Atomic physics

$1u = \frac{1}{12}$ mass of $^{12}_{6}C$

A - Mass
G - Symbol
Z - protons

Flux (# particles)

$F = \frac{\Delta N_p}{\Delta t\, A}$

Hard shell scattering

$\sigma = \pi (r_A + r_p)^2$

Rate of hits

$R = F \cdot \sigma$, $R = \frac{\text{numb. Hits}}{\text{time}}$

$n = \frac{N_p}{V}$

$N_p(x) = N_p(0) e^{-\sigma \cdot n x}$

Attenuation length:

$\frac{N_p(L)}{N_p(0)} \overset{!}{=} \frac{1}{e} \Rightarrow L = \frac{1}{n\sigma}$

Hard shell in Gas

$N(x) = N(0)\, e^{-\frac{p}{k_B T}\sigma x}$

Van der Waals

$\left(p + \frac{a}{V_m^2}\right)(V_m - b) = RT$ (b: covolume)

$V_m = \frac{V}{n}$ (molar volume), $b = \frac{4}{3}\pi r^3 \cdot N_A$ (volume of 1 mol gas)

• non zero radius and realistic interactions.

Chemical identity

$N_p = n \cdot N_A$ (Avogadro; n in mol)

$R = k_B N_A$

Rutherford scattering

$k = \frac{zZe^2}{4\pi\varepsilon_0}$

• V_0 = initial velocity

• m = mass of the α-particle

$d\sigma = \frac{1}{4}\left(\frac{k}{mV_0^2}\right)^2 \frac{1}{\sin^4\left(\frac{\theta}{2}\right)}\, d\Omega$, $d\Omega = \sin\theta\, d\theta\, d\gamma$

($d\sigma$: cross section)

Ideal Gas law

$pV = N_p k_B T$

• point masses with no interactions

Probability

$P(3|4)$ from state 4 to 3

Since 2 coins 2 coils?

States

A microstate is a particular configuration of a system.
A macrostate is a describtion in "bulk" properties

Fundamental postulate of statistical physics

For a closed system, every microstates which satisfies the global constraints is equally likely to be occupied.

The probability of a macrostate is equal to the number of microstates compatible with the macrostates, divided by the number of microstates.

Systems where the fundamental postulate is true are said to be in thermodynamic equilibrium

The macrostate that is occupied in thermal equilibrium is the one with the largest number of microstates.

Irreversibility

With passage of time, a closed thermodynamic system will evolve toward the macrostate with the largest number of microstates

Thermodynamic equilibrium for two systems

If two systems reached thermodynamic equilibrium:

$\left(\frac{\partial\sigma_1}{\partial U_1}\right)_{N_1} = \left(\frac{\partial\sigma_2}{\partial U_2}\right)_{N_2}$

$\frac{1}{T} = k_B\left(\frac{\partial\sigma}{\partial U}\right)_{N,V} = \left(\frac{\partial S}{\partial U}\right)_{N,V}$

Entropy

$S = k_B \cdot \sigma$

Ω : # particles × V × Energy → $\mathbb{N}$

Ω gives the number of microstates for given N_p and U_0

$\sigma = \log(\Omega)$

Representation of temperature

$\tau = k_B \cdot T$, $\beta = \frac{1}{\tau} = \frac{1}{k_B T}$

Law of thermodynamics

0: thermal equilibrium ⟺ same temperature

I: $\Delta U = Q - W$ (Q: heat, W: work)

$dU = TdS - pdV$ (thermo. identity)

II: Entropy never decreases

Microscopic derivation

$\frac{1}{2} m \langle v_x^2 \rangle = \frac{1}{2} k_B T$

$\langle v_x \rangle = \int_{\mathbb{R}} v_x\, p(v_x)\, dv_x$

Partition function

BF is ∝ probability to find with energy E

$Z = \sum_s \underbrace{e^{-\beta \cdot \varepsilon_s}}_{\text{Boltzmann factor}}$

$P(\varepsilon_i) = \frac{e^{-\beta\varepsilon_i}}{Z}$, $Z = \int_{\mathbb{R}^3} BF\, dr^3$

$U = \langle \varepsilon \rangle = -\frac{\partial}{\partial\beta}\log(Z) = \frac{1}{Z}\sum_s \varepsilon_s e^{-\beta\varepsilon_s} = \sum_j P(\varepsilon_j)\varepsilon_j$ (n_j)

h planck

Entropy

$S = \frac{\partial}{\partial T}\left(k_B T \cdot \log(Z)\right)$

Single particle

$Z_{sp} = \frac{V}{h^3}\int_0^\infty 4\pi p^2 e^{-\beta p^2/2m}\, dp = V\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}$

N particles

$Z = \frac{Z_{sp}^N}{N!}$ (indistinguishable)

$Z = Z_{sp}^N$ (distinguishable)

Energy of the ideal gas

$U = \frac{3}{2} N k_B T$ (in distinguishable)

Maxwell-Boltzmann distribution

$P(p)dp = \frac{2\pi V p^2 dp}{h^3}\frac{e^{-\beta p^2/2m}}{Z_{sp}}$ Probability to find particle with momentum p ⟺ dp

$n(v)dv = 4\pi N v^2 dv \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-mv^2/2k_B T}$ expected number of particles with speed between v ⟺ dv

$P(v)dv = \frac{4\pi v^2 dv\, e^{-Mv^2/2k_B T}}{Z}$

$n_j = \frac{N}{Z}e^{-\beta\varepsilon_j} \Rightarrow U = \sum n_j \cdot \varepsilon_j$

Speed $|\vec{v}|$

$\langle v \rangle = \sqrt{\frac{8 k_B T}{m}}$ (average)

$v_{max} = \sqrt{\frac{2 k_B T}{m}}$ (most probable)

$\langle v \rangle \neq v_{max}$ ← Distr. not symmetric

$\frac{\langle v \rangle}{v_{max}} \approx 1{,}13$

Energy of Rotation

$E = \frac{L^2}{2J} = \frac{\hbar^2 L(L+1)}{2m\left(\frac{d}{2}\right)^2}$

Energy levels of a single axis of rotation

Temperature at which rotation contribute to heat capacity:

$(L=1 - L=0) = k_B T$

$E(L=1)$

Scattering

$dR_\theta = F 2\pi b\, db$

$\frac{dR_\theta}{d\theta} = F\frac{d\sigma}{d\theta}$

Differential cross section

Light (interfero)

$I = A^* A$

$A = \frac{A_0}{2}(1 + e^{i\delta\varphi})$

$I = \frac{I_0}{2}(1 + \cos\delta\varphi)$

Optics

$\omega = 2\pi\nu$

$c = \lambda \cdot \nu$

$k = \frac{2\pi}{\lambda}$

$v = \frac{c}{n_i}$

$D = n_i \cdot s$

phase displacement

$\varphi = k \cdot L$

Paraxial approximation

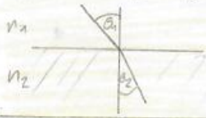
$\theta \ll 1$ is small

$c - a \approx \frac{b^2}{2a}$ incident rays have a small to optical axis

$a \approx c$

Snells law

$n_1 \sin\theta_1 = n_2 \sin\theta_2$



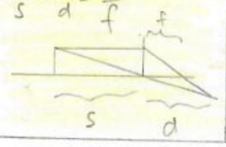
Magnification

$M = -\frac{d}{s}$

$M = -\prod_i \frac{d_i}{s_i}$

Lensmaker, (virtual image)

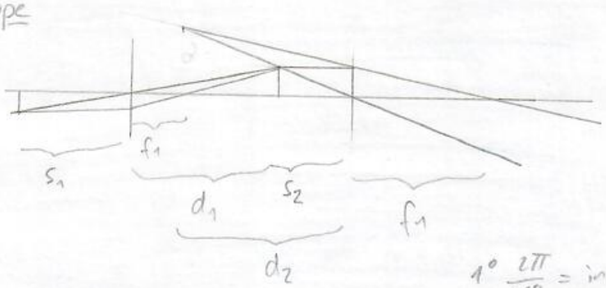
$\frac{1}{s} + \frac{1}{d} = \frac{1}{f}$



Fermat

Light travels by the path which is extremal in the optical path length D.

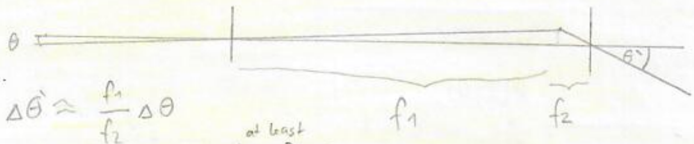
Microscope



$1° \; \frac{2\pi}{360°} =$ in rad

Telescope

$S \gg f$ "$s_1 = \infty$", $M = \frac{\Delta\theta'}{\Delta\theta}$

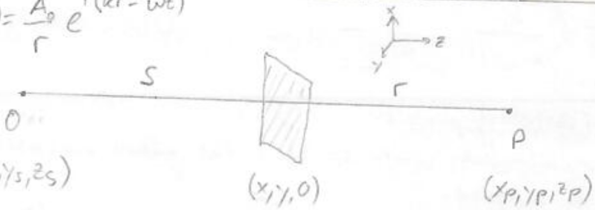


$\Delta\theta' \approx \frac{f_1}{f_2}\Delta\theta$

at least $L = f_1 + 2f_2$

Wave optics

$E(r,t) = \frac{A_0}{r} e^{i(kr - \omega t)}$



Fraunhofer Diffraction at aperature

$t(x,y) = \begin{cases} 1 & \text{else} \\ 0 & \text{opaque} \end{cases}$

$U(P) \propto e^{ik(s_0 + r_0)} \iint_{\mathbb{R}\,\mathbb{R}} t(x,y)\, e^{ik(Xx + Yy)} dx dy$

$X = \frac{x_S}{s_0} + \frac{x_P}{r_0} \qquad Y = \frac{y_S}{s_0} + \frac{y_P}{r_0}$

Huygen

$U(P) \propto A_0 \iint_{\text{Aperature}} \frac{e^{iks}}{s} \frac{e^{ikr}}{r} dx dy$

Simplification

$U(x_P, y_P) \propto A_0 \iint e^{iks} e^{ikr} dx dy$

Fraunhofer Approx.

- Surface of constant phase are planes
- Wave components arriving at P from different parts of A are out of phase which varies linearly.
- $\lambda, \Delta x \ll d, s$

Square Aperature

$U(P) \propto \frac{\Delta x^2 \Delta y^2 e^{ik(s_0 + r_0)}}{s_0 r_0} \operatorname{sinc}\left(\frac{k X \Delta x \Delta y}{2}\right) \operatorname{sinc}\left(\frac{k Y \Delta x \Delta y}{2}\right)$

First Minima

$\sin\theta = \frac{\lambda}{D}$

D is the diameter

for circular, multiply by a factor of 1,22

Rayleigh criterion

Two objects are resolved if the maximum from the intensity pattern of one falls on the first minimum of the pattern of the other:

$\theta = \sin\theta > \frac{\lambda}{D} \cdot (1{,}22)$ circular lens

D – lens diameter

Polarization (in $\hat{z}$-direction)

$E = E_x \hat{x} \cos(k_x z - \omega t) + E_y \hat{y} \cos(k_y z - \omega t + \alpha)$

$k_x = n_x k \quad , \quad k_y = n_y k$

$\alpha = 0$ linear polarization

$\alpha = \frac{\pi}{2}$ σ^+, right circular, counterclockwise

$\alpha = -\frac{\pi}{2}$, σ^-, left circular, clockwise

neither: elliptical

Boundary condition

$E_{\parallel 1} = E_{\parallel 2}$

$D_{\perp 1} = D_{\perp 2}$

$H_{\parallel 1} = H_{\parallel 2}$

$B_{\perp 1} = B_{\perp 2}$

Abbé resolution criteria in Microscope

$\delta z = \frac{\lambda}{2NA}$, $N_A = \sin(\theta_{lens}) \approx \frac{w_{lens}}{2d_{lens}}$

Brewsters angle

For p polarized, no reflection at: $\tan(\theta_i) = \frac{n_2}{n_1}$

Fresnel equations

S is senkrecht E to the plane

P-polarized:

$\frac{E_r}{E_i} = \frac{n_2 \cos\theta_i - n_1 \cos\theta_t}{n_2 \cos\theta_i + n_1 \cos\theta_t}$

$\frac{E_t}{E_i} = \frac{2 n_1 \cos\theta_i}{n_2 \cos\theta_i + n_1 \cos\theta_t}$

S-polarized:

n_i are all swap but the blue marked

$B = \frac{n \cdot E}{c}$

Take the $\hat{x}$-component for derivation and for S

Grating

$N = \frac{L}{d} = \frac{\text{length grating}}{\text{gap between grating}}$

$m \cdot \lambda = d(\sin\theta_r - \sin\theta_i)$, $m \in \mathbb{N}$ is the order

$I(\theta_r) = I(0) \frac{\sin^2\left(\frac{\delta\varphi N}{2}\right)}{\sin^2\left(\frac{\delta\varphi}{2}\right)}$, $N\delta\varphi = 2\pi n$, $n \in \mathbb{Z}$

Michelson interferometer

$\delta\varphi = 2k(d_2 - d_1)$, $I(\delta\varphi) = \frac{I_{max}}{2}(1 + \cos(\delta\varphi))$

$m = \frac{2(d_2 - d_1)}{\lambda}(n-1)$ index of refr.

numb. of fringes

$I \propto \frac{I_0}{2}\left(1 + \cos\left(\frac{4\pi(d_2 - d_1)}{\lambda}\right)\right)$

$I = A^* A$

Grating resolution

$\Delta\nu = \frac{c}{N \cdot d(\sin\theta_i - \sin\theta_f)}$

$\left(\frac{\delta\nu}{\nu}\right)_{min} = \frac{\lambda}{2Nd}$

biggest possible path difference

Resolution

$\Delta\nu_{min} = \frac{c}{\text{max path length in apparatus difference}}$

$x_{max} = d_2 - d_1$

Fourier transform spectrometer

$S(\nu)d\nu =$ light power emitted between ν and $d\nu$

$S(\nu) \propto \int_0^{x_{max}} (2I(x) - I_0) \cos\left(\frac{4\pi\nu x}{c}\right) dx$

$= \operatorname{sinc}\left(\frac{2\pi(\nu - \nu_0)x_{max}}{c}\right) + \operatorname{sinc}\left(\frac{2\pi(\nu + \nu_0)x_{max}}{c}\right)$

Resolution for Michelson

$\frac{\delta\nu}{\nu} = \frac{\delta\lambda}{\lambda} \gg \frac{\lambda}{2x_{max}}$, $\Delta\nu = \frac{c}{2x_{max}}$

Wave-function

$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\Psi(x,t) = 0$

Equipartition theorem

$U = \frac{f}{2} N k_B T$

$f = \underset{\text{translation}}{a} + \underset{\text{rotation}}{b} + \underset{\text{vibration}}{2c}$

Every quadratic term contributes a value of $\frac{1}{2} k_B T$ to the internal Energy

Degrees of freedom

1atom 3

2atom 7

3atom linear 11

3atom angled 12

Heat capacity

$C_V = \left(\frac{\partial u}{\partial T}\right)_V$

$\varepsilon_i = h \cdot \nu$

Planck Distribution

Idea: Energy is discrete.

$U = \sum_i^N \frac{h \cdot \nu_i}{e^{\beta h \nu_i} - 1}$

$\Rightarrow \rho(\nu) d\nu = \frac{8\pi h}{c^3} \frac{\nu^3 d\nu}{e^{\beta h \nu} - 1}$

Blackbody

Boundary condition: $E_\parallel = 0$, $\nabla \cdot E = 0$

$g(k) dk = \frac{V}{\pi^2} k^2 dk$, $g(\nu) d\nu = \frac{8\pi V}{c^3} \nu^2 d\nu$

number of modes with wavevector magnitudes between $k \leftrightarrow dk$

$\rho(\nu) d\nu = k_B T \frac{g(\nu) d\nu}{V} \overset{R.J.}{=} k_B T \frac{8\pi \nu^2}{c^3} d\nu$ (Rayleigh-Jeans)

Energy density in Box within cycle frequency between $\nu \leftrightarrow d\nu$

A blackbody is in thermal equilibrium if $P_{emit} = P_{received}$

Photoelectric effect

$E = h \cdot \nu$

$E^{kin}_{electron} = \underset{\text{Photon}}{h \cdot \nu} - \underset{\text{often negligible}}{\Phi}$

$p = \frac{h \cdot \nu}{c}$

$E_{tot} = mc^2 + E_{ext} = \sqrt{m^2c^4 + p^2c^2}$

Rayleigh Scattering

- frequency of photon doesn't change

$E \propto \frac{q E_0 \omega^2}{m(\omega^2 - \omega_0^2)} \cos \omega t$, $I = |E|^2$

$\omega_0 = \sqrt{\frac{k}{m}}$ eigenfrequency of the atom

Wien displacement law

The maximum of the Planck Distribution is at $\nu_{max} \approx 2{,}822 k_B T$

Stefan-Boltzmann Law

Total energy density (EM) is

$u = \underbrace{\frac{8\pi^5 k_B^4}{15 h^3 c^3}}_{a} T^4$

$j = \sigma T^4 = \frac{\text{Power}}{\text{Area of BB}}$

$\sigma = \frac{ac}{4}$ (Stefan's constant)

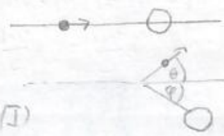
$P_{em} = j A$ total power emmited

$P_{received} = P_{em} \frac{A}{S(r)}$

A: Area perpendicular to j

$S(r)$: total Surface of sphere with radius r (distance)

Compton scattering



$$\begin{cases} h\nu + mc^2 = h\nu' + \sqrt{m^2c^4 + p^2c^2} & (I) \\ \frac{h\nu}{c} + 0 = \frac{h\nu'}{c}\cos\theta + p\cos\varphi & (II) \\ 0 + 0 = \frac{h\nu'}{c}\sin\theta - p\sin\varphi & (III) \end{cases}$$

$m = m_{electron}$

θ observation angle

$\overset{II}{\Longrightarrow} p^2\cos^2\varphi = \frac{h^2}{c^2}(\nu - \nu'\cos\theta)^2$

$\overset{III}{\Longrightarrow} p^2\sin^2\varphi = \frac{h^2\nu'^2}{c^2}\sin^2\theta$

$\overset{II+III}{\Longrightarrow} p^2c^2 = h^2[\nu^2 - 2\nu\nu'\cos\theta + \nu'^2\cos^2\theta + \nu'^2\sin^2\theta]$

$\Rightarrow p^2c^2 = h^2(\nu - \nu')^2 + 2h^2\nu\nu'(1 - \cos\theta)$

$\overset{I}{\Longrightarrow} p^2c^2 = (h(\nu - \nu') + mc^2)^2 - m^2c^4$

$\overset{\text{above}}{=} h^2(\nu - \nu')^2 + 2h(\nu - \nu')mc^2$

$\Rightarrow h\nu\nu'(1 - \cos\theta) = (\nu - \nu')mc^2$

$\Rightarrow \Delta\nu = \frac{h\nu\nu'}{mc^2}(1 - \cos\theta)$

$\Rightarrow \Delta\lambda = \frac{c}{\nu'} - \frac{c}{\nu} = c\frac{\nu - \nu'}{\nu\nu'} = \frac{c\Delta\nu}{\nu\nu'}$

if proton, use m_p not m_e

$\Rightarrow \Delta\lambda = \lambda_c(1 - \cos\theta)$, $\lambda_c = \frac{h}{m_e c}$ (compton wavelength)

X-Ray diffraction (Bragg's Law)

$\lambda < 2d$

$2 \cdot d \sin\theta = n \cdot \lambda$

Matter waves

$E = \frac{h^2}{\lambda^2 2m}$

$E = h\nu$, $p = \frac{h\nu}{c} \Rightarrow \lambda_{dB} = \frac{h}{p}$

$p = \hbar k_{dB}$, $\hbar = \frac{h}{2\pi}$

$E = \frac{p^2}{2m}$ is actual energy

Davison-Germer

$d\sin\varphi = n \cdot \lambda_{dB}$

Wave packets

- Group velocity (maximum of the envelop) has the same velocity as the particle

- $\Psi(x,t) = \int_{k_0 - \Delta k}^{k_0 + \Delta k} A e^{i(kx - \omega(k)t)} dk$

Photon: $\omega(k) = \frac{h\nu}{\hbar} = c \cdot k$

Matter: $\omega(k) = \frac{p^2}{2m\hbar} = \frac{\hbar k^2}{2m}$

k_0 is an average

$\Psi(x,t) \approx A e^{ik_0x - \omega_0 t} \int_{-\Delta k}^{\Delta k} e^{i(kx - \frac{\hbar k_0}{m} t k)} dk$

$\approx \frac{A}{2\Delta k} e^{i(k_0x - \omega_0 t)} \underbrace{\operatorname{sinc}\left(\Delta x\left(x - \frac{\hbar k_0 t}{m}\right)\right)}_{\text{envelope}}$

$\frac{dx_{max}}{dt} = \frac{\hbar k_0}{m} = v_0$

$x_{max} = \frac{\hbar k_0 t}{m}$

Wave functions (Math)

$|\Psi(x,t)| = \Psi^*(x,t)\,\Psi(x,t)$

$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx \overset{!}{=} 1$

$\delta(x) = \int_{-\infty}^{\infty} e^{2\pi i x y} dy$

$\delta(ax) = \frac{\delta(x)}{|a|}$

$\int \delta(x - y) g(y) dx = g(x)$

Operator

$\hat{p} = -i\hbar \frac{\partial}{\partial x}$ $\quad p = \hbar k$

$\hat{E} = i\hbar \frac{\partial}{\partial t}$ $\quad E = h \cdot \nu$

Probability

$P(x,t) dx = |\Psi(x,t)|^2 dx$

Heisenberg

$\Delta x \Delta p \geq \frac{\hbar}{2}$

Observables

All physical observables are associated with Hermitian Operators. The Eigenvalues of these operators give the results of all possible measurements of the observable. The eigenvalues are real-valued (not complex).

Spectral theorem

The set of eigenfunctions of an observable operator form a complete, orthonormal basis.

Condition of orthonormality

$\int \varphi^*(p,x)\varphi(p',x) dx \overset{!}{=} \delta(p' - p)$

ONB of $\hat{p}$

Eigvals of $\hat{p}$

$$\varphi(p,x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

$$\tilde{\Psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-ipx/\hbar} \Psi(x)\,dx$$

F.T.

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{ipx/\hbar} \tilde{\Psi}(p)\,dp$$

Schrödinger (1D)

$$\hat{H}\Psi(x,t) = i\hbar \frac{\partial}{\partial t}\Psi(x,t)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(\hat{x}) = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

time independant:

$$\hat{H}\varphi_E(x) = E\varphi_E(x)$$

$$\Psi(x,t) = e^{-i\frac{E_n t}{\hbar}}\varphi_E(x)$$

Parity

$$\hat{\Pi}\Psi(x,t) = \Psi(-x,t)$$

$\Pi = 1 \Rightarrow$ even "cos"

$\Pi = -1 \Rightarrow$ odd "sin"

Continuity condition

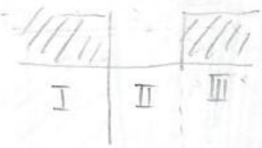
$\Psi(x,t)$ is continuous in x.

$\frac{\partial\Psi(x,t)}{\partial x}$ is continuous in x

$$[\hat{a}^\dagger, \hat{a}^\dagger\hat{a}] = -\hat{a}^\dagger$$

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

Not infinity square



$\mathrm{I}: Be^{\kappa x}$

$\mathrm{III}: Ae^{-\kappa x}$

$$\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$$

$\mathrm{II}: Ce^{ikx} + \tilde{C}e^{-ikx}$

$$k = \sqrt{2mE/\hbar^2}$$

often discrete

Probability of observables

$$\hat{O}\Psi(O,t) = O\Psi(O,t)$$

$$P_O(O)\,dO = |\Psi_O(O,t)|^2\,dO$$

probability of measuring an observable O between $O \Leftrightarrow dO$

Eigenstates of Hamiltonian

The probability distribution of an eigenstate of the Hamiltonian does not evolve in time

Free particle (1D)

$$V(x) = 0$$

$$\Rightarrow \varphi_E(x) = Ae^{ikx} + Be^{-ikx}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Psi(x,t) = Ae^{i(kx - \frac{E}{\hbar}t)} + Be^{i(kx + \frac{E}{\hbar}t)}$$

Tunneling

$$T = \left|\frac{A_{trans}}{A_{inc}}\right|^2$$

$$T \propto 16\frac{E}{V_0} e^{-2\sqrt{2m(V_0-E)}\,a/\hbar}$$

If $A_{\mathrm{III}} = 1$ and $B_{\mathrm{III}} = 0$

$$\Rightarrow R = \left|\frac{A_{refl}}{A_{inc}}\right|^2 = T \cdot |A_{refl}|^2$$

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x} + x\right)$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial x} + x\right)$$

$\hat{a}$ and $\hat{a}^\dagger$ are not observables!

$$[\hat{a}, \hat{a}^\dagger] = 1 \neq 0$$

$$\Rightarrow \hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1$$

$$\varphi_0(x) = \sqrt[4]{\frac{m\omega}{\pi\hbar}}\, e^{-m\omega x^2/2\hbar}$$

$$\hat{a}^\dagger\varphi_n = \sqrt{n+1}\,\varphi_{n+1}$$

$$\hat{a}\varphi_n = \sqrt{n}\,\varphi_{n-1}$$

$$\hat{a}\hat{a}^\dagger\varphi_n = n\varphi_n$$

Expectation value of Operator

$$\langle\Psi|\hat{O}|\Psi\rangle = \int_{\mathbb{R}} \Psi^* \hat{O}\Psi\,dx = \langle\hat{O}\rangle$$

Commutator

If $[\hat{O}, \hat{Q}] = 0$, there exists a set of Basis functions for both $\hat{O}$ and Q.

I: antisymmetric

II: bilinear

III: Jacobi identity

IV: Product

$$[A,B] = -[B,A]$$

$$[AB,C] = A[B,C] + [A,C]B$$

$$[A,BC] = [A,B]C + B[A,C]$$

Infinite square

$$V(x) = \begin{cases} 0 & 0 \le x \le a \\ \infty & \text{else} \end{cases}$$

$0 \to a$: $\varphi_E = A\cos kx + B\sin kx$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}$$

$$\varphi_E \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) & 0 \le x \le a \\ 0 & \text{else} \end{cases}$$

Harmonic Oscillator

$$V(x) = \frac{1}{2}m\omega^2x^2 \Rightarrow \omega^2 = \frac{k}{m}$$

natural frequency

$$\hat{\chi} = \sqrt{\frac{m\omega}{\hbar}}\,\hat{x}, \quad [\chi] = -$$

number operator

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) = \hbar\omega\left(\hat{n} + \frac{1}{2}\right)$$

$$\hat{a} = \frac{i}{\sqrt{2m\omega\hbar}}\hat{p} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}$$

$$\hat{a}^\dagger = -\frac{i}{\sqrt{2m\omega\hbar}}\hat{p} + \sqrt{\frac{m\omega}{2\hbar}}\hat{x}$$

$$\boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right)} \qquad E_{n+1} - E_n = \hbar\omega$$

$$\Psi_n(x) = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\Psi_0$$

Hermite

$$\varphi_n(x) = \left(\frac{m\omega}{\pi 2^{2n}(n!)^2\hbar}\right)^{1/4} e^{-\chi^2/2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

Expectation values

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

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

$$\langle\hat{x}\rangle = 0, \quad \langle\hat{p}\rangle = 0$$

orthonormality and $\hat{a}^{(\dagger)}$ operator

$$\langle\hat{x}^2\rangle = \left(\frac{\hbar}{2m\omega}\right)(1+2n)$$

$$\langle\hat{p}^2\rangle = \frac{m\hbar\omega}{2}(1+2n)$$

$$H_0(\chi) = 1$$

$$H_1(\chi) = 2\chi$$

$$H_2(\chi) = -2(1-2\chi^2)$$

$$H_3(\chi) = -12(\chi - \frac{2}{3}\chi^3)$$

$$\sigma_x\sigma_p = \frac{\hbar}{2}(1+2n)$$

for $n=0$

$$\sigma_x\sigma_p = \frac{\hbar}{2}$$

Rules of Quantum measurement

$$\Psi(x,t) = a_1\varphi_1(x) + a_2\varphi_2(x)$$

$$|a_1|^2 + |a_2|^2 \overset{!}{=} 1$$

complex but not eigvals

$$\hat{O}\varphi_1 = O_1\varphi_1$$

if O_1 was measured ($|a_1|^2$ probability) the wave-function collapses to:

$$\Psi(x,t) = \varphi_1(x), \quad P_{\varphi_i} = \left|\int_{\mathbb{R}}\varphi_i^*\Psi(x,t)\,dx\right|^2$$

Measurements with degeneracy

if O_i is eigenvalue for multiple φ_n the wavefunction collapses to

$$\Psi(x,t) = \frac{\sum_j a_j\varphi_j(x,t)}{\sqrt{\sum_j |a_j|^2}}$$

where j runs over all φ which have the same eigenvalue $O_i = O_j$

$$P(O_i) = \sum_j |a_j|$$

— again over $O_i = O_j$

Uncertainties

$w_x = |\Psi(x,0)|^2$

w_x

$$\sigma_x = \sqrt{\langle x^2\rangle} \qquad \sigma_p = \sqrt{\langle p^2\rangle}$$

$$\sigma_x\sigma_p \geq \frac{\hbar}{2}, \quad \sigma_O = \sqrt{\langle\hat{O}^2\rangle - \langle\hat{O}\rangle^2}$$

Robertson

Schrödinger (3D)

$$\hat{r} = (\hat{x}, \hat{y}, \hat{z}), \quad \hat{p} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$$

$$\hat{p} = -i\hbar\,\mathrm{grad}(\cdot)$$

$$[\hat{x},\hat{y}] = [\hat{x},\hat{z}] = [\hat{y},\hat{z}] = 0$$

$$[\hat{p}_x,\hat{p}_y] = [\hat{p}_y,\hat{p}_z] = [\hat{p}_x,\hat{p}_z] = 0$$

$[\hat{p}_x,\hat{y}] = [\hat{p}_x,\hat{z}] = 0$ and similar

$$[\hat{p}_x,\hat{x}] = [\hat{p}_y,\hat{y}] = [\hat{p}_z,\hat{z}] = i\hbar \neq 0$$

$$\hat{H} = \frac{\hat{p}\cdot\hat{p}}{2m} + V(\hat{r})$$

scalar product

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\hat{r})$$

Fourier transform from $\hat{x} \to \hat{p}$

$$\varphi(p,0) = \frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}} e^{-ipx/\hbar}\Psi(x,0)\,dx$$

not eigenfunction of momentum

Probability of finding a state

1.) Check whether the energy is possible

2.) $\int_{-\infty}^{\infty}\Psi_k^*\Psi_0\,dx$, Ψ_k is the state, Ψ_0 is general solution

3.) Beware of odd/even while integrate

4.) Probability is $|\int\ldots|^2$ (!)

Optical spectrum of hydrogen

$$\nu = \frac{c}{\lambda} = c \cdot R_\infty \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$n_2 > n_1$, R_∞ Rydberg const.

$R_e := h \cdot c \cdot R_\infty \approx 13{,}6\,eV$

Energy according to Rydberg

$$E_n = -R_e \left(\frac{1}{n^2} \right), \quad n = 1,2,3$$

$$h \cdot \nu = E_{n_2} - E_{n_1}$$

Bohr radius

$$r_n = \frac{4\pi \varepsilon_0 \hbar^2 n^2}{m e^2}$$

$$r_1 = \frac{4\pi \varepsilon_0 \hbar^2}{m e^2} \equiv a_0$$

Fine structure constant

$$\alpha = \frac{v}{c} = \frac{\hbar}{a_0 m c} = \frac{e^2}{4\pi \varepsilon_0 c \hbar} \approx \frac{1}{137}$$

Bohr Atom Postulates

I: discrete circular orbit are stable.

II: $E_n = -\frac{R_e}{n^2}$, $n = 1,2,3$

III: $h\nu = E_{n_2} - E_{n_1}$, $n_2 > n_1$

IV: for great radius, the emitted radiation frequency between adjacent orbits should equal the inverse of the period of the orbit.

Correspondance principle

Quantum systems should behave like classical systems as the system becomes macroscopic.

R_e by Bohr

$m = m_e$

$$E = \frac{1}{2} m v^2 - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$\frac{e^2}{4\pi\varepsilon_0 r^2} = m \frac{v^2}{r}, \quad \omega = \frac{v}{r}$$

$$E = -\frac{1}{2} \sqrt[3]{\frac{e^4 m}{16\pi^2 \varepsilon_0^2}}\, \omega^{2/3}$$

$$E_{n+1} - E_n = \hbar\omega$$

$$-R_e \left(\frac{1}{(n+1)^2} - \frac{1}{n^2} \right) = \hbar\omega$$

$n \gg 1$

$$\Rightarrow -R_e \left(\frac{1}{n^2} \right) \left(\frac{1}{(1+\frac{1}{n})^2} - 1 \right) = \hbar\omega$$

$$\frac{R_e}{n^2} \left(1 + \frac{2}{n} - 1 \right) = \hbar\omega$$

$$\frac{2R_e}{n^3} = \hbar\omega$$

$$-\frac{R_e}{n^2} = -\frac{1}{2} \sqrt[3]{\frac{e^4 m}{16\pi^2 \varepsilon_0^2}}\, \omega^{2/3}$$

$$-\frac{(2R_e)^{3/2}}{n^3} = -\sqrt{\frac{e^4 m}{16\pi^2 \varepsilon_0^2}}\, \omega$$

$$(2R_e)^{-1/2} = \frac{\hbar}{\sqrt{\frac{e^4 m}{16\pi^2 \varepsilon_0}}}$$

$$R_e = \frac{e^4 m}{32\pi^2 \hbar^2 \varepsilon_0^2} \approx 13{,}6\,eV$$

Hydrogen Atom

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{r})$$

$$\frac{-\hbar^2}{2m_e} \nabla^2 \psi_E + V(r)\psi_E = E\psi_E$$

Ansatz: $\psi_E(r,\theta,\varphi) = R(r)\, Y(\theta,\varphi)$

Orbital angular momentum

$\hat{H}$ has spherical symmetry.

$$\Rightarrow [\hat{H}, R^2_{\Delta\varphi}] = 0$$

$$\hat{L} = \hat{r} \times \hat{p} = \begin{pmatrix} \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{pmatrix}$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial\varphi}$$

$$[\hat{H}, \hat{L}_z] = [\hat{H}, \hat{L}_y] = [H, \hat{L}_x] = 0$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

$$[\hat{L}_x, \hat{L}_z] = -i\hbar \hat{L}_y$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$

Spherical function

$$\hat{L}^2 Y_{l,m} = \hbar^2 l(l+1) Y_{l,m}, \quad \hat{L}_z^2 Y_{l,m} = \hbar^2 m^2 Y_{l,m}$$

$$\hat{L}_z Y_{l,m} = m\hbar Y_{l,m} \quad 2l+1 \text{ eigenfunctions}$$

$$Y_{l,l}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}} \frac{\sqrt{(2l+1)!}}{l!\, 2^l} \sin^l\theta\, e^{il\varphi}$$

for different m, apply $\hat{L}_-$.

$\hat{L}^2$-operator

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$[\hat{L}^2, \hat{L}_z] = 0$$

$$[\hat{H}, \hat{L}^2] = 0$$

Ladder-operator

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y$$

$$\hat{L}_- = \hat{L}_x - i\hat{L}_y$$

$$[\hat{L}_+, \hat{L}_z] = -\hbar \hat{L}_+$$

$$[\hat{L}_-, \hat{L}_z] = \hbar \hat{L}_-$$

$$[\hat{L}_+, \hat{L}_-] = 2\hbar \hat{L}_z$$

$$[\hat{L}_+, \hat{L}^2] = 0$$

$$[\hat{L}_-, \hat{L}^2] = 0$$

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,1} = -\frac{3}{\sqrt{8\pi}} \sin\theta\, e^{i\varphi}$$

$$Y_{1,0} = \frac{3}{\sqrt{4\pi}} \cos\theta$$

$$Y_{1,-1} = \frac{3}{\sqrt{8\pi}} \sin\theta\, e^{-i\varphi}$$

$$Y_{2,2} = \frac{1}{4} \sqrt{\frac{15}{8\pi}} \sin^2\theta\, e^{2i\varphi}$$

Radial eigenfunctions

$$E_n = -\frac{1}{n^2} \frac{mc^2\alpha^2}{2}$$

Laguerre polynom

$$R_{n,l}(r) = C\, r^l\, L^{2l+1}_{n-l-1}\left(\frac{2r}{n a_0} \right) e^{-r/n a_0}$$

Normalization: $\int_0^\infty |R_n(r)|^2 r^2\, dr = 1$

Beware!

Perturbation theory (degenerate)

The operator has to commute with $\hat{H}_0$ and $\delta\hat{H}$, i.e.: $[\hat{H}_0, Q] = [\delta\hat{H}, Q] = 0$

Ladder operator

$$\hat{L}_- \hat{L}_+ = \hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z$$

$$\hat{L}_+ \hat{L}_- = \hat{L}^2 - \hat{L}_z^2 + \hbar \hat{L}_z$$

Perturbation theory

$$\hat{H} = \hat{H}_0 + \delta\hat{H}$$

$$\hat{H}_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$$

$$\hat{H}\psi_n = E_n \psi_n$$

$$\delta E_n = E_n - E_n^{(0)}$$

$$\delta\psi_n = \psi_n - \psi_n^{(0)}$$

Degeneracy of Hydrogen

$n > l$, $-l \le m \le l$

$\Rightarrow n^2$ number of eigenstate

First order energy shift

$$\delta E_n = \int \psi_n^{(0)*}\, \delta\hat{H}\, \psi_n^{(0)}\, dx$$

maybe $= 0$ cause $\frac{1}{2}$

First order wavefunction shift

$$\delta\psi_n = \sum_{m \neq n} \frac{\int \psi_m^{(0)*}\, \delta\hat{H}\, \psi_n^{(0)}\, dx}{E_n^{(0)} - E_m^{(0)}} \psi_m$$

Normal Zeemann effect

$$\hat{\vec{\mu}} = -\frac{e}{2m_e} \hat{L} = -\mu_B \frac{\hat{L}}{\hbar}$$

$$\delta\hat{H} = \delta V = -\hat{\vec{\mu}} \cdot B$$

$$\delta E_m = \mu_B B \cdot m$$

$$\mu_B = \frac{e\hbar}{2m_e} \quad \text{(Bohr magneton)}$$

Problem: degeneracy

B in x-direction:

Use linear combination of the degenerate eigenfunctions to make them eigenfunctions of $\hat{L}_x$ rather than $\hat{L}_z$.

Time dependant perturbation

$$\omega_j = \frac{E_j^{(0)}}{\hbar}$$

$$\hat{H} = \hat{H}_0 + \hat{H}_1(t)$$

$$\Psi(x,t) = \sum_j c_j(t) e^{-i\frac{E_j^{(0)}}{\hbar}t} \psi_j^{(0)}(x)$$

$$\frac{\partial c_j}{\partial t} = \frac{1}{i\hbar}\sum_j c_j e^{i(\omega_k-\omega_j)t}\int \psi_k^{(0)}(x)^* \hat{H}_1(t)\psi_j^{(0)}(x)dx$$

$$M_{jk}(t) = \int (\psi_j^{(0)}(x))^* \hat{H}_1(t)\psi_k^{(0)}(x)\,dx$$

$j \neq k$. if $M_{jk} = 0 \overset{\text{for all } t}{\Rightarrow}$ direct transition forbidden

$M_{jk} \neq 0 \Rightarrow$ allowed
for a general t

Inversion

spherical:
$$\hat{\Pi} = \begin{pmatrix} r \to r \\ \theta \to \pi - \theta \\ \varphi \to \pi + \varphi \end{pmatrix}$$

$$\hat{\Pi}\, Y_{l,l}(\theta,\varphi) = (-1)^l\, Y_{l,l}(\theta,\varphi)$$

$$[\hat{\Pi}, \hat{L}] = 0 \Rightarrow \hat{\Pi}\, Y_{l,m} = (-1)^l\, Y_{l,m}$$

Einstein-de Haas

Angular momentum conserved.

Stern-Gerlach

$B(z)$ varies strongly on z.

$l=0 \Rightarrow m=0$

$\Rightarrow \vec{\mu} = 0 \Rightarrow$ ↯

there is still a seperation

Spin-Orbit-coupling

$$B_{nucleus} = \frac{1}{2}\frac{\mu_0}{4\pi}\frac{Ze}{r^3 m_e} L$$

numb. protons; ang. momentum

$$\delta\hat{H} = \frac{g_s \mu_0 Z e^2}{16\pi m_e^2 r^3}\hat{S}\cdot\hat{L}$$

$$\delta\hat{H} = -\mu_S \cdot B_{nucleus}$$

Magnetic moment spin

$$\mu_S = -g_S \frac{\mu_B}{\hbar}\hat{S}$$

$\hat{S} = m_s \hbar$

$-g_S \approx 2$, μ_B Bohr magneton

$U = -\mu \cdot B$

j-operator

$$\hat{j}^2 \psi = \hbar^2 j(j+1)\psi$$

$$\hat{j}_z \psi = \hbar m\, \psi$$

half Integer

$j = l \pm \frac{1}{2}$, m_j; $-l \leq m_j \leq l$

Commutator

$$[\hat{L}, \hat{S}] = 0$$

$$[\hat{L}^2, \hat{S}\cdot\hat{L}] = 0$$

$$[\hat{L}_z, \hat{S}\cdot\hat{L}] \neq 0$$

$$[\hat{S}_z, \hat{S}\cdot\hat{L}] \neq 0$$

$$\hat{j} = \hat{L} + \hat{S}$$

$$[\hat{j}_z, \hat{S}\cdot\hat{L}] = 0$$

$$\hat{j}_z Y = \hbar(m + m_s)\, Y$$

$$\hat{j}^2 = \hat{L}^2 + \hat{S}^2 + 2\hat{S}\cdot\hat{L}$$

Probability Stern Gerlach

$$P(x_1|x_2) = |x_1 x_2|^2$$

m_L

$$m_L = -L, \dots, L$$

gross

Electron in magn. field

$$\hat{H} = g_S \mu_B \hat{S}_z B$$

$$E = \pm \mu_B B$$

Optical transitions

$$\delta V = -p_0 \cdot E - \vec{\mu}_0 \cdot B$$

electric dipolemoment

no change in strength of field in space for $\lambda \gg 0{,}5\,\text{Å}$

Electric dipole Approximation

$$\boxed{\hat{H}_1(t) = e\,E(t)\cdot\hat{r}}$$

$p_0 = -e\cdot\hat{r}$ displacement vector

$$\vec{\mu}_0 = -\frac{e}{2m_e}L$$

$(n,l,m) \longrightarrow (n',l',m')$ allowed $\Leftrightarrow \neq 0$

$$\int_0^\infty\int_0^\pi\int_0^{2\pi} \psi_{n',l',m'}(r,\theta,\varphi)(e\hat{r}\cdot E(t))\psi_{n,l,m}(r,\theta,\varphi)\, r^2 dr \sin\theta\, d\theta\, d\varphi \overset{?}{=} 0$$

Linear polarized

possible when $m = m'$, $\Delta L = L' - L = \pm 1$, n arbitrary

Circular polarized

possible when $m' = m \pm 1$ (before, after) — right circular, clockwise, σ^+ / left circular counterclock σ^-

$L = L' \pm 1$ not dependant on polarization

Polarize along z

possible when $m' = m$, $L = L' \pm 1$

Spin

$$\hat{S} = \begin{pmatrix} \hat{S}_x \\ \hat{S}_y \\ \hat{S}_z \end{pmatrix}$$

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$$

$$[\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x$$

$$[\hat{S}_x, \hat{S}_z] = -i\hbar\hat{S}_y$$

$$[\hat{S}^2, \hat{S}_z] = 0$$

$$\hat{S}^2 \chi_{s,m_s} = s(s+1)\hbar^2 \chi_{s,m_s}$$

$$\hat{S}_z \chi_{s,m_s} = m_s \hbar\, \chi_{s,m_s}$$

Quantum numbers

: $s = \frac{1}{2}$, $m_s = \pm\frac{1}{2}$, $j = l \pm s$, $m_j = \{-j, \dots, j\}$

Pauli matrices

$$\chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Spin operator matrices (raising)

$$\hat{S}_x = \frac{\hbar}{2}\sigma_x \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\hat{S}_y = \frac{\hbar}{2}\sigma_y$$

$$\hat{S}_z = \frac{\hbar}{2}\sigma_z \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad S_+\chi_{1/2} = 0, \quad S_-\chi_{-1/2} = 0$$

$$\hat{S}_+ = \hat{S}_x + i\hat{S}_y = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{S}_- = \hat{S}_x - i\hat{S}_y = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Rules for j:

$l = 0 \Rightarrow j = s = \frac{1}{2}$, $l > 0 \Rightarrow j = l + 1/2$ or $j = l - 1/2$

Energy level shift

$$\delta E_{n,j,l,s} = \frac{1}{4}\alpha^4 m_e c^2 Z^4 \frac{j(j+1) - l(l+1) - s(s+1)}{n^3 l(l+1/2)(l+1)}$$

Corrections to hydrogen

$$E_{nj} = -E_n \frac{Z^2\alpha^2}{n}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right) \quad \text{(Darwin-Term)}$$

Lamb shift: fluctuations of the EM-Field

Multiple electron atoms

$$\psi^{\pm}_{1,2}(r_1,r_2)=\frac{1}{\sqrt{2}}\left(\psi_1(r_1)\psi_2(r_2)\pm\psi_2(r_1)\psi_1(r_2)\right)$$

symmetric – singlet – $S=0$

antisymmetric → triplet → $S=1$

Energies for first excited state

symmetric spatial wavefunction has non zero propability of finding two electron at the same location. Therefore symmetric wavefunction have higher energy ⇒ singlet higher energy than triplet

L-S coupling – repulsive coulomb interaction

$$^{(2S+1)}L \quad , \quad \hat{S}=\sum_{j=1}^{N}\hat{s}_j \quad , \quad \hat{L}=\sum_{j=1}^{N}\hat{l}_j$$

Spin orbit coupling (neutrons not included)!

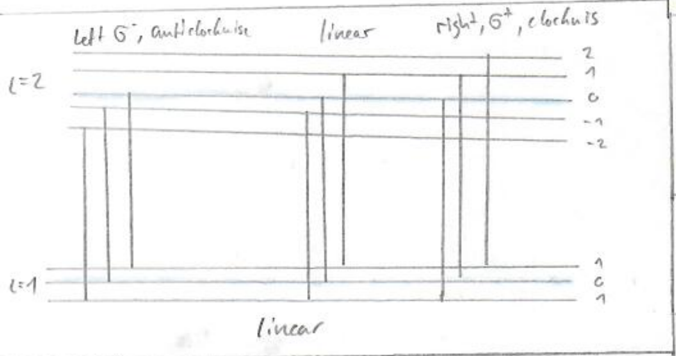
interaction of the electron spins from the effective magnetic field created by the electron orbits

$$\hat{H}_{SO}=\underbrace{\xi}_{\text{constant}}\hat{L}\cdot\hat{S} \quad , \quad \hat{J}=\hat{L}+\hat{S}$$

$$\hat{J}_z\rightarrow M_J\hbar \quad , \quad \hat{J}^2\rightarrow J(J+1)\hbar^2$$

Good quantum number

v_j for H and OP. O if every eigenvector $|v_j\rangle$ remains an eigenvector of O with the same eigenvalues as time evolves



Spin-Orbit coupling for hydrogen

$$\delta\hat{H}_1=\frac{g_s\mu_0 Z e^2}{16\pi m^2 r^3}\hat{l}\cdot\hat{s}$$

$$\delta E_{n,l,j,1/2}=-E_n\frac{(Z\alpha)^2}{2nl(l+1/2)(l+1)}\cdot\begin{cases} l, & j=l+1/2 \\ -l-1, & j=l-1/2\end{cases} \qquad \underbrace{\quad}_{l\neq 0}$$

Spin-Spin interaction

For neutrons, there is no spin-orbit nor LS-coupling. The degeneracy can be broken by spin-spin

Normal Zeeman effect

$S=0$. Split in spectral lines when a homogeneous magn. field is applied

Exchange Operator

$$\hat{X}\psi(r_1,r_2)=\psi(r_2,r_1)$$

Pauli exclusion principle

No two identical fermions can be simultaneously in the same single particle state.

Quantum numbers

L	letter	# single electron states
0	s	2
1	p	6
2	d	10
3	f	14
4	g	18

Optical transitions

only one electron makes a transition.

$\Delta l=\pm 1$

$\Delta m_s=0$

$\Delta L=\pm 1$

$\Delta L=0$ for $L\neq 0$

$\Delta S=0$

$\Delta J=\pm 1$

$\Delta J=0$ for $J\neq 0$

j selection rules

$$j=|L-S|,\dots,|L+S|$$

Energy shift for optical transitions:

$$\Delta\nu=\frac{\mu_B\cdot B}{h}$$

j-operator

$$j=l\pm\frac{1}{2}, \quad l=0\Rightarrow j=\frac{1}{2}$$

correct J-operator (term symbol)

$$j\in\{|L-S|,\dots,|L+S|\}$$

LS-coupling

Spin statistic theorem

Wavefunction of identical particles will always be an Eigenfunction of $\hat{X}$. Eigenvalue depends on the spin of the particles

- Fermions: (antisymmetric), $\hat{X}\psi=-\psi$
  half integer spin
  electrons, protons, neutrons
- Bosons: integer spin
  symmetric, $\hat{X}\psi=\psi$
  photons, α-particle, gluons

Exchange symmetry

$$\psi_{1,2}(r_1,r_2)\,\chi(1;2)$$

the exchange symmetry of the spatial part of the wavefunction is always opposite to that of the spin part

Spin states

symmetric (triplet): $\uparrow_1\uparrow_2$, $\downarrow_1\downarrow_2$, $\frac{1}{\sqrt{2}}(\uparrow_1\downarrow_2+\downarrow_1\uparrow_2)$

antisymmetric (singlet): $\frac{1}{\sqrt{2}}(\chi_{\uparrow_1\downarrow_2}-\chi_{\downarrow_1\uparrow_2})$

Quantum number

$$n\,l^{\#}\dots\,{}^{2S+1}L_j$$

$m_j=m+\frac{1}{2}$, $j=L+S$ aligned

$m_j=m-\frac{1}{2}$, $j=L-S$ not aligned

Boson ground state

$S=\pm 1, 0$

$$\psi_1=\chi_{\downarrow\downarrow}, \quad \psi_2=\chi_{\uparrow\uparrow}, \quad \psi_3=\chi_{..}$$

$$\psi_4=\frac{1}{\sqrt{2}}(\chi_{\downarrow .}+\chi_{.\downarrow})$$

$$\psi_5=\frac{1}{\sqrt{2}}(\chi_{.\uparrow}+\chi_{\uparrow .})$$

$$\psi_6=\frac{1}{\sqrt{2}}(\chi_{\uparrow\downarrow}+\chi_{\downarrow\uparrow})$$

Orbital momentum quantization

Reason is, same wavefunction after Rotation of 360 degrees.

⇒ angular function has periodicity of $2\pi n$ $n\in\mathbb{Z}$

This quantizes orbital angular momentum.

Tunneling

$$H\psi_{I,III} = -\frac{\hbar^2}{2m}\frac{d\psi_{I,III}}{dx^2} = E\psi_{I,III}$$

$$\Rightarrow \psi_{I,III} = \underset{\longrightarrow}{A_{I,III}e^{ik_1x}} + B_{I,III}e^{-ik_1x} \quad \longleftarrow \text{direction}$$

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$H\psi_{II} = -\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} + V_0\psi_{II} = E\psi_{II}$$

$$\Rightarrow \psi_{II} = A_{II}e^{ik_2x} + B_{II}e^{-ik_2x}$$

$$k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

Set $B_{III} = 0$ and $A_{III} = 1$

Use continuity at border a

$$\Rightarrow A_{II} = \frac{1}{2}\frac{k_2+k_1}{k_2}e^{-i(k_2-k_1)a}$$

$$\Rightarrow B_{II} = \frac{1}{2}\frac{k_2-k_1}{k_2}e^{i(k_2+k_1)a}$$

Continuity at $x=0$

$$\Rightarrow A_{II} + B_{II} = A_I + B_I$$

$$\frac{k_2}{k_1}(A_{II} - B_{II}) = A_I - B_I$$

$$A_I = \frac{1}{4}\left(\frac{(k_2+k_1)^2}{k_1k_2}e^{-i(k_2-k_1)a} - \frac{(k_2-k_1)^2}{k_1k_2}e^{i(k_2+k_1)a}\right)$$

$$B_I = \frac{1}{4}\left(-\frac{(k_2^2-k_1^2)}{k_1k_2}e^{-i(k_2-k_1)a} + \frac{(k_2^2-k_1^2)}{k_1k_2}e^{i(k_2+k_1)a}\right)$$

$$T = \left|\frac{A_{III}}{A_I}\right|^2 = \frac{|16e^{-2ik_1a}|}{\left|\frac{(k_2+k_1)^2}{k_1k_2}e^{-ik_2a} - \frac{(k_2-k_1)^2}{k_1k_2}e^{ik_2a}\right|^2}$$

$E \ll V_0$

$$\Rightarrow T \simeq 16\frac{E}{V_0}e^{-2a\sqrt{2m(V_0-E)}/\hbar}$$

$$k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}, \quad k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$R = \left|\frac{B_I}{A_I}\right|^2 = T|B_I|^2$$

1.) Find total energy

2.) Solve for ψ_k while setting E_k as know

3.) Solve for E_k

k has to be integer

Chromatic aberration and spherical aberration

Wave function of a free particle

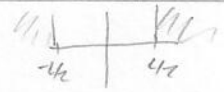
$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\varphi(k)\, e^{-i\omega_k t}e^{ikx}dk = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\varphi(k)\, e^{i(kx - \frac{\hbar k^2}{2m}t)}dk$$

$$\varphi(k) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\psi(x,0)e^{-ikx}dx$$

Rotation functions

$$\psi_k(\varphi) = Ae^{ik\varphi} + Be^{-ik\varphi}$$

Square Well



$$\varphi_n(x) = \sqrt{\frac{2}{L}}\begin{cases}\cos(n\pi x/L) & n \text{ odd}\\ \sin(n\pi x/L) & n \text{ even}\end{cases}$$

this if not stated clearly