Física de Partículas
Aula 4
Brief overview of non-relativistic Quantum Mechanics

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Topics for the class

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Basic principles of Quantum Mechanics

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We list the basic principles of QM:

- For a given state of the system there is state function $|\Phi\rangle$ that contains all the possible information about the system
  - In many cases we deal with the representation of $|\Phi\rangle$ in terms of the coordinates and time, the so-called wave function $\Psi(q_i, s_i, t)$.
  - $|\Psi(q_i, s_i, t)|^2 \geq 0$ has an interpretation in terms of the probability density for finding the particle in a given state with coordinates q_i, internal quantum numbers s_i at time t
- The physical observables are represented by hermitian operators

$$p_i \to -i\hbar \frac{\partial}{\partial q_i} \ , \qquad E \to i\hbar \frac{\partial}{\partial t}$$

- The state $|\Phi_n\rangle$ is an eigenstate of the operator Ω if

$$\Omega \, |\Phi_n\rangle = \omega_n \, |\Phi_n\rangle$$

where $|\Phi_n\rangle$ is the eigenstate that corresponds to the eigenvalue ω_n. If Ω is hermitian then the ω_n are real.

Basic principles of Quantum Mechanics ...

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- For a complete set of operators that commute among themselves, $\{\Omega_1, \Omega_2, \ldots\}$, there exist a complete set of simultaneous eigenfunctions Ψ_n. An arbitrary state (or wave function) can be expanded in this basis as

$$\Psi = \sum_n a_n \Psi_n$$

- The result of a measurement of the observable Ω is any of its eigenvalues ω_n with probability $|a_n|^2$. The average value of an observable is

$$< \Omega >_\Psi = \sum_s \int dq_1 ... \Psi^*(q_i, s_i, t) \Omega \Psi(q_i, s_i, t) = \sum_n |a_n|^2 \omega_n$$

- The time evolution of the system is given by

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$$

(The Hamiltonian H is a linear and hermitian operator)

- The linearity implies the superposition principle and the hermiticity leads to the conservation of probability,

$$\frac{d}{dt} \sum_s \int dq_1 \cdots \Psi^* \Psi = \frac{i}{\hbar} \sum_s \int dq_1 \cdots [(H\Psi)^* \Psi - \Psi^* (H\Psi)] = 0$$

Schrödinger Equation

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- Schrödinger equation in 3 dimensions

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\Psi(\vec{r},t), \qquad \int d^3r|\Psi|^2 = 1$$

- Spherical symmetry

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{L^2}{\hbar^2 r^2}$$

where $\vec{L} = \vec{r}\times\vec{p}$ is the angular momentum operator.

- The eigenfunctions of the operator L^2 are the spherical harmonics

$$L^2 Y_{lm}(\theta,\phi) = \hbar^2\, l(l+1)\, Y_{lm}(\theta,\phi)$$

$$L_z Y_{lm}(\theta,\phi) = \hbar\, m\, Y_{lm}(\theta,\phi)\ .$$

The spherical harmonics are simultaneous eigenfunctions of the operators L_z and L^2, as these commute.

Schrödinger equation for the Central Potential

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- For the case of spherical symmetry $V(\vec{r}) = V(r)$, the Schrödinger equation can be separated in the three variables r, θ and ϕ,

$$\psi(r,\theta,\phi) = R(r)\ Y_{lm}(\theta,\phi)$$

where the radial function satisfies

$$-\frac{\hbar^2}{2m}\left(\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr}\right) + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right] R = ER$$

- It is sometimes convenient to write $R(r) = u(r)/r$. The the function $u(r)$ satisfies

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right] u = Eu$$

that is a one dimensional equation for a potential that includes the centrifugal barrier.

Spherical Harmonics

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The spherical harmonics are the product of the solutions for the equations for θ and ϕ

$$\frac{d}{d\theta}(\sin\theta\frac{d\Theta}{d\theta}) + \ell(\ell+1)\sin\Theta - \frac{m_\ell^2}{\sin\theta}\Theta = 0 \ .$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2} = -m_\ell^2 \ ,$$

conveniently normalized,

$$Y_{\ell m_\ell}(\theta,\varphi) \equiv N_{\ell m_\ell} P_\ell^{m_\ell}(\theta) e^{i m_\ell \varphi}$$

$$N_{\ell m_\ell} = (-1)^m \left[\frac{2\ \ell+1}{4\pi}\frac{(\ell-m_\ell)!}{(\ell+m_\ell)!}\right]^{1/2} \ ,$$

where $P_\ell^{m_\ell}(\theta)$ are the associated Legendre polynomials and the normalization is conventional

Schrödinger equation for the hydrogen atom

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- In our simplified study we consider the proton fixed with the electron orbiting around
- The potential energy of the electron in the field of the proton is

$$V(r) = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$$

where r is the distance between the proton and electron.

- As we are dealing with a potential with spherical symmetry (central potential) the solutions are of the general form,

$$\psi_{n,l,m}(r,\theta,\phi) = R_{nl}(r)\ Y_{lm}(\theta,\phi)$$

where the radial equation is

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR}{dr}) - \frac{2m}{\hbar^2}\left[V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right]R + \frac{2mE}{\hbar^2}R = 0\ .$$

- The spherical harmonics are the eigenfunctions of L^2 and L_z. θ e ϕ

Results from the solution of the problem

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- The only solutions that satisfy the proper boundary conditions in ϕ are those for which m_l is an integer,

$$m_l = 0, \pm 1, \pm 2, \ldots$$

- The only solutions finite everywhere (for all the $\theta' s$) are those where,

$$\ell = 0, 1, 2 \ldots, \quad \ell \geq |m_\ell|$$

- When we solve the radial equation for $R(r)$ the only solutions finite everywhere $(0 \leq r \leq \infty)$ are those for which

$$E_n = -\frac{1}{2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{m^2}{\hbar^2}\frac{1}{n^2} \qquad ; \qquad n = 1, 2, 3, \ldots \quad \ell < n$$

- The restrictions for m_ℓ and ℓ can be written as,

$$m_\ell = 0, \pm 1, \pm 2, ..., \pm \ell \quad \text{e} \quad \ell = 0, 1, 2, ..., n-1 \ .$$

Physical meaning of the results

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- The most important fact about these results is that the energy of the atom is quantized. This originates from physical requirements on the wave function.
- The second fact is that the expression for the energy is exactly the one found in the Bohr atom. The energy depends on the integer n, the principal quantum number.
- As for each value of n there are several values of ℓ and m_ℓ, it is possible for the electron to have different characteristics and have the same energy (degenerate states).

$$\text{Degree of degenerescency} = \sum_{\ell=0}^{n-1} \sum_{m_\ell=-\ell}^{+\ell} 1 = \sum_{\ell=0}^{n-1} (2\ell+1) = n^2 \ .$$

- The physical observable that distinguishes among these states is the angular momentum. One can show that the square of the angular momentum, L^2,

$$L^2 \equiv L_x^2 + L_y^2 + L_z^2 \ , \quad [L^2, L_z] = 0, \quad [L^2, H] = 0, \quad [L_z, H] = 0$$

  and L_z, commute simultaneously with the Hamiltonian
- Therefore the eigenfunctions $\psi_{n\ell m_\ell}$ should be simultaneous eigenfunctions of H, L^2 and L_z.

The Spin

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- To solve the contradictions in the observed spectra for hydrogen atom in a magnetic field, the so-called Zeeman effect, G. Uhlenbeck and S. Goudsmit proposed that the electron had an intrinsic angular momentum called *spin*, $\vec{S}$.
- This word in QM just means this property, the electron is not really spinning.
- More precisely, in Quantum Mechanics, $\vec{S}$ is an hermitian operator that obeys the angular momentum algebra,

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y$$

- The eigenvalues are

$$\begin{aligned} S^2 &= \vec{S}\cdot\vec{S} = s(s+1)\hbar^2 \qquad \text{com} \qquad s = \tfrac{1}{2} \\ S_z &= m_s\hbar \qquad ; \qquad m_s = \pm\tfrac{1}{2} \end{aligned}$$

That is, it takes half-integers values.

Spin ···

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- Associated to the spin $\vec{S}$ there exists a magnetic moment $\vec{\mu}_s$ given by,

$$\vec{\mu}_s = -\frac{|e|}{m}\vec{S}.$$

- Sometimes we write in an equivalent form

$$\vec{\mu}_s = -\frac{|e|}{2m} g\ \vec{S} \qquad ; \qquad g = 2$$

where g is the so-called gyro-magnetic ratio. The value $g = 2$ for the electron was determined experimentally to explain the spectra of the atoms.

- At the level of the Schrödinger equation the spin is an additional quantum number and the factor g experimentally determined. The spin only appears naturally in the context of the relativistic equation of Dirac, that predicts the value $g = 2$ for the electron.

- The state of the electron is then specified by the quantum numbers n, ℓ, m_ℓ e m_s (has $s = 1/2$ always). Note that $[\vec{L}, \vec{S}] = 0$ as $\vec{L}$ and $\vec{S}$ act on different spaces. This explains why it is possible to have simultaneous eigenfunctions of $\vec{L}$ and $\vec{S}$.

Addition of Angular Momentum

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- We saw that the state of the electron can be described by two angular momenta, $\vec{L}$ (orbital angular momentum) and $\vec{S}$ (spin).
- In many applications it is important to define the so-called *total angular momentum*,

$$\vec{J} \equiv \vec{L} + \vec{S} \ .$$

- $\vec{J}$ is an angular momentum has it obeys the usual algebra

$$[J_x, J_y] = i\hbar J_z \quad [J_y, J_z] = i\hbar J_x \quad [J_z, J_x] = i\hbar J_y \ ,$$

- What are the possible values for $\vec{J}$? It is outside this introduction to explain all the details.
- The results are however simple and are important in the applications. We will present them in the form of theorems without demonstration.

Theorems for the Angular Momentum

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Theorem 1

Let $\vec{J}$ be an operator with the angular momentum algebra. Then the eigenvalues of $J^2 = \vec{J} \cdot \vec{J}$ and J_z are

$$J^2 = j(j+1)\hbar^2, \quad J_z = m_j \hbar$$

where j is an integer or half-integer and m_j takes the $(2\ j+1)$ values

$$m_j = -j, -j+1, ..., j-1, j \ .$$

- Particular cases for this theorem are the cases where $\vec{J} = \vec{L}$ where $j = \ell =$ integer and $\vec{J} = \vec{S}$ where $j = s = \frac{1}{2} =$ half-integer.

Theorem 2

Let $\vec{J} = \vec{J}_1 + \vec{J}_2$ be the angular momenta corresponding to the sum of two angular momenta with values j_1 e j_2. Then the value j that corresponds to $\vec{J}$ can take the values

$$|j_1 - j_2| \leq j \leq j_1 + j_2 \ .$$

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- **Theorem 3**
  Let $\vec{J} = \vec{J}_1 + \vec{J}_2$. Then the number of possible values for m_j obeys the relation

$$\sum_{|j_1 - j_2|}^{j_1 + j_2} (2\,j + 1) = (2\,j_1 + 1)\,(2\,j_2 + 1)\ .$$

- Example: Table for the possible values of j and m_j for an electron ($s = 1/2$) with orbital angular momentum $\ell = 0, 1$ and 2.

ℓ	j	m_j
0	$\frac{1}{2}$	$-\frac{1}{2}, \frac{1}{2}$
1	$\frac{1}{2}$	$-\frac{1}{2}, \frac{1}{2}$
	$\frac{3}{2}$	$-\frac{3}{2}, -\frac{1}{2}\ \ \frac{1}{2}, \frac{3}{2}$
2	$\frac{3}{2}$	$-\frac{3}{2}, -\frac{1}{2}\ \ \frac{1}{2}, \frac{3}{2}$
	$\frac{5}{2}$	$-\frac{5}{2}, -\frac{3}{2}\ \ -\frac{1}{2}, \frac{1}{2},\ \ \frac{3}{2}, \frac{5}{2}$

The Clebsch-Gordon coefficients

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- A state $|J, M\rangle$ where $\vec{J} = \vec{J}_1 + \vec{J}_2$ can be expressed in terms of the eigenstates of $\vec{J}_1$ and $\vec{J}_2$, denoted by $|j_1, m_1\rangle$ and $|j_2, m_2\rangle$, respectively.
- This relation is normally written in the form,

$$|J, M\rangle = \sum_{m_1=-j_1}^{m_1=j_1} \sum_{m_2=-j_2}^{m_2=j_2} |j_1, m_1\rangle \otimes |j_2, m_2\rangle \langle j_1 j_2, m_1 m_2 | J, M\rangle$$

  where $m_1 + m_2 = M$ and $\langle j_1 j_2, m_1 m_2 | JM\rangle$ are the Clebsh-Gordon coefficients.
- Their value can be obtained from the rules of the angular momentum operator, but normally we use tables to read the coefficients.
- Normally to obtain the coefficients one has to take the square root, with the convention that the minus sign is outside the square root. We will give one example.

Use of the Table of Clebsch-Gordon Coefficients

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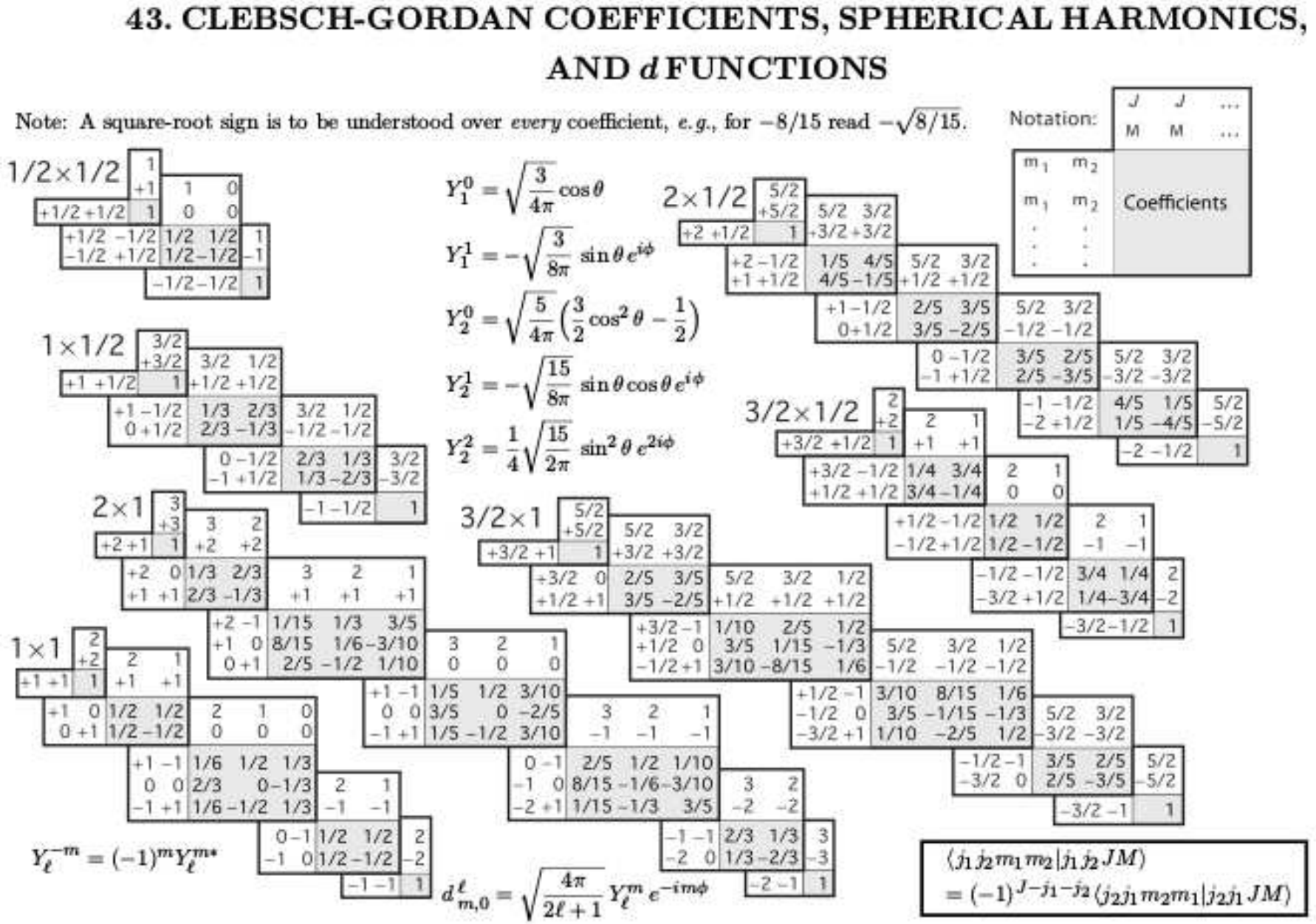

Use of the Table of Clebsch-Gordon Coefficients: Case $1 \times 1/2$

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$$1 \times 1/2 = 3/2 + 1/2$$

$J = 3/2$	$J = 1/2$	
$\|3/2, 3/2\rangle$		
$\|3/2, 1/2\rangle$	$\|1/2, 1/2\rangle$	Orthogonal
$\|3/2, -1/2\rangle$	$\|1/2, -1/2\rangle$	Orthogonal
$\|3/2, -3/2\rangle$		

Use of the Table of Clebsch-Gordon Coefficients: Case $1 \times 1/2$

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- We have $(2 \times 1 + 1) \times 2 = (2 \times 3/2 + 1) + (2 \times 1/2 + 1) = 6$ states.
- We get

$$|3/2, 3/2\rangle = |1, 1\rangle\, |1/2, 1/2\rangle$$

$$|3/2, 1/2\rangle = \sqrt{1/3}\, |1, 1\rangle\, |1/2, -1/2\rangle + \sqrt{2/3}\, |1, 0\rangle\, |1/2, 1/2\rangle$$

$$|1/2, 1/2\rangle = \sqrt{2/3}\, |1, 1\rangle\, |1/2, -1/2\rangle - \sqrt{1/3}\, |1, 0\rangle\, |1/2, 1/2\rangle$$

$$|3/2, -1/2\rangle = \sqrt{2/3}\, |1, 0\rangle\, |1/2, -1/2\rangle + \sqrt{1/3}\, |1, -1\rangle\, |1/2, 1/2\rangle$$

$$|1/2, -1/2\rangle = \sqrt{1/3}\, |1, 0\rangle\, |1/2, -1/2\rangle - \sqrt{2/3}\, |1, -1\rangle\, |1/2, 1/2\rangle$$

$$|3/2, -3/2\rangle = |1, -1\rangle\, |1/2, -1/2\rangle$$

Fermi Golden Rule in Non-Relativistic QM

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- In Particle Physics we are normally interested in decay rates and scattering cross sections. In NRQM we calculate the transition rates using the Fermi's golden rule. We will sketch below its derivation.
- Let $|\phi_k\rangle$ be normalized solutions of the SE for the unperturbed Hamiltonian H_0,

$$H_0 |\phi_k\rangle = E_k |\phi_k\rangle , \quad \langle\phi_j|\phi_k\rangle = \delta_{jk}$$

- Now consider the time dependent perturbation $H'(\vec{x}, t)$ that can induce transitions. The SE becomes

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = [H_0 + H'] |\psi\rangle$$

- $|\psi\rangle$ can be expressed in the complete set of unperturbed states

$$|\psi(\vec{x}, t)\rangle = \sum_k c_k(t) |\phi_k\rangle e^{-\frac{i}{\hbar}E_k t}$$

- Substituting we have,

$$i\hbar \sum_k \left[\frac{dc_k}{dt} |\phi_k\rangle e^{-\frac{i}{\hbar}E_k t} - \frac{i}{\hbar} E_k c_k |\phi_k\rangle e^{-\frac{i}{\hbar}E_k t} \right] = \sum_k \left[c_k H_0 |\phi_k\rangle + H' c_k |\phi_k\rangle \right] e^{-\frac{i}{\hbar}E_k t}$$

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- This gives a differential equation for the coefficients c_k

$$i\hbar \sum_k \frac{dc_k}{dt} |\phi_k\rangle e^{-\frac{i}{\hbar}E_k t} = \sum_k H' c_k |\phi_k\rangle e^{-\frac{i}{\hbar}E_k t}$$

- Consider that at $t = 0$ the initial state is $|i\rangle = |\phi_i\rangle$ and that $c_k(0) = \delta_{ik}$. If the perturbation is constant for $t > 0$ and is small enough that $c_i(t) \simeq 1$ and $c_{k\neq i}(t) = 0$, we obtain to first approximation,

$$i\hbar \sum_k \frac{dc_k}{dt} |\phi_k\rangle e^{-\frac{i}{\hbar}E_k t} \simeq H' |\phi_i\rangle e^{-\frac{i}{\hbar}E_i t}$$

- The differential equation for the coefficient of the transition from an initial state $|i\rangle$ to a final state $|f\rangle = |\phi_f\rangle$, is obtained using the orthogonality of the states $|\phi_k\rangle$. We multiply on the left by $\langle\phi_f|$ to get,

$$\frac{dc_f}{dt} = -\frac{i}{\hbar} \langle f|H'|i\rangle e^{\frac{i}{\hbar}(E_f - E_i)t}$$

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- We define the transition matrix element (dimensions of energy)

$$T_{fi} = \langle f|H'|i\rangle = \int_V d^3x \phi_f^*(\vec{x}) H' \phi_i(\vec{x})$$

- At time $t = T$ the amplitude for transitions to state $|f\rangle$ is,

$$c_f(T) = -\frac{i}{\hbar}\int_0^T dt\, T_{fi} e^{\frac{i}{\hbar}(E_f - E_i)t} = -\frac{i}{\hbar} T_{fi} \int_0^T dt e^{\frac{i}{\hbar}(E_f - E_i)t}$$

where the last step holds for time-independent perturbing Hamiltonian H'.

- The probability for the transition to the state $|f\rangle$ is,

$$\begin{aligned} P_{fi} =& c_f^*(T) c_f(T) = |T_{fi}|^2 \frac{1}{\hbar^2} \int_{-T/2}^{T/2} \int_{-T/2}^{T/2} dt dt' e^{\frac{i}{\hbar}(E_f - E_i)t} e^{\frac{i}{\hbar}(E_f - E_i)t'} \\ =& |T_{fi}|^2 \; T^2 \frac{1}{\hbar^2} \frac{\sin^2 x}{x^2} \end{aligned}$$

where $x = \frac{(E_f - E_i)T}{2\hbar}$

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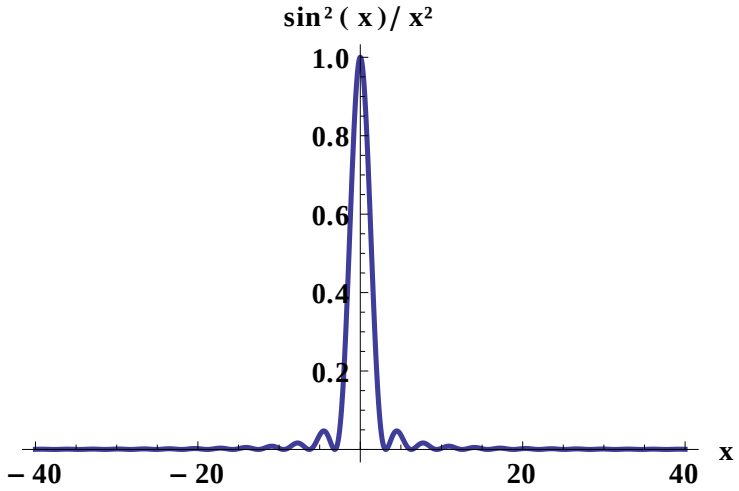
- In the figure we show the plot of $\sin^2 x/x^2$, with $x = (E_f - E_i)T/(2\hbar)$



- It is peaked at $E_f = E_i$, that is, energy is conserved within the limits of the energy-time uncertainty relation

$$\Delta E \Delta t \sim \hbar$$

- This means that we can take one of the integrals as a delta function

$$\lim_{T\to\infty} \int_{-T/2}^{T/2} dt' e^{\frac{i}{\hbar}(E_f - E_i)t'} = 2\pi\hbar\delta(E_f - E_i)$$

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- Therefore the transition rate (probability per unit time) will be

$$d\Gamma_{fi} = \lim_{T\to\infty} \frac{P_{fi}}{T} = \frac{2\pi}{\hbar}|T_{fi}|^2 \lim_{T\to\infty} \left[\frac{1}{T}\int_{-T/2}^{T/2} dt e^{\frac{i}{\hbar}(E_f-E_i)t}\delta(E_f-E_i)\right]$$

- If there are dn accessible final states in the range $E_f \to E_f + dE_f$ then the total transition rate is

$$\begin{aligned}
\Gamma_{fi} =& \frac{2\pi}{\hbar}\int |T_{fi}|^2 \frac{dn}{dE_f} \lim_{T\to\infty}\left[\frac{1}{T}\int_{-T/2}^{T/2} dt e^{\frac{i}{\hbar}(E_f-E_i)t}\delta(E_f-E_i)\right] dE_f \\
=& \frac{2\pi}{\hbar}\int |T_{fi}|^2 \frac{dn}{dE_f}\delta(E_f-E_i) \lim_{T\to\infty}\left[\frac{1}{T}\int_{-T/2}^{T/2} dt\right] dE_f \\
=& \frac{2\pi}{\hbar}\int |T_{fi}|^2 \frac{dn}{dE_f}\delta(E_f-E_i) dE_f \\
=& \frac{2\pi}{\hbar}|T_{fi}|^2 \left|\frac{dn}{dE_f}\right|_{E_i}
\end{aligned}$$

Density of States: $\rho(E_i) = \left|\frac{dn}{dE_f}\right|_{E_i}$

- Fermi Golden Rule: $\Gamma_{fi} = \frac{2\pi}{\hbar}|T_{fi}|^2\rho(E_i)$

Rutherford Scattering: Classical derivation

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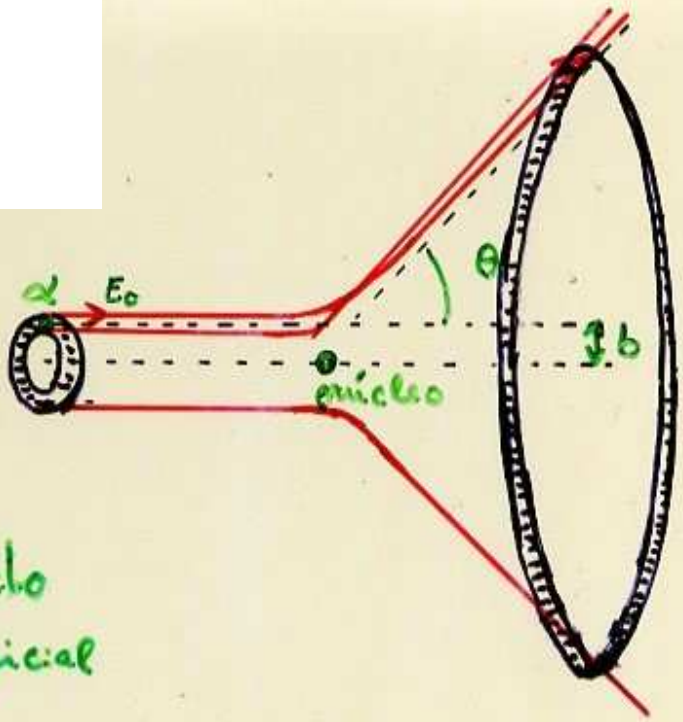
Classical derivation: Kepler Problem



θ - ângulo de difusão
b - parâmetro de impacto
E₀ - Energia cinética inicial

Mecânica clássica (prob. Kepler)

$\vec{E}$ = cte
$\vec{L}$ = cte

$$b = \frac{Q_1 Q_2}{4\pi\epsilon_0 2E_0} \cot\frac{\theta}{2}$$

trajs. determinísticas

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- The number of particles in the area between b and $b + db$ is

$$dN = 2\pi\, b\, db\, n_{\text{beam}}$$

where n_{beam} is the number of particles/unit area/unit time in the beam.

- Therefore

$$\frac{dN}{db} = 2\pi\, b\, n_{\text{beam}} = 2\pi\, \frac{Q_1 Q_2}{4\pi\epsilon_0 2E_0} \cot\frac{\theta}{2}\; n_{\text{beam}}$$

- Now

$$\begin{aligned}\frac{dN}{d\theta} =& \frac{dN}{db}\frac{db}{d\theta}\\ =& \frac{dN}{db}\frac{Q_1 Q_2}{4\pi\epsilon_0 2E_0}\frac{1}{2}\frac{1}{\sin^2\frac{\theta}{2}}\\ =& \pi\left(\frac{Q_1 Q_2}{4\pi\epsilon_0 2E_0}\right)^2 \frac{\cos\frac{\theta}{2}}{\sin^3\frac{\theta}{2}}\; n_{\text{beam}}\end{aligned}$$

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- In terms of the solid angle Ω,

$$d\Omega = 2\pi \sin\theta d\theta, \quad \frac{d\Omega}{d\theta} = 4\pi \sin\frac{\theta}{2}\cos\frac{\theta}{2}$$

- We get

$$\begin{aligned}\frac{dN}{d\Omega} &= \frac{dN}{d\theta}\frac{d\theta}{d\Omega} \\ &= \left(\frac{1}{4\pi\epsilon_0}\frac{Q_1Q_2}{2E_0}\right)^2 \frac{1}{4\,\sin^4\frac{\theta}{2}}\, n_{\text{beam}} \\ &= \left(\frac{1}{4\pi\epsilon_0}\frac{Q_1Q_2}{4E_0}\right)^2 \frac{1}{\sin^4\frac{\theta}{2}}\, n_{\text{beam}}\end{aligned}$$

- Finally the differential cross section is

$$\frac{d\sigma}{d\Omega} \equiv \frac{\frac{dN}{d\Omega}}{n_{\text{beam}}} = \left(\frac{1}{4\pi\epsilon_0}\frac{Q_1Q_2}{4E_0}\right)^2 \frac{1}{\sin^4\frac{\theta}{2}}$$

Rutherford cross section

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- To derive the Rutherford cross section in non-relativistic QM we start by an intermediate result for the Fermi Golden Rule,

$$d\Gamma = \frac{2\pi}{\hbar}|T_{fi}|^2\, dN_f\, \delta(E_f - E_i)$$

- The cross section for scattering by a potential is obtained dividing by the incident flux j_i, and number of particles in the target, N_t,

$$d\sigma \equiv \frac{d\Gamma}{j_i N_t} = \frac{d\Gamma}{j_i} = \frac{1}{j_i}\frac{2\pi}{\hbar}|T_{fi}|^2\, dN_f\, \delta(E_f - E_i)$$

  where the last step is just for one particle in the target $N_t = 1$.

- We are going to use plane waves for the incident and outgoing particles. As it is well known this brings a normalization problem. The solution is to normalize in a box of volume V. Then we write

$$\phi_i(\vec{x}) = \frac{1}{\sqrt{V}} e^{\frac{i}{\hbar}\vec{p}_i\cdot\vec{x}}, \quad \phi_f(\vec{x}) = \frac{1}{\sqrt{V}} e^{\frac{i}{\hbar}\vec{p}_f\cdot\vec{x}},$$

- We are going to show that the factors of V cancel out in the cross section and in the end we can take the limit $V \to \infty$

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- We start by evaluating dN_f. The normalization of one particle in a box of volume $V = L^3$, implies that the wave function should satisfy periodic boundary conditions, that is

$$\phi(x + L, y, z) = \phi(x, y, z), \text{ etc}$$

- This in turn implies that, for example,

$$e^{\frac{i}{\hbar} p_x x} = e^{\frac{i}{\hbar} p_x (x+L)}$$

leading to the quantization of the momenta

$$(p_x, p_y, p_z) = (N_x, N_y, N_z) \frac{2\pi\hbar}{L}$$

where N_x, N_y, N_z are integers.

- Each state in momentum space occupies a volume

$$\Delta^3 p = \Delta p_x \, \Delta p_y \, \Delta p_z = \left(\frac{2\pi\hbar}{L} \right)^3 = \frac{(2\pi\hbar)^3}{V}$$

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- Then the number of states with magnitude of momentum in the interval p and $p + dp$, is obtained dividing the element of volume d^3p in momentum space by the volume occupied by one state

$$dN = \frac{d^3p}{\Delta^3 p} = V\frac{d^3p}{(2\pi\hbar)^3} = V\frac{d\Omega p^2 dp}{(2\pi\hbar)^3}$$

where in the last expression we used spherical coordinates in momentum space.

- The next step is the incident flux. With the normalization we use, the density of the initial particles is $n_i = 1/V$, and therefore the flux is

$$j_i = n_i v_i = \frac{v_i}{V}, \quad \frac{1}{j_i} = \frac{V}{v_i}$$

where v_i is the velocity of the initial particle.

- Finally, assuming scattering by a time independent potential $H' = U(\vec{x})$

$$T_{fi} = \int_V d^3x \phi_f^*(\vec{x}) U(\vec{x}) \phi_i(\vec{x}) = \frac{1}{V}\int d^3x U(\vec{x}) e^{\frac{i}{\hbar}\vec{q}\cdot\vec{x}} \equiv \frac{1}{V}\mathcal{T}_{fi}(\vec{q})$$

where $\mathcal{T}_{fi}(\vec{q})$ is the Fourier transform of the potential, and $\vec{q} \equiv \vec{p}_i - \vec{p}_f$

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- Putting everything together we get

$$d\sigma = \frac{2\pi}{\hbar}\frac{V}{v_i}\frac{1}{V^2}\left|\mathcal{T}_{fi}(\vec{q})\right|^2 V\frac{d\Omega p_f^2 dp_f}{(2\pi\hbar)^3}\delta(E_f - E_i)$$

- As promised the volume V disappears and we can drop it from now on, and take $V \to \infty$ in the integrals. The differential cross section is obtained by integrating in the final momentum using the delta function. From $p^2 = 2mE$ we obtain $pdp = mdE$ and,

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \frac{1}{4\pi^2 v_i \hbar^4}\int p_f^2 dp_f \delta(E_f - E_i)|\mathcal{T}_{fi}(\vec{q})|^2 \\ &= \frac{1}{4\pi^2 v_i \hbar^4}\int p_f\, m\, dE_f\, \delta(E_f - E_i)|\mathcal{T}_{fi}(\vec{q})|^2 \\ &= \frac{1}{4\pi^2 v_i \hbar^4} p_f m |\mathcal{T}_{fi}(\vec{q})|^2\end{aligned}$$

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{p_f^2}{4\pi^2\, v_i v_f\, \hbar^4}|\mathcal{T}_{fi}(\vec{q})|^2}$$

Valid for any potential in NRQM

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- We are now in position to evaluate the Rutherford cross section in NRQM. The potential energy is

$$U(\vec{x}) = \frac{Q_1 Q_2}{4\pi\epsilon_0 \, |\vec{x}|}$$

where Q_1 is the electric charge of the particle in the beam and Q_2 that of the fixed target.

- The evaluation of the Fourier transform of the Coulomb potential is left as exercise. We get

$$\mathcal{T}_{fi}(\vec{q}) = \frac{Q_1 Q_2}{4\pi\epsilon_0} \int d^3x \, \frac{e^{\frac{i}{\hbar}\vec{q}\cdot\vec{x}}}{|\vec{x}|} = \frac{Q_1 Q_2}{4\pi\epsilon_0} \frac{4\pi\hbar^2}{|\vec{q}|^2}$$

- We get then for the QM Rutherford differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{p_f^2}{4\pi^2 v_i v_f \, \hbar^4} \left(\frac{Q_1 Q_2}{4\pi\epsilon_0}\right)^2 \frac{(4\pi\hbar^2)^2}{|\vec{q}|^4} = \left(\frac{Q_1 Q_2}{4\pi\epsilon_0}\right)^2 \frac{4m^2}{|\vec{q}|^4}$$

where we have used $p_i = p_f = m v_i = m v_f$

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- To compare with the classical result, we write this in terms of the transfered momentum $\vec{q} = \vec{p}_i - \vec{p}_f$ with $|\vec{q}|^2 = 8mE_0 \sin^2 \frac{\theta}{2}$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{Ruth}} = \left(\frac{1}{4\pi\epsilon_0}\frac{Q_1 Q_2}{4E_0}\right)^2 \frac{1}{\sin^4 \frac{\theta}{2}} = \left(\frac{Q_1 Q_2}{4\pi\epsilon_0}\right)^2 \frac{4m^2}{|\vec{q}|^4}$$

- We obtain therefore the important result that the Rutherford cross section has exactly the same expression in non-relativistic QM as in classical physics. Notice that the $\hbar$ disappears.

Bibliography for this class

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