Quantum Mechanics (P304H)
Part 2 – Revision

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Quantum Mechanics - Part II

Applications of the Schrödinger Equation:

- Solution of the 1-dimensional Time Independent Schrödinger Equation (TISE) for the potential step and potential barrier.
- Interpret the solutions: the tunneling process.
- Solve the TISE for potential square wells of finite and infinite depth.
- Discuss the resulting quantised and continuous energy levels, eigenvalues and quantum numbers.
- Show that the TISE for the (1d) simple harmonic oscillator results in Hermite's equation, with solutions which are Hermite functions.
- Show that the boundary conditions result in the quantization of its energy levels.
- Use the optical spectroscopy of quantum wells in semiconductors and alpha particle decay as examples.

Angular Momentum:

- Review "Classical" angular momentum.
- Motivate the angular momentum operators in quantum mechanics and derive their commutation relations.
- Solve the angular part of the TISE for a central potential and define spherical harmonics and Legendre polynomials in terms of eigenfunctions of angular momentum.
- Provide an elementary treatment of the addition of angular momenta by analogy to vectors.

Wave functions

- In Quantum Mechanics, all information about a particle is contained in its wave function: $\Psi(x,t)$
- Probability of finding particle in region x to $x+dx$ is

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

- The particle must be somewhere in space (normalization condition):

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

- The behaviour of a particle is described by the time-dependent Schrödinger equation:

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

where $\hat{H}$ is the Hamiltonian operator: $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

Operators

- In QM, dynamical variables are replaced by *operators*, e.g. $\hat{O}$
- The eigenvalue equation is: $\hat{O}\Psi(x,t) = O_n\Psi(x,t)$
- Operators:

Quantity	Operator	Representation
Momentum	$\hat{p}_x$	$-i\hbar\frac{\partial}{\partial x}$
Position	$\hat{x}$	x
Kinetic energy	$\hat{T} = \frac{\hat{p}_x^2}{2m}$	$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
Potential energy	$\hat{V}$	$V(x)$
Total energy (Hamiltonian)	$\hat{H} = \hat{T} + \hat{V}$	$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

The Schrödinger Equation

We performed a separation of variables

$$\Psi(x,t) = T(t)\,\psi(x)$$

and

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) \Rightarrow$$

$$i\hbar\frac{\partial T(t)}{\partial t}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}T(t) + V(x)\psi(x)T(t)$$

We have separated the spatial part of the Schrödinger equation. This is called the Time-Independent Schrödinger Equation - **TISE** (in 1D):

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = E$$

This is an eigenvalue problem $\hat{H}\psi(x) = E\psi(x)$

Free particle

- In this case $V(x)=0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - E\psi(x) = 0 \quad \Rightarrow \quad \psi(x) = Ae^{ikx} + Be^{-ikx} \quad \text{with} \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

- Full wave function including the time-dependant part was:

$$\Psi(x,t) = \left(Ae^{ikx} + Be^{-ikx}\right)e^{-i\omega t} \quad \text{where} \quad \omega = \frac{E}{\hbar} \qquad (2)$$

i.e. the sum of two plane waves. *E* is the energy of the system.

- This solution is not normalisable: we can normalise the wavefunction only if the particle is confined to a region of space.
- Momentum can be defined with:

$$\overline{p}_x = \int \Psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\Psi(x,t)\right)dx = \int A^* e^{-ikx} k\hbar A e^{ikx} dx = \hbar k$$

Probability density

- The probability density, when $B=0$ in eq. (2), was defined as:

$$P(x,t) = |\Psi(x,t)|^2 = \left|Ae^{i(kx-\omega t)}\right|^2 = |A|^2$$

- The probability current density was defined as

$$\mathbf{J}(x,t) = \frac{\hbar}{i2m}\left[\Psi^*(x,t)(\nabla\Psi(x,t)) - \left(\nabla\Psi^*(x,t)\right)\Psi(x,t)\right] = \mathrm{Re}\left[\Psi^*(x,t)\left(\frac{\hbar}{im}\nabla\Psi(x,t)\right)\right]$$

and in this case

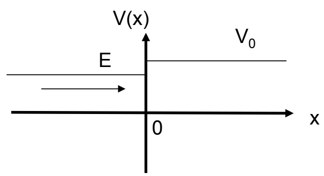
$$J(x,t) = \mathrm{Re}\left[A^* e^{-i(kx-\omega t)}\frac{\hbar}{im}Aike^{i(kx-\omega t)}\right] = \frac{\hbar k}{m}|A|^2 = v|A|^2$$

from which

$$J(x,t) = vP(x,t) \qquad \frac{\partial P(x,t)}{\partial t} + \frac{\partial J(x,t)}{\partial x} = 0$$

Potential step

$E<V_0$



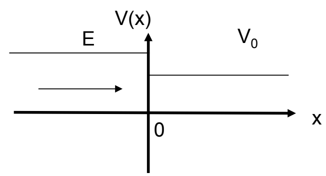
$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \quad , x<0$$

$$\frac{d^2\psi(x)}{dx^2} - \kappa^2\psi(x) = 0 \quad , x\geq 0$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \quad \kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$k,\kappa \in \mathbb{R}^+$$

$E>V_0$



$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \quad , x<0$$

$$\frac{d^2\psi(x)}{dx^2} + k'^2\psi(x) = 0 \quad , x\geq 0$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \quad k' = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

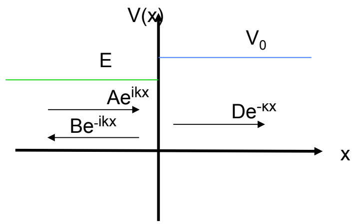
$$E > V_0 \quad k,k' \in \mathbb{R}^+$$

Potential step

$E<V_0$

$$\psi(x)=\begin{cases}Ae^{ikx}+Be^{-ikx} & ,x<0\\ Ce^{\kappa x}+De^{-\kappa x} & ,x\geq 0\end{cases}$$

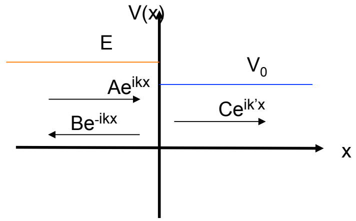
Coefficient C must be zero, else this term grows to infinity when $x\to\infty$



$E>V_0$

$$\psi(x)=\begin{cases}Ae^{ikx}+Be^{-ikx} & ,x<0\\ Ce^{ik'x}+De^{-ik'x} & ,x\geq 0\end{cases}$$

This would be a plane wave coming from the right, which we don't have, so D must be 0.



Potential step

$E<V_0$

Probability current density:

$$J(x,t)=\text{Re}\left[\psi^*\frac{\hbar}{im}\frac{\partial}{\partial x}\psi\right]$$

$$\kappa\in\mathbb{R}^+,\quad |A|^2=|B|^2 \leftarrow \text{Standing wave}$$

$$J(x,t)=\begin{cases}v\left(|A|^2-|B|^2\right)=0, & x<0\\ 0, & x\geq 0\end{cases}$$

Reflection and transmission coefficients:

$$R=\frac{v|B|^2}{v|A|^2}=\frac{|B|^2}{|A|^2}=1,\quad T=0$$

The wave is totally reflected, even though there is a non-zero probability of finding the particle at x>0.

$E>V_0$

Probability current density:

$$J(x,t)=\begin{cases}v\left(|A|^2-|B|^2\right), x<0, & v=\dfrac{\hbar k}{m}\\ v'|C|^2 \quad ,x\geq 0, & v'=\dfrac{\hbar k'}{m}\end{cases}$$

$$k,k'\in\mathbb{R}^+,\quad J(x,t)\neq 0$$

Reflection and transmission coefficients:

$$R=\frac{v|B|^2}{v|A|^2}=\frac{|B|^2}{|A|^2}=\frac{(k-k')^2}{(k+k')^2}$$

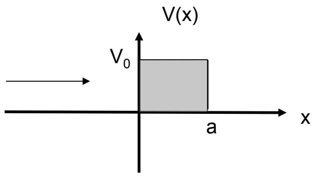
$$T=\frac{v'|C|^2}{v|A|^2}=\frac{4kk'}{(k+k')^2}$$

$$R+T=1$$

Potential Barrier

– The potential is defined as:

$$V(x)=\begin{cases}0 \text{ if } x<0\\ V_0 \text{ if } 0<x<a\\ 0 \text{ if } x\geq a\end{cases}$$



– The 1D Schrödinger equation is: $\dfrac{d^2\psi(x)}{dx^2}+\dfrac{2m}{\hbar^2}[E-V(x)]\psi(x)=0$

– The particle is free in the regions $x<0$ and $x>a$. We assume that the particle is incident from the left, with amplitude A, that there is a reflected wave of amplitude B from left to right, and that there is a transmitted wave of amplitude C and wave number k:

$$\psi(x)=\begin{cases}Ae^{ikx}+Be^{-ikx} & ,x<0\\ Ce^{ikx} & ,x>a\end{cases}\qquad k=\sqrt{\frac{2mE}{\hbar^2}}$$

Potential Barrier with $E<V_0$

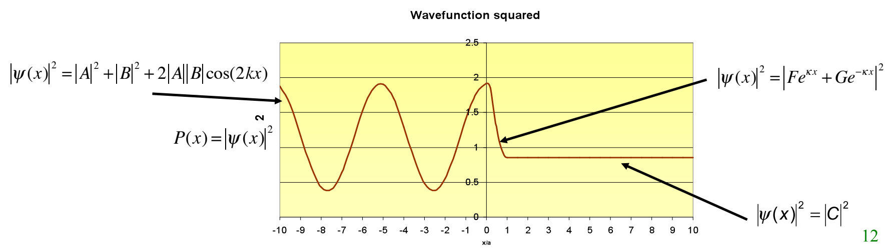
The reflection and transmission coefficients:

$$R=\frac{|B|^2}{|A|^2}=\left[1+\frac{4k^2\kappa^2}{(k^2+\kappa^2)\sinh^2(\kappa a)}\right]^{-1}=\left[1+\frac{4E(V_0-E)}{V_0^2\sinh^2(\kappa a)}\right]^{-1}$$

$$T=\frac{|C|^2}{|A|^2}=\left[1+\frac{(k^2+\kappa^2)\sinh^2(\kappa a)}{4k^2\kappa^2}\right]^{-1}=\left[1+\frac{V_0^2\sinh^2(\kappa a)}{4E(V_0-E)}\right]^{-1}$$

$$\Rightarrow\quad R+T=1$$

There is a <u>non-zero probability</u> of the particle leaking through the potential barrier (barrier penetration, or tunnel effect). This is one of the remarkable consequences of Quantum Mechanics.



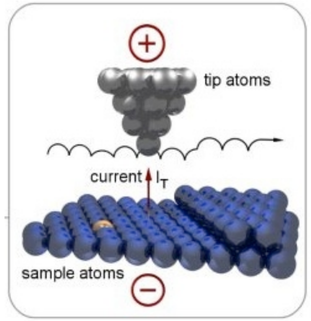
Potential Barrier with E<V_0

- For small values of the energy $(E \to 0)$ we have: $T \to 0$
- When the energy E approaches V_0 (the top of the barrier), then:

$$\lim_{E\to V_0} T = \lim_{E\to V_0}\left[1+\frac{V_0^2\,2m(V_0-E)a^2}{4E(V_0-E)\hbar^2}\right]^{-1} = \left[1+\frac{mV_0a^2}{2\hbar^2}\right]^{-1}$$

- Also, when the opacity $\frac{mV_0a^2}{\hbar^2}$ is very large ($\kappa a \gg 1$) then:

$$\sinh(\kappa a) \approx \frac{e^{\kappa a}}{2} \Rightarrow T \approx \frac{16E(V_0-E)}{V_0^2}e^{-2\kappa a}$$



- This formula was relevant for **scanning electron microscopy** where contour maps as accurate as 10^{-11}m can be made.

Potential Barrier with E>V_0

- Solution in the barrier region is similar to the case when E<V_0, but now:

$$\psi(x) = Fe^{ik'x} + Ge^{-ik'x}, \quad 0<x<a \qquad \text{with } k' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

- The solutions are:

$$R = \frac{|B|^2}{|A|^2} = \left[1+\frac{4k^2k'^2}{(k^2-k'^2)^2\sin^2(k'a)}\right]^{-1} = \left[1+\frac{4E(E-V_0)}{V_0^2\sin^2(k'a)}\right]^{-1}$$

$$T = \frac{|C|^2}{|A|^2} = \left[1+\frac{(k^2-k'^2)^2\sin^2(k'a)}{4k^2k'^2}\right]^{-1} = \left[1+\frac{V_0^2\sin^2(k'a)}{4E(E-V_0)}\right]^{-1}$$

$$\Rightarrow R+T=1$$

The transmission coefficient is less than unity: $T \leq 1$. In classical physics, when $E>V_0$, the particle would always pass the barrier.

$T=1$ only when $k'a=\pi, 2\pi, 3\pi, \ldots$(when the thickness of the barrier is equal to a half-integral or integral number of de Broglie wavelengths: $\lambda' = 2\pi/k'$

- Case $E=V_0$ can only be investigated as a limit case for $E \lessgtr V_0$

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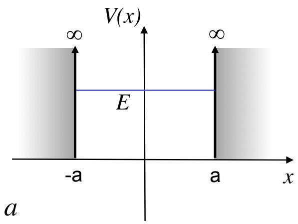
Infinite Potential Well

Potential

$$V(x) = \begin{cases} 0 & \text{if} \quad -a<x<a \\ \infty & \text{if} \quad |x|>a \end{cases}$$



Schrödinger equation:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0 \quad \text{for} \quad -a<x<a$$

Solution:

$$\psi(x) = A'e^{ikx} + B'e^{-ikx} = A\cos kx + B\sin kx \qquad k=\sqrt{\frac{2mE}{\hbar^2}}$$

Boundary conditions (wave function must be zero at both walls) has as consequence the quantisation of the wave number:

$$\cos(\text{ka}) = 0 \Rightarrow k_n = \frac{n\pi}{2a} = \frac{n\pi}{L}, \quad n=1,3,5,\ldots$$

$$\sin(\text{ka}) = 0 \Rightarrow k_n = \frac{n\pi}{2a} = \frac{n\pi}{L}, \quad n=2,4,6,\ldots$$

Infinite Potential Well

Wave functions can be normalised:

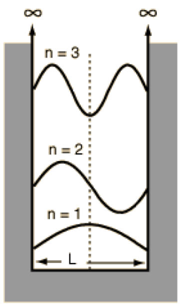
$$\psi_n(x) = \frac{1}{\sqrt{a}}\cos\left(\frac{n\pi}{2a}x\right), \quad n = 1,3,5,\ldots$$

symmetric (even function) $\psi_n(x) = \psi_n(-x)$

$$\psi_n(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}x\right), \quad n = 2,4,6,\ldots$$

antisymmetric (odd function) $\psi_n(x) = -\psi_n(-x)$

The solutions have a definite *parity* (either odd or even).



Corresponding de Broglie wavelength:

$$k_n = \frac{n\pi}{2a} \Rightarrow \quad \lambda_n = \frac{2\pi}{k_n} = \frac{2L}{n} \quad n = 1,2,3,4,\ldots.$$

Only half integer and integer wavelengths fit in the box.

The energy is quantized

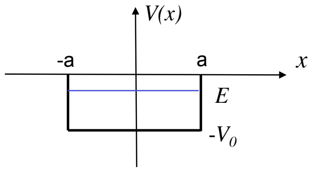
$$E_n = \frac{p^2}{2m} = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2\pi^2 n^2}{8ma^2} = \frac{\hbar^2\pi^2 n^2}{2mL^2}$$

Wavefunctions are normalisable for a confined particle.

Finite Potential Well

E<V_0

Bound state where E is the binding energy:



Schrödinger equation inside the well:

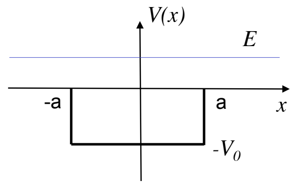
$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + \alpha^2\psi(x) = 0, \quad |x| < a$$

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

E>V_0

Scattering in a potential well:



The Schrödinger equation:

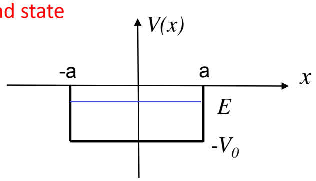
$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0$$

use $k = \sqrt{\frac{2mE}{\hbar^2}}$, $\alpha = \sqrt{\frac{2m(V_0 + E)}{\hbar^2}}$

Finite Potential Well

E<V_0

Bound state



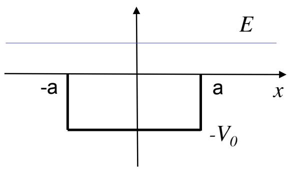
Schrodinger equation outside the well:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} - \beta^2\psi(x) = 0, \quad |x| > a$$

with $\beta = \sqrt{-\frac{2m}{\hbar^2}E} = \sqrt{\frac{2m}{\hbar^2}|E|}$

E>V_0



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Finite Potential Well

E<V_0

Solutions (even and odd):

$$\psi(x) = \begin{cases} A\cos(\alpha x), & 0 < |x| < a \\ Ce^{-\beta|x|}, & |x| > a \end{cases}$$

$$\psi(x) = \begin{cases} B\sin(\alpha x), & 0 < |x| < a \\ Ce^{-\beta|x|}, & |x| > a \end{cases}$$

Continuity conditions lead to transcedental equations which could be solved graphically or numerically.

$$\alpha a\tan(\alpha a) = \beta a$$

$$\alpha a\cot(\alpha a) = -\beta a$$

For $V_0 \to \infty \Rightarrow \gamma \to \infty$ we recover the infinite well solution.

E>V_0

Solutions:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < -a \\ Fe^{i\alpha x} + Ge^{-i\alpha x}, & -a < x < a \\ Ce^{ikx}, & x > a \end{cases}$$

Reflection and transmission coefficients:

$$R = \frac{|B|^2}{|A|^2} = \left[1 + \frac{4E(E+V_0)}{V_0^2\sin^2(\alpha L)}\right]^{-1}$$

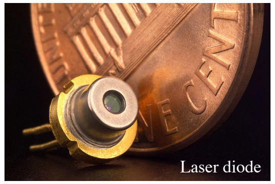
$$T = \frac{|C|^2}{|A|^2} = \left[1 + \frac{V_0^2\sin^2(\alpha L)}{4E(E+V_0)}\right]^{-1}$$

$T<1$ with maxima ($T=1$) occurring when αL=nπ, i.e. when L is an integral or half-integral number of de Broglie wavelengths. As $E \gg V_0$, T tends asymptotically to 1.

Finite Potential Well effects and applications

- Ramsauer effect: the scattering of low energy electrons off atoms in a gas could not be explained classically, since they behave as QM finite potential wells

- Semiconductor applications: "quantum wells" - obtained by sandwiching materials with different energy gaps - have applications in specialised semiconductor devices like: laser diodes, HFET and MODFET transistors, QWIPs (quantum well infrared photodetectors)



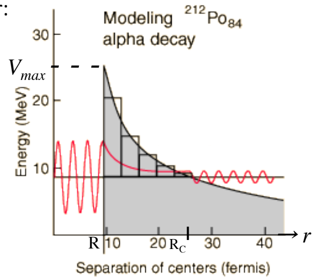
- Alpha decay: radioactive half-time can be calculated by modelling alpha as a particle behind a potential barrier:

$$nT \approx \frac{1}{2} \qquad T \simeq \prod_i T_i(V_i, a)$$

$$\Delta t = \frac{2R}{v} = 2R\sqrt{\frac{M}{2E_\alpha}}$$

$$t_{1/2} \approx n\Delta t \approx \frac{\Delta t}{2T}$$

Such a simplistic model does not always work though



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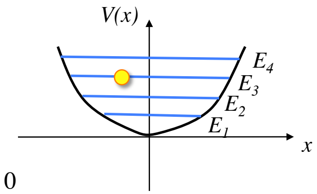
Harmonic Oscillator

- Defined by a quadratic potential:

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



- Schrödinger equation:

$$\left(\frac{m\omega}{\hbar}\right)\frac{d^2\psi(x)}{dy^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}x^2\right)\psi(x) = 0$$

$$\alpha = \frac{2E}{\hbar\omega}, \quad \beta = \sqrt{\frac{m\omega}{\hbar}} \quad \text{and} \quad y = \beta x \quad \Rightarrow \quad \frac{d^2\psi}{dy^2} + \left(\alpha - y^2\right)\psi = 0$$

- The solutions involve Hermite polynomials

$$\psi_n(y) = \sqrt{\frac{1}{2^n n!}}\left(\frac{\beta^2}{\pi}\right)^{1/4} e^{-y^2/2} H_n(y), \qquad n = 0, 1, 2, \ldots$$

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n}\left(e^{-y^2}\right)$$

Wave functions are normalisable because the particle is confined.

Harmonic Oscillator

- Energies are quantised (because again, the particle is confined):

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

- The energy levels are equidistant: $E_{n+1} - E_n = \hbar\omega$

- Ground state energy is non-zero: $E_0 = \frac{\hbar\omega}{2} > 0$

- This is a very important physical result because it tells us that the energy of a system described by a harmonic oscillator potential cannot have null energy.
- There is no classical equivalent to this.
- Physical systems such as atoms in a lattice or in molecules of a diatomic gas cannot have zero energy even at absolute zero temperature ($T=0K$).
- For example this zero point energy is what prevents liquid 4He from freezing at atmospheric pressure, no matter how low the temperature.

Harmonic Oscillator

- The Hermite polynomials can be calculated recursively
- The first four normalised wave function solutions:

$$x = y\left(\frac{m\omega}{\hbar}\right)^{-1/2}$$

$$H_0(y) = 1 \quad H_1(y) = 2y \quad H_2(y) = 4y^2 - 2 \quad H_3(y) = 8y^3 - 12y \quad \Rightarrow$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

$$\psi_1(x) = \left(\frac{4}{\pi}\right)^{1/4}\left(\frac{m\omega}{\pi\hbar}\right)^{3/4} x \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

$$\psi_2(x) = \left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left[\left(\frac{2m\omega}{\hbar}\right)x^2 - 1\right]\exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

$$\psi_3(x) = \left(\frac{1}{9\pi}\right)^{1/4}\left(\frac{m\omega}{\hbar}\right)^{3/4}\left[\left(\frac{2m\omega}{\hbar}\right)x^3 - 3x\right]\exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

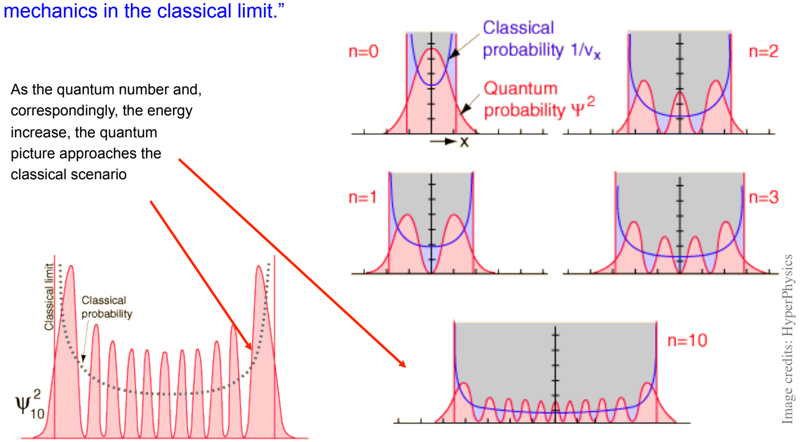
with the corresponding energies:

$$E_0 = \frac{1}{2}\hbar\omega, \quad E_1 = \frac{3}{2}\hbar\omega, \quad E_2 = \frac{5}{2}\hbar\omega, \quad E_3 = \frac{7}{2}\hbar\omega$$

Discrete energy levels are a characteristic of confined particles in QM.

Harmonic Oscillator at the classical limit

The correspondence principle: "results of quantum mechanics tend towards classical mechanics in the classical limit."



Uncertainty principle and the harmonic oscillator

- The harmonic oscillator offers a nice illustration of the Uncertainty Principle:

For the ground state:

$$\langle x^2\rangle = \frac{\hbar}{2m\omega}, \quad \langle p_x^2\rangle = \frac{1}{2}m\hbar\omega, \quad \langle x\rangle = 0 \quad \text{and} \quad \langle p_x\rangle = 0$$

Then

$$\Delta x \Delta p = \sqrt{\left(\langle x^2\rangle - \langle x\rangle^2\right)\left(\langle p_x^2\rangle - \langle p_x\rangle^2\right)} =$$

$$= \sqrt{\frac{\hbar}{2\,m\omega}\times\frac{1}{2}\,m\omega\,\hbar} = \sqrt{\frac{\hbar^2}{4}} = \frac{\hbar}{2}$$

The non-zero ground state energy can be interpreted as the smallest energy allowed by the uncertainty principle.

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Angular Momentum:

- Review "Classical" angular momentum.
- Motivate the angular momentum operators in quantum mechanics and derive their commutation relations.
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- Provide an elementary treatment of the addition of angular momenta by analogy to vectors.

Operators and their properties

- Commutation relations for operators:
  - The commutator was defined as: $\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}$

  In general, for operators in QM: $\left[\hat{A},\hat{B}\right]\neq 0$ (non-Abelian algebra)
  - Momentum and position operators do not commute:

$$\left[\hat{x},\hat{p}_x\right]=i\hbar \text{ with } \hat{x}=x \text{ and } \hat{p}_x=(-i\hbar)\frac{d}{dx}$$

(Shown in QM Part 1)

  - Commutator algebra reminders:

$$1)\left[\hat{A},\hat{B}\right]=-\left[\hat{B},\hat{A}\right];$$
$$2)\left[\alpha\hat{A},\beta\hat{B}\right]=\alpha\beta\left[\hat{A},\hat{B}\right];$$
$$3)\left[\hat{A},\hat{B}\pm\hat{C}\right]=\left[\hat{A},\hat{B}\right]\pm\left[\hat{A},\hat{C}\right]$$
$$4)\left[\hat{A},\hat{B}\hat{C}\right]=\left[\hat{A},\hat{B}\right]\hat{C}+\hat{B}\left[\hat{A},\hat{C}\right];$$
$$5)\left[\hat{A},\left[\hat{B},\hat{C}\right]\right]+\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]+\left[\hat{C},\left[\hat{A},\hat{B}\right]\right]=0$$

Hermitian operators and compatible observables

- Quantum mechanical operators are Hermitian, i.e.

$$\int_{-\infty}^{\infty}\psi^*(x)\left(\hat{Q}\varphi(x)\right)dx=\int_{-\infty}^{\infty}\left(\hat{Q}\psi\right)^*\varphi(x)dx$$

- Eigenvalues of Hermitian operators are real.

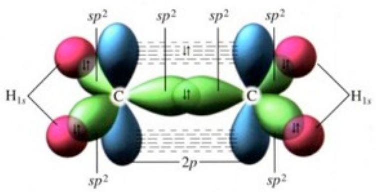
- A complete set of commuting observables is a set of commuting operators whose eigenvalues completely specify the state of a system.
- If there exists a complete set of functions ψ_n, such that each function is an eigenfunction of two operators Â and B, then the observables of the operators are said to be compatible

$$\hat{A}\psi_n=a_n\psi_n \qquad \hat{B}\psi_n=b_n\psi_n \quad \Rightarrow \hat{A}\hat{B}\psi_n=\hat{A}b_n\psi_n=a_nb_n\psi_n=b_na_n\psi_n=\hat{B}\hat{A}\psi_n$$

Two compatible observables commute!

Switching to 3D: Angular Momentum

- Angular momentum is important and a concept necessary in many domains of physics to describe atomic, molecular and nuclear spectra, the spin of elementary particles, magnetism, etc.
- Classically, it is a *constant of motion*, *i.e.* a conserved quantity in an isolated system
- In a central potential $dL/dt=0$
- There are also typical QM angular momenta with no classical equivalents
- Stern-Gerlach experiment
- Zeeman effect



Angular Momentum

- General QM properties of angular momenta follow purely from commutation relations between the associated operators
- Starting from the classical definition of $\underline{L}$, we have constructed our operator $\hat{L}$
- We've constructed various observables, we have found that $\left[\hat{L}_z,\hat{L}^2\right]=0$ and have chosen $\hat{L}^2$ and $\hat{L}_z$ for our set of compatible observables
- In polar coordinates

$$\hat{L}^2=-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right) \qquad (1)$$

$$\hat{L}_z=-i\hbar\frac{\partial}{\partial\varphi} \qquad (2)$$

- We were looking for the eigenfunctions and eigenvalues of these operators

$$\hat{L}^2Y_{lm}(\theta,\varphi)=l(l+1)\hbar^2Y_{lm}(\theta,\varphi) \qquad (3)$$

$$\hat{L}_zY_{lm}(\theta,\varphi)=m\hbar Y_{lm}(\theta,\varphi) \qquad (4)$$

where by $Y_{lm}(\theta,\phi)$ we have denoted the wave function (for reasons we will discover later on).

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Polar coordinates

- It is convenient to work in polar coordinates:

$$x = r\sin\theta\cos\varphi \qquad y = r\sin\theta\sin\varphi \qquad z = r\cos\theta$$

$$\Rightarrow \quad \underline{\nabla} = \underline{u}_r\frac{\partial}{\partial r} + \underline{u}_\theta \frac{1}{r}\frac{\partial}{\partial\theta} + \underline{u}_\varphi \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi} \qquad \underline{r} = \underline{u}_r r$$

– Therefore:

$$\hat{\underline{L}} = -i\hbar\underline{r}\times\underline{\nabla} = -i\hbar\left(\underline{u}_\varphi\frac{\partial}{\partial\theta} - \underline{u}_\theta\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}\right)$$

no radial dependence - L does not depend on $\underline{u}_r$

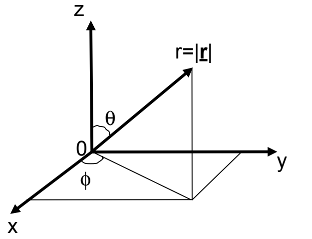
– The components of the L operator were:

$$\hat{L}_x = -i\hbar\left(-\sin\varphi\frac{\partial}{\partial\theta} - \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)$$

$$\hat{L}_y = -i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)$$

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

simplest



$$r \geq 0, \quad 0 \leq \theta \leq \pi, \quad 0 \leq \varphi \leq 2\pi$$

Angular Momentum Solutions

– Without implying any properties for the numbers l and m, we have chosen for <u>convenience</u> to write the eigenvalues of $\hat{L}^2$ and $\hat{L}_z$ as

$$\lambda' = l(l+1)\hbar^2$$
$$\lambda = m\hbar$$

– We've performed a separation of variables by writing $Y_{lm}(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi)$

– With (2), we've solved the eigenvalues equation (4) for $\Phi(\varphi)$ and from boundary conditions we've found out that m must be quantised $m=0,\pm1,\pm2, \dots$

– Using the substitution $F_{lm}(w) = \Theta_{lm}(\theta)$ with $w = \cos\theta \quad (-1 \leq w \leq 1)$ we have obtained from (1) and (3) the equation

$$\left((1-w^2)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + l(l+1) - \frac{m^2}{1-w^2}\right)F_{lm}(w) = 0$$

– This we have identified as Legendre's equation - the solutions of which are known.

Solutions for m=0

– For the special case $m=0$

$$\left((1-w^2)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + l(l+1)\right)F_{l0}(w) = 0$$

we had the solution (normalised)

$$F_{l0}(w) = \left(\frac{2l+1}{2}\right)^{1/2} P_l(w) \qquad (5)$$

where by $P_l(w)$ we denote the Legendre polynomial or order l, given by the formula:

$$P_l(w) = \frac{1}{2^l\,l!}\frac{d^l}{dw^l}\left[(w^2-1)^l\right]$$

where

$$P_0(w) = 1, \quad P_1(w) = w \qquad (l+1)P_{l+1}(w) = (2l+1)wP_l(w) - lP_{l-1}(w)$$

Solutions when m≠0

- When $m \neq 0$:

$$\left((1-w^2)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + l(l+1) - \frac{m^2}{1-w^2}\right)F_{lm}(w) = 0 \qquad (6)$$

  – Note that this equation is independent of the sign of m; its solutions depend only on l and $|m|$.

- The solutions of this equation are known to be of the form $F_{lm}(w) = P_l^{|m|}(w)$ or more exactly:

Phase factor — *Normalisation* — *Associated Legendre polynomial*

$$F_{lm}(w) = (-1)^m\left[\frac{(2l+1)(l-m)!}{2(l+m)!}\right]^{1/2} P_l^m(w), \quad m \geq 0$$

$$F_{lm}(w) = (-1)^m F_{l|m|}(w), \qquad m < 0$$

where $P_l^m(w)$ are called associated Legendre functions.

Associated Legendre Functions

- The associated Legendre functions are defined as:

$$P_l^{|m|}(w) = \left(1-w^2\right)^{\frac{|m|}{2}} \frac{d^{|m|}}{dw^{|m|}} P_l(w)$$

where $P_l(w)$ is the Legendre polynomial defined in (5).

- They satisfy the orthogonality relation:

$$\int_{-1}^{1} P_l^{|m|}(w) P_{l'}^{|m|}(w)\, dw = \frac{2}{2l+1}\frac{(l+|m|)!}{(l-|m|)!}\delta_{ll'}$$

- They can be obtained by recurrence

$$(2l+1)wP_l^m = (l+1-m)P_{l+1}^m + (l+m)P_{l-1}^m$$

$$(2l+1)\sqrt{1-w^2}\,P_l^{m-1} = P_{l+1}^m - P_{l-1}^m$$

- There are $2l+1$ allowed values for m:

$$|m| \leq l \quad \Rightarrow \quad -l, -l+1, ..., 0, ..., l-1, l$$

Full solution

- Remember that the full solution for the wave function was

$$Y_{lm}(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi) \quad \text{where} \quad \Theta(\theta) = F_{lm}(w), \quad w = \cos\theta$$

- Hence, the normalised eigenfunctions $Y_{lm}(\theta,\varphi)$ common to the operators L^2 and L_z are:

$$Y_{lm}(\theta,\varphi) = (-1)^m\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\,P_l^m(\cos\theta)e^{im\varphi}, \quad m \geq 0$$

$$Y_{lm}(\theta,\varphi) = (-1)^m Y_{l|m|}^*(\theta,\varphi), \qquad m < 0$$

- These functions are called spherical harmonics. They are orthonormal:

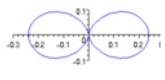
$$\int_{-1}^{1} Y_{l'm'}^*(\theta,\varphi)Y_{lm}(\theta,\varphi)d\Omega = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta\, Y_{l'm'}^*(\theta,\varphi)Y_{lm}(\theta,\varphi) = \delta_{ll'}\delta_{mm'}$$

3D Plots

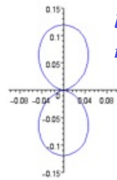
- The expressions and 3D-graphs of some spherical harmonics:

$Y_0^0 = \sqrt{\frac{1}{4\pi}}$	$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos(\theta)$	$Y_2^0 = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$
	$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$	$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$
	$Y_1^{-1} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\phi}$	$Y_2^{-1} = \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{-i\phi}$
		$Y_2^2 = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{2i\phi}$
		$Y_2^{-2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{-2i\phi}$

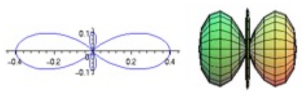
l=0; m=0



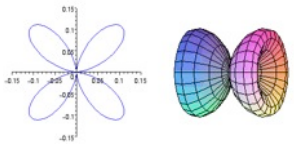
l=1; m=0



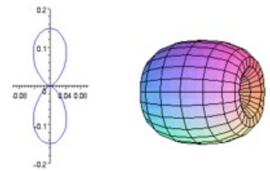
l=1; m=+1



l=2; m=0



l=2; m=+1



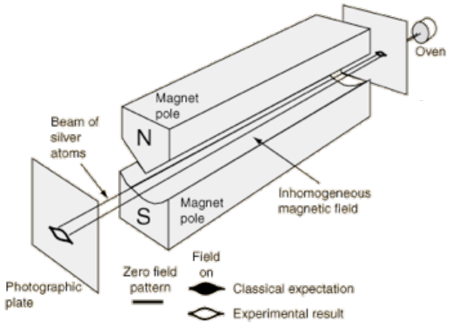
l=2; m=+2

The Stern-Gerlach experiment

- Experiment performed in 1922 by Otto Stern and Walter Gerlach to test the Bohr–Sommerfeld hypothesis that the direction of the angular momentum of a silver atom is quantised.
- Neutral atoms do not get deflected in a uniform magnetic field
- However, if an atom with a magnetic moment μ_z is in an inhomogeneous magnetic field $B(x)$ parallel to z, then a force emerges:

$$F = \mu_z \frac{\partial B(x)}{\partial x}$$

- Stern and Gerlach used a beam of Ag atoms that was passing through a non-uniform magnetic field before falling onto a collection plate

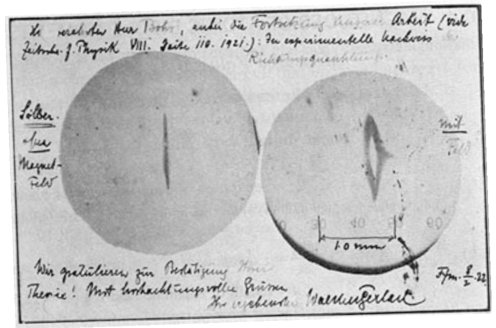


Spin

- Classically, if the atom is in the ground state (l=0) then the deflection should be random and the image on the collection plate should be symmetrical about the centre
- Quantum Mechanics predicts that the beam will split into $2l+1$ parts
- The two lines observed by Stern and Gerlach observed two lines fited with neither the classical case nor with any possible $2l+1$ multiplicity
- The two lines observed implied that

$$2l+1=2 \quad \Rightarrow \quad l=\frac{1}{2}$$

- The explanation required a new, purely QM concept: the spin s=1/2
- The spin is an intrinsic QM property with no classical equivalent



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Matrix representation

- The matrix representation of angular momentum:
  - A general angular momentum state can be written as:

$$|\psi\rangle = a_1|l,l\rangle + a_2|l,l-1\rangle + \ldots + a_{2l}|l,-l+1\rangle + a_{2l+1}|l,-l\rangle \qquad (1)$$

  - We can write this "$|ket\rangle$" function as a column matrix:

$$|\psi\rangle = \begin{bmatrix} a_1 \\ \vdots \\ a_{2l+1} \end{bmatrix}$$

  - And the "$\langle bra|$" function as a row matrix:

$$\langle\psi| = \begin{bmatrix} a_1^* & \cdots & a_{2l+1}^* \end{bmatrix}$$

Hermitian conjugate

- An operator acting on the wave function is then represented as a matrix multiplying the vector.
- The eigenvalue equation takes the form:

$$\hat{A}|\psi\rangle = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix}\begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} = \lambda \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} \quad \text{with} \quad n = 2l+1$$

λ is the eigenvalue

which is equivalent to:

$$\begin{vmatrix} A_{11}-\lambda & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn}-\lambda \end{vmatrix} = 0$$

- The Hermitian conjugate of matrix $\hat{A}$ is defined as:

$$\hat{A}^{+} \triangleq \hat{A}^{*T} = \begin{bmatrix} A^{*}_{11} & \cdots & A^{*}_{n1} \\ \vdots & \ddots & \vdots \\ A^{*}_{1n} & \cdots & A^{*}_{nn} \end{bmatrix}$$

Complex conjugate, transpose

- Therefore a matrix is called Hermitian if: $A_{ij} = A^{*}_{ji}$

Spin in matrix representation

- Similar to orbital angular momentum $\hat{L}$
- We denoted by χ_{s,m_s} the simultaneous eigenstates of $\hat{S}^2$ and $\hat{S}_z$:

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

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

- For spin 1/2 we have only two states:

$$\chi_{1/2,1/2}, \quad \chi_{1/2,-1/2} \qquad \left|\frac{1}{2},+\frac{1}{2}\right\rangle, \left|\frac{1}{2},-\frac{1}{2}\right\rangle$$

'spin up' (↑) 'spin down' (↓)

- Where we introduced:

$$\chi_{s,m_s} \doteq |s,m_s\rangle \qquad \left|\frac{1}{2},+\frac{1}{2}\right\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \left|\frac{1}{2},-\frac{1}{2}\right\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$|s,m_s\rangle = a_{1/2}\begin{bmatrix} 1 \\ 0 \end{bmatrix} + a_{-1/2}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} a_{1/2} \\ a_{-1/2} \end{bmatrix}$$

Ladder Operators

- We introduced *ladder operators* defined by:

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

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

The ladder operator S_+ increases eigenvalue of S_z by $\hbar$ and operator S_- lowers it by $\hbar$.

with the property

$$\hat{S}_{-} = \hat{S}_{+}^{+}$$

- Then we have: $\hat{S}_x = \frac{1}{2}\left(\hat{S}_{+} + \hat{S}_{-}\right)$ $\quad \hat{S}_y = \frac{1}{2i}\left(\hat{S}_{+} - \hat{S}_{-}\right)$

$$\left[\hat{S}_z,\hat{S}_{+}\right] = \left[\hat{S}_z,\hat{S}_x\right] + i\left[\hat{S}_z,\hat{S}_y\right] = i\hbar\hat{S}_y + i(-i\hbar)\hat{S}_x = +\hbar\hat{S}_{+}$$

$$\left[\hat{S}_z,\hat{S}_{-}\right] = -\hbar\hat{S}_{-} \qquad \hat{S}_{+} = \hbar\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \qquad \hat{S}_{-} = \hbar\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$\hat{S}_x = \frac{1}{2}\left(\hat{S}_{+} + \hat{S}_{-}\right) = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{S}_y = \frac{1}{2i}\left(\hat{S}_{+} - \hat{S}_{-}\right) = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Pauli Spin Matrices

The Pauli Spin Matrices are 2×2 complex matrices, Hermitian and unitary:

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- Such that $\underline{\hat{S}} = \frac{\hbar}{2}\underline{\hat{\sigma}}$
- And we had the properties

$$\left[\hat{S}_x,\hat{S}_y\right] = \frac{1}{4}\hbar^2\left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} - \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right)$$

$$= \frac{1}{4}\hbar^2\left(\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} - \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix}\right) = i\hbar\frac{1}{2}\hbar\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = i\hbar\hat{S}_z$$

$$\underline{\hat{S}}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = \frac{3}{4}\hbar^2\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \Rightarrow \left[\underline{\hat{S}}^2,\hat{S}_x\right] = \left[\underline{\hat{S}}^2,\hat{S}_y\right] = \left[\underline{\hat{S}}^2,\hat{S}_z\right] = 0$$

Addition of Angular Momenta

- We can have particles with both orbital angular momentum and intrinsic angular momentum (spin).
- We need to calculate the total angular momentum $\hat{\underline{J}} = \hat{\underline{L}} + \hat{\underline{S}}$

$$\hat{L}^2|l,m_l\rangle = l(l+1)\hbar^2|l,m_l\rangle \qquad \hat{S}^2|s,m_s\rangle = s(s+1)\hbar^2|s,m_s\rangle$$
$$\hat{L}_z|l,m_l\rangle = m_l\hbar|l,m_l\rangle \qquad \hat{S}_z|s,m_s\rangle = m_s\hbar|s,m_s\rangle$$

- L and S are independent, so any component of L commutes with any component of S, i.e. L^2, L_z, S^2 and S_z form a complete set of observables with eigenstates that will be the *direct product* of the individual eigenstates:

$$|(l,m_l);(s,m_s)\rangle \equiv |j,m\rangle \quad \Rightarrow \quad \begin{cases} \hat{J}^2|j,m\rangle = j(j+1)\hbar^2|j,m\rangle \\ \hat{J}_z|j,m\rangle = m\hbar|j,m\rangle \end{cases}$$

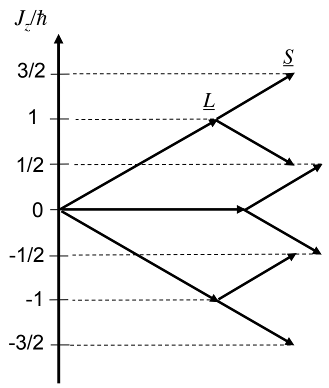
We use m_l for the L_z quantum numbers and m for the eigenvalues of J_z!

$$\left.\begin{aligned} j_{max} &= l+s \\ j_{min} &= |l-s| \end{aligned}\right\} \Rightarrow \quad |l-s| \le j \le l+s \qquad m = m_l + m_s$$

+ examples ....

Vector interpretation

- Take as example $j=l+s$, with $l=1$ and $s=1/2$



- The orbital angular momentum vector $\underline{L}$ has 3 possible orientations.
- The spin $\underline{S}$ can have **2** possible orientations.
- The total angular momentum $\underline{J}$ can then have **6** possible orientations.
- The component J_z can have **4** distinct values:

  $-3/2\hbar$, $-1/2\hbar$, $1/2\hbar$, $3/2\hbar$

Zeeman Effect

- Splitting of a spectral line into several components in the presence of a static magnetic field.
- When the magnetic interaction is stronger than the spin-orbit interaction (strong field):

$$\Delta E = \mu_B B(m_l + 2m_s)$$

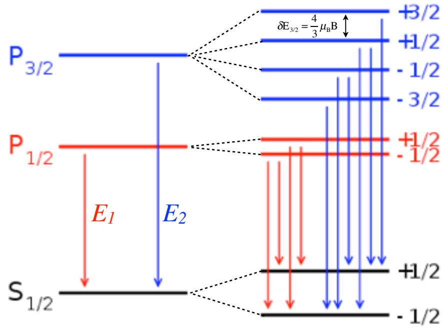
- In the case of a weak magnetic field (when the spin-orbit term dominates):

$$\Delta E_{m_j} = g\mu_B B m_j$$

with the *Landé* g factor given by

$$g = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}$$

Referred to as the 'anomalous' Zeeman effect before the electron spin was discovered.



Transitions between the energy levels of atomic hydrogen. The r.h.s. split occurs in the presence of a weak magnetic field

Heisenberg is out for a drive when he's stopped by a traffic cop. The cop says: *"Do you know how fast you were going?"* Heisenberg says: *"No, but I know where I am."*

Quantum Mechanics is easy.

If you have any questions before the exams please feel free to email me or drop by my office:

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