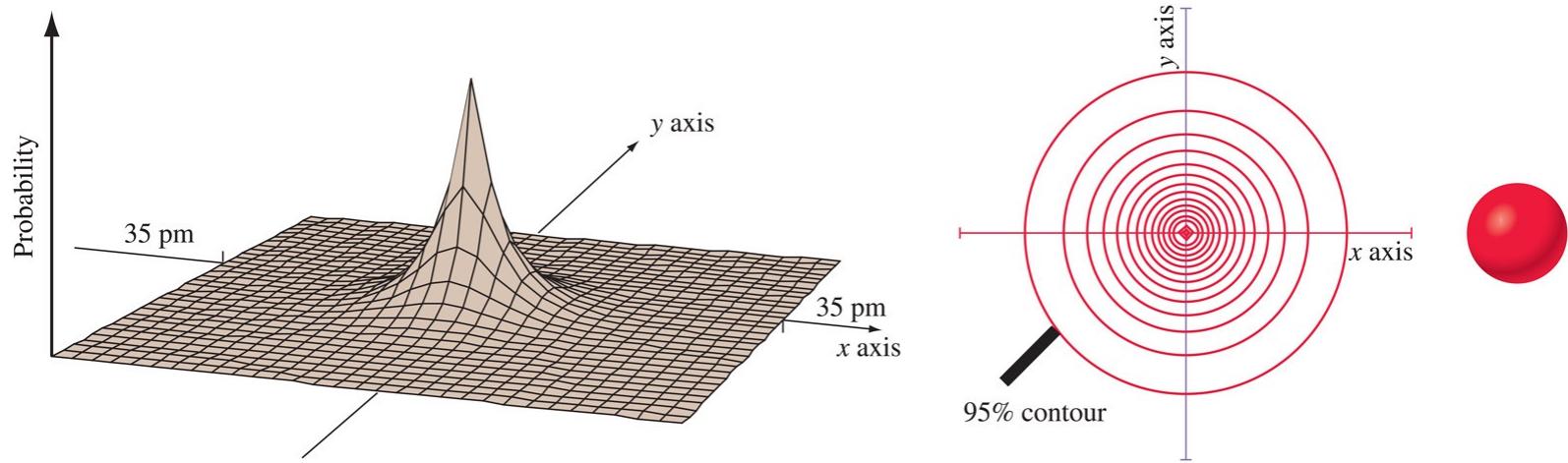
Subshell $\ell = 0 \quad \ell = 1 \quad \ell = 2$

Each subshell is made
up of $(2\ell + 1)$ orbitals.



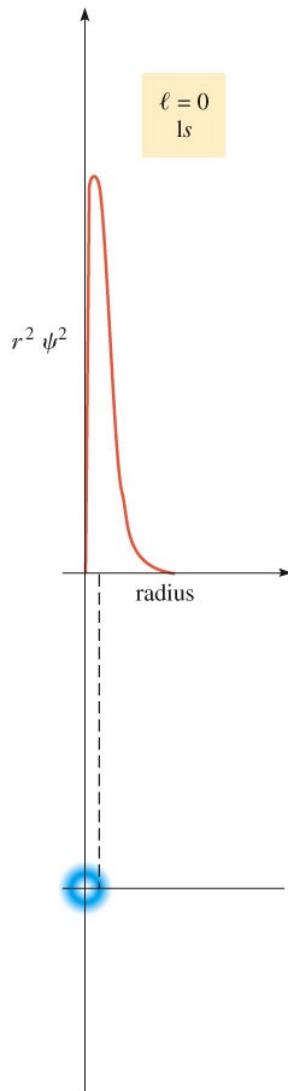
Schalen und Unterschalen eines Wasserstoff-Atoms

s Orbitale



3 Repräsentation für die Elektronen-Wahrscheinlichkeits-Dichten für das 1s-Orbital

s Orbitale



1s, 2s und 3s mit Querschnitten

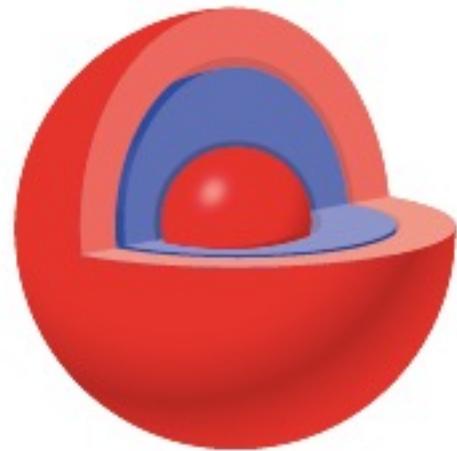
2s Orbitale



$1s$



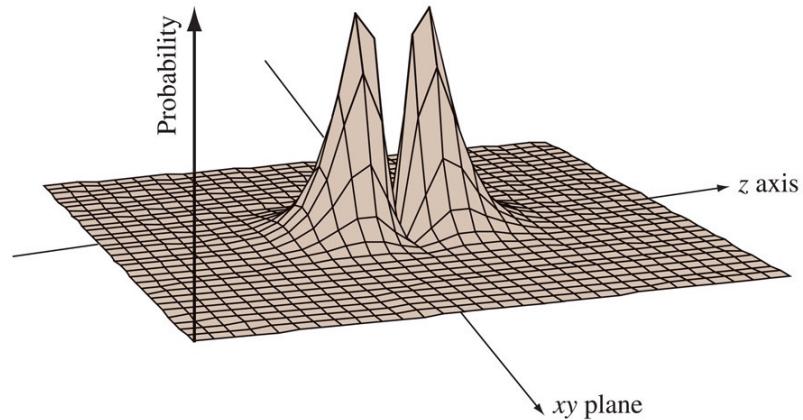
$2s$



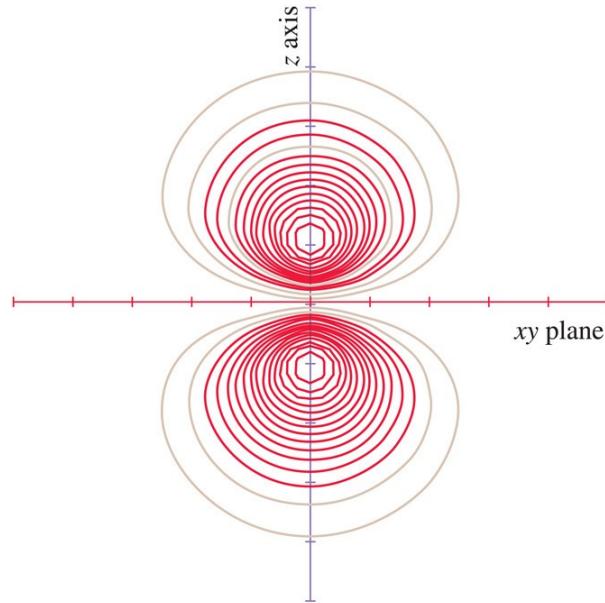
$3s$



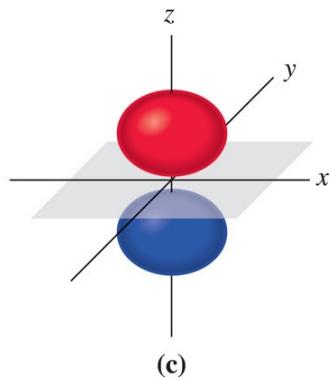
95% Elektronenwahrscheinlichkeitsdichten für 1s, 2s und 3s Orbitale



(a)

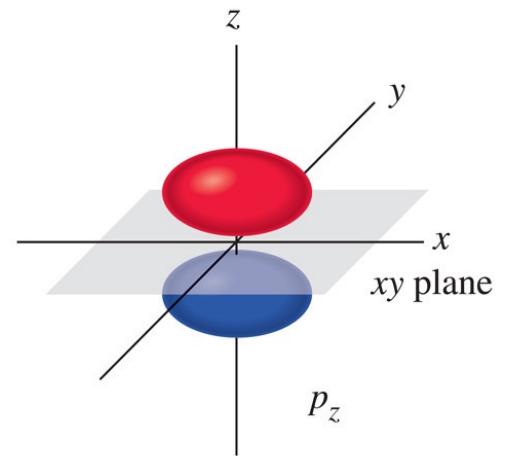
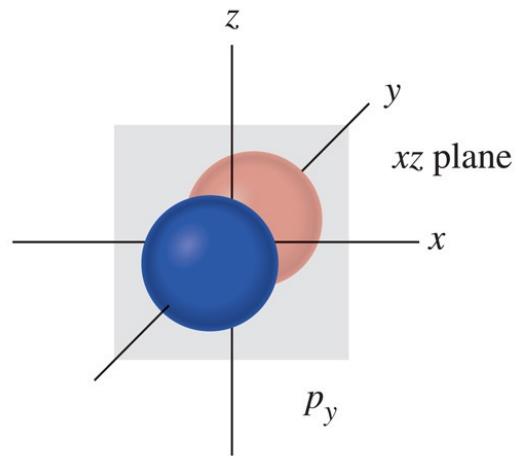
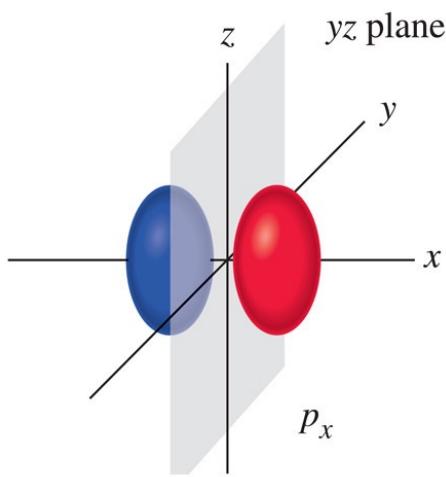


(b)

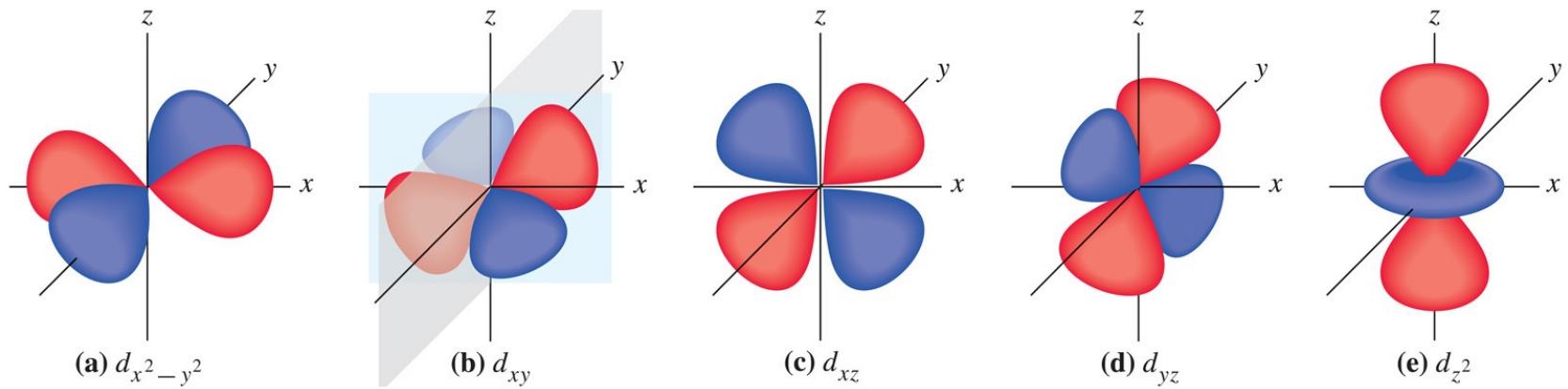


(c)

▲
2p Orbital

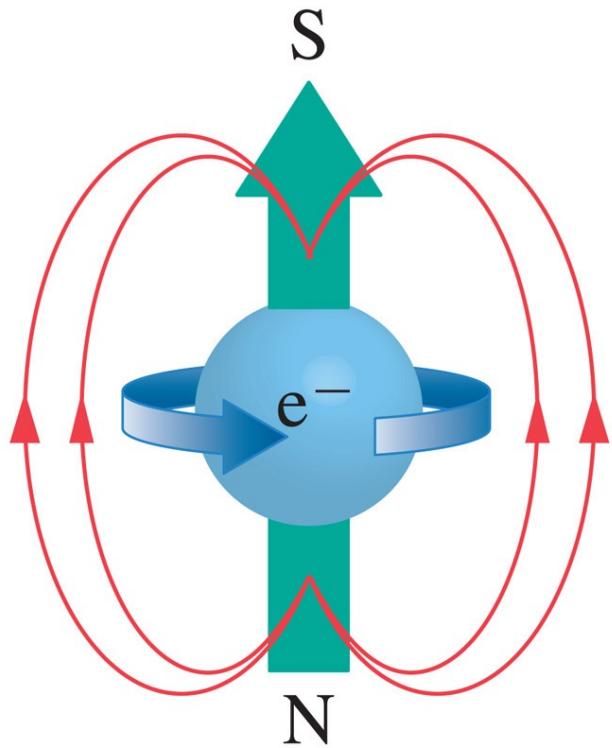


Die drei 2p-Orbitale

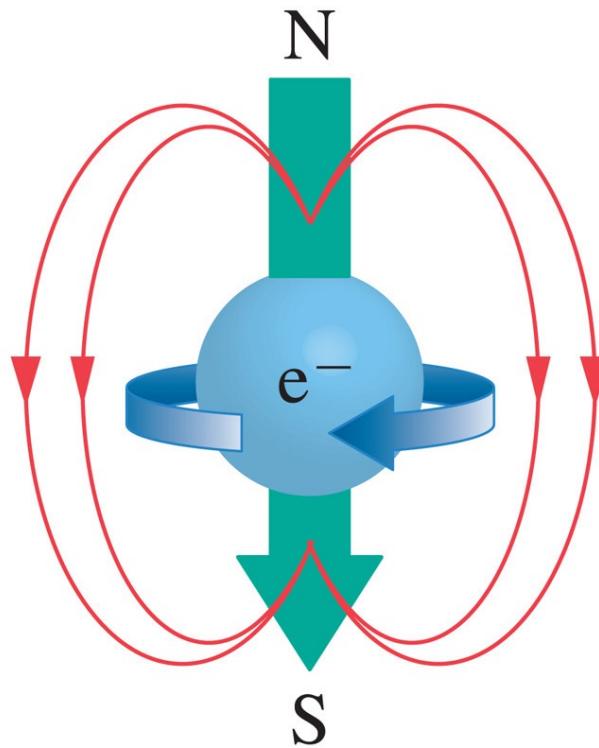


Fünf d-Orbitale

Elektronenspin: Eine vierte Quantenzahl



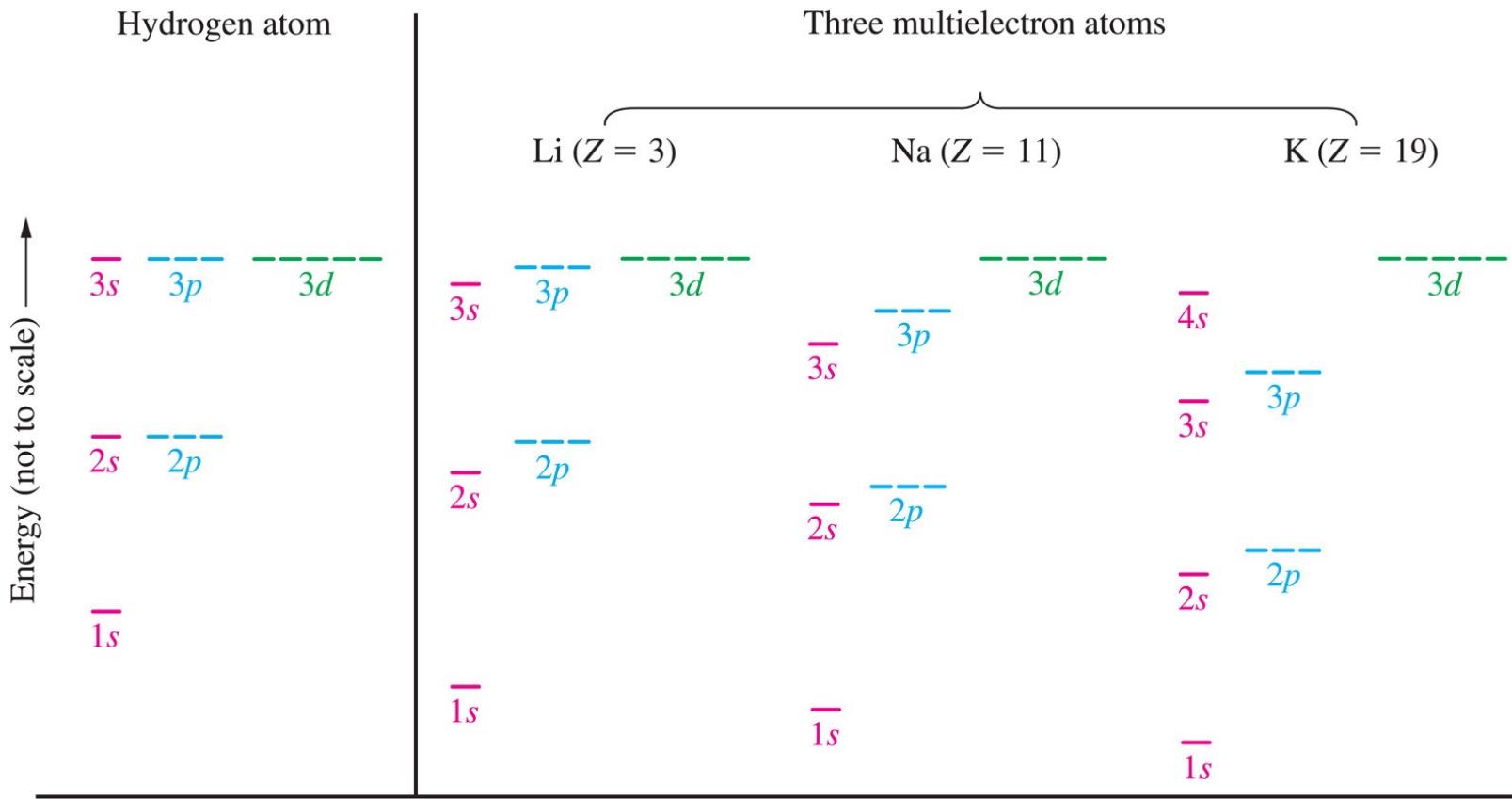
$$m_s = +\frac{1}{2}$$



$$m_s = -\frac{1}{2}$$



Elektronenspin



Energiediagramm für die ersten drei Schalen.

Elektronenkonfigurationen

Aufbau-Prinzip

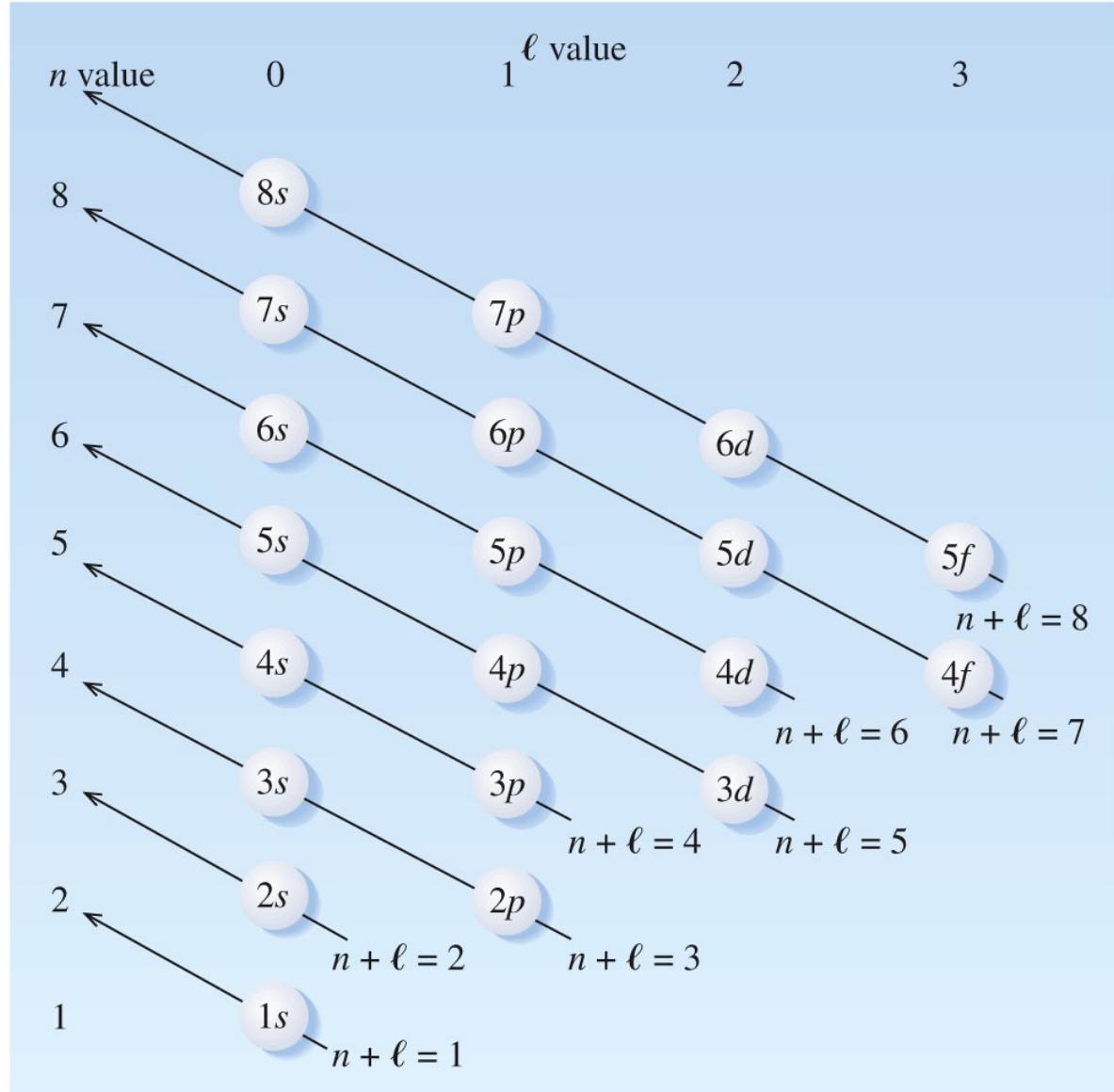
Von unten nach oben auffüllen.

Pauli-Prinzip

Elektronen müssen sich in mindestens einer Quantenzahl unterscheiden.

Hundsche Regel

Orbitale zuerst einzeln mit parallelen Spins besetzen.



Auffüllen von Unterschalen

Notation von Elektronenkonfigurationen

Hauptquantenzahl n

1s²

Anzahl Elektronen
im Orbital

Nebenquantenzahl l

Notation von Elektronenkonfigurationen

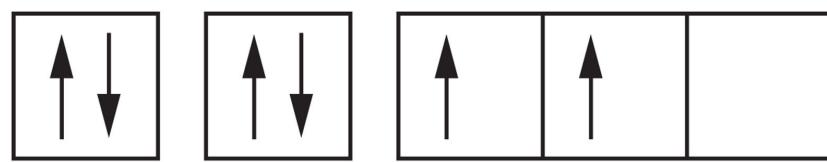
spdf Notation

$1s^2 2s^2 2p^2$

spdf Notation (erweitert)

$1s^2 2s^2 2p_x^1 2p_y^1$

spdf Notation (Kästchen)

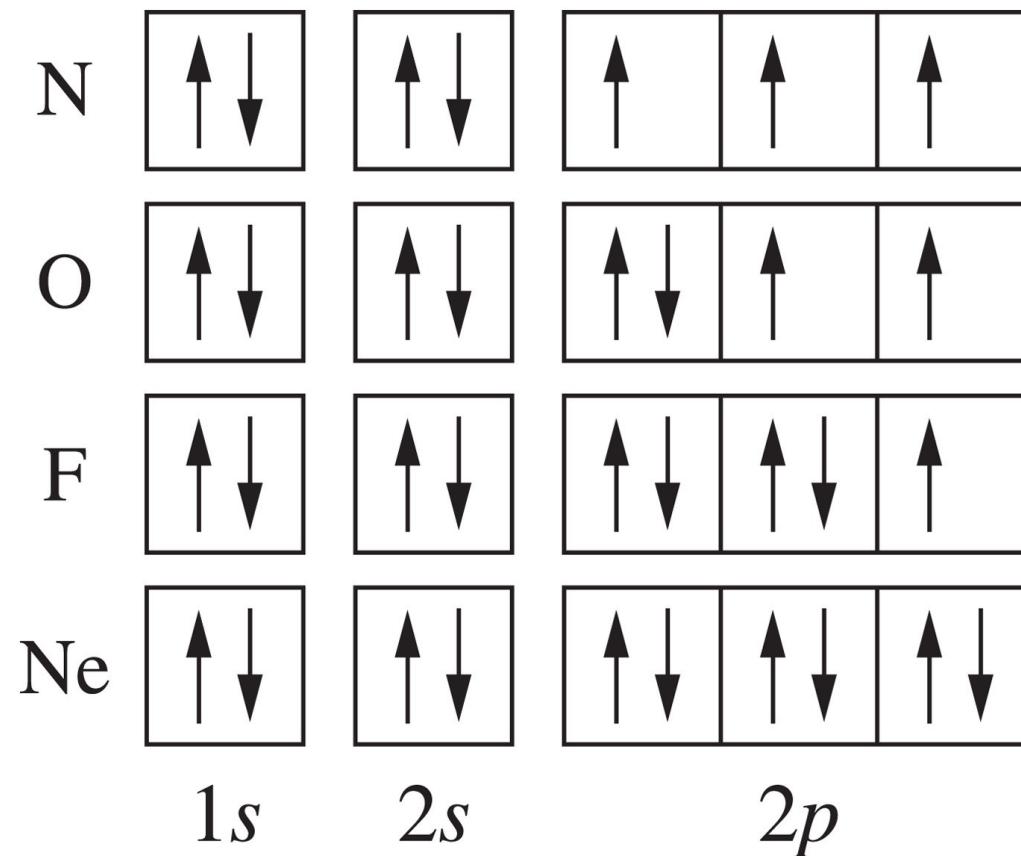


$1s$

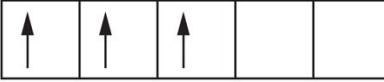
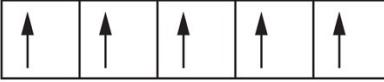
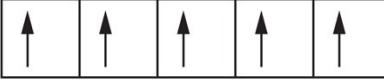
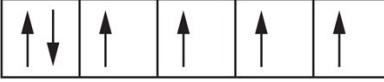
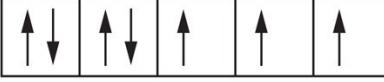
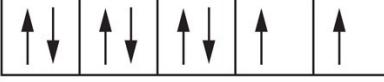
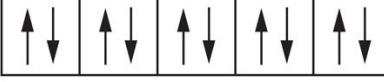
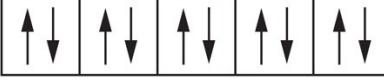
$2s$

$2p$

Aufbau-Prinzip



Aufbauprinzip – Sc bis Zn

Sc:	[Ar]			[Ar]3d ¹ 4s ²
Ti:	[Ar]			[Ar]3d ² 4s ²
V:	[Ar]			[Ar]3d ³ 4s ²
Cr:	[Ar]			[Ar]3d ⁵ 4s ¹
Mn:	[Ar]			[Ar]3d ⁵ 4s ²
Fe:	[Ar]			[Ar]3d ⁶ 4s ²
Co:	[Ar]			[Ar]3d ⁷ 4s ²
Ni:	[Ar]			[Ar]3d ⁸ 4s ²
Cu:	[Ar]			[Ar]3d ¹⁰ 4s ¹
Zn:	[Ar]			[Ar]3d ¹⁰ 4s ²

3d

4s

Elektronenkonfiguration und das PSE



Orbital-Blöcke

TABLE 8.2 Electron Configurations of Some Groups of Elements

Group	Element	Configuration
1	H	$1s^1$
	Li	$[\text{He}]2s^1$
	Na	$[\text{Ne}]3s^1$
	K	$[\text{Ar}]4s^1$
	Rb	$[\text{Kr}]5s^1$
	Cs	$[\text{Xe}]6s^1$
	Fr	$[\text{Rn}]7s^1$
17	F	$[\text{He}]2s^22p^5$
	Cl	$[\text{Ne}]3s^23p^5$
	Br	$[\text{Ar}]3d^{10}4s^24p^5$
	I	$[\text{Kr}]4d^{10}5s^25p^5$
	At	$[\text{Xe}]4f^{14}5d^{10}6s^26p^5$
18	He	$1s^2$
	Ne	$[\text{He}]2s^22p^6$
	Ar	$[\text{Ne}]3s^23p^6$
	Kr	$[\text{Ar}]3d^{10}4s^24p^6$
	Xe	$[\text{Kr}]4d^{10}5s^25p^6$
	Rn	$[\text{Xe}]4f^{14}5d^{10}6s^26p^6$