Quantum Effects

Alessio Cimma

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1.1 $[\ \]$ Introduction to quantum mechanic

Examples: Transistors, LASERs, atomic clocks, NMR (medical), Quantum computers, Superconductors

What led to discrepancies: Before quantum mechanics, there was classical physics (electromagnetism). The emission spectra put scientist in front of a problem that could not be explained called "Ultraviolet catastrophy"

Formulas: The emission lines for Hydrogen are discrete and obtained using: $\frac{1}{\lambda} = Ry \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$ where $Ry = 11 * 10^6 \text{ m}^{-1}$ is the Rydberg constant.

Duality of light: Many experiments reveal that light is both a particle (photon) and a wave.

Experiments we will analyze:

- Double-slit experiment
- Photoelectric effect

1.2 $[\checkmark]$ Maxwell's equation

Generic case of Wave equation in the void:

$$\frac{\partial^2}{\partial t^2} \vec{E}(\vec{r}, t) = c^2 \nabla^2 \vec{E}(\vec{r}, t)$$

Case 1D:

$$\frac{\partial^2}{\partial t^2} \vec{E}(x,t) = c^2 \frac{\partial^2}{\partial x^2} \vec{E}(x,t)$$

The general solution of a monochromatic wave would be:

$$E(x,t) = F(x-ct) + G(x+ct)$$

Where F and G are arbitrary functions describing a progressive wave and regressive wave. It is our interest to study a set of stationary waves, the periodic waves (signals). These are great because we can analyze them using Fourier's transform, obtaining something like:

$$A\cos(kx - \omega t + \phi) = A\cos\left(k\left[x - \frac{\omega}{k}t\right] + \phi\right)$$
$$A\sin(kx - \omega t + \phi)$$

Where:

• k: wave number

• ω : angular frequency $\rightarrow \omega = kc$

• ϕ : phase shift

• A: amplitude of the wave

Symbols you should remember:

• λ : wavelenght (also equal to $\frac{2\pi}{k}$)

• ν : frequency (also equal to $\frac{1}{T} = \frac{\omega}{2\pi}$)

• T: time period

Superposition Principle: If you have 2 solution (both true but with different wave numbers) that propagates with the same speed, we can sum them and obtain a correct solution. $|\vec{k}|c = \omega$ and $|\vec{k'}|c = \omega'$

Interference: If in a single point 2 waves collide, the result of their sum will generate interferences, which can be *positive* or *negative*.

Useful notation: Using complex numbers to represent monochromatic waves, like this:

$$Ae^{i(\vec{k}\vec{x}-\omega t+\phi)}$$

Remembering the Euler's formula:

$$e^{i\alpha} = \cos(\alpha) + i\sin(\alpha)$$

1.3 $[\checkmark]$ Interference

$$A_1 * e^{i(\vec{k}\vec{x} - \omega t + \phi_1)} + A_2 * e^{i(\vec{k}\vec{x} - \omega t + \phi_2)} = A_{1+2} * e^{i(\vec{k}\vec{x} - \omega t + \phi_3)}$$

To obtain A_{1+2} we must solve $A_{1+2}^2 = |A_1e^{ia_1} + A_2e^{ia_2}|^2 = A_1^2 + A_2^2 + 2A_1A_2\cos(a_2 - a_1)$



Figure 1: Plot of phase difference



Figure 2: Double split experiment

1.4 $[\checkmark]$ Double - slit experiment

Phase difference: $k(\Delta l)$ and $\Delta l = d \sin(\theta) = d \frac{x}{L}$.

Intensity: $|A_{1+2}|^2$ and $A_1^2(2+2\cos(k\Delta l))$. This means that $I=A_1^2(2+2\cos(k\frac{xd}{L}))$

1.5 $[\checkmark]$ Photoelectric effect



Figure 3: Photoelectric experiment

What is interesting is that it doesn't matter how much tension we apply or the intensity of light. Below a certain ν electrons are NOT extracted. We must then assume that light is made of photons that are bound by the formula $E=h\nu$ where h is known as Planck constant. Once it is reached then there's enough energy to extract an electron and separate it from its atom. This is known as the W work function $\to h\nu \ge W$

The maximum energy of the photon will then be: $h\nu - W = E_{kin}$. In the experiment we can generate an electric field that generates an equal and opposite force $(eV_{stop} = E_{kin,max})$, to obtain the value of E_{kin} .

We can then extract our result remembering that: $h\nu - W = E_{kin} = eV_{stop}$ and discover that the slope will always be the same equals to h, and the intercept is equal to W. Remember that h is equal to: $6.626 * 10^{-34} \text{Js}$



Figure 4: Photoelectric function result

Particle momentum: $\frac{h\nu}{c} = \frac{h}{\lambda}$, since photons have no mass and move at speed of light: $E = |\vec{p}|c$.

Debroglie relation: $\vec{p} = \frac{h}{2\pi} \vec{k}$.

This informations, gives us everything we need to know for translating it into a wave equation:

$$\Psi(\vec{r},t) = Ae^{i(\vec{k}r - \omega t + \phi)} = Ae^{i\phi}e^{i(\frac{\vec{p}\vec{x} - Et}{\hbar})}$$

$2 \quad 2/10/24$

2.1 [\checkmark] Ripasso eq. Schrödinger

From last time we can change the $(\vec{k}\vec{r} - Et)$ into $(\vec{p}\vec{r} - Et)/\hbar$ from de Broglie relations.

So what about particles that moves much slower than the speed of light and consequentely have mass?

$$E = \frac{1}{2}mv^2$$

Considering that $\vec{v} = \frac{\vec{p}}{m}$ we can rewrite the previous formula as:

$$E = \frac{(\vec{p})^2}{2m}$$

If we then consider that $E = \hbar \omega$ since $\vec{p} = \hbar \vec{k}$, we can write what is now called a "Matter Wave":

$$\Psi_n(\vec{r},t) = Ae^{i\left(\frac{\vec{p}\vec{x} - Et}{\hbar}\right)}$$

Where the terms of energy and momentum are the formulas described for the matter equations.

Il prof. spiega roba in maniera non estremamente chiara, per il ripassone, leggi il PDF di Uccirati.

- Linear operator is something that operates in a linear way towards a function (taking a derivative, or multiplying by a certain factor)
- Wave packet → is a group of superposed waves which together form a travelling localized disturbance, especially one described by Schrödinger's equation and regarded as representing a particle
- Probability density \longrightarrow is the formula $(|\Psi(\vec{r},t)|^2)$ that determines the probability to find a particle in a position \vec{r} at the time t. In all the universe this equals to 1.

2.1.1 Regole interessanti

- 2 waves which differ only by the phase, represent the SAME state ($|x|^2$)
- If we check that a wave is valid at a certain time, it will be valid for any time.

2.2 $[\checkmark]$ Course objectives

2.2.1 Complex vectors

Complex vectors can be:

- vertical "KET" and symbolized with $|v\rangle$, and it's easy to immagine them as a column vector.
- horizontal "BRA" and symbolized with $\langle v|$, and it's easy to immagine them as a row vector of the complex conjugate.
- the combination (BRAKET): $\langle w|v\rangle$ is a scalar product (dot).

2.2.2 Dagger

 $\langle v|=(|v\rangle)^{\dagger}$ which is the simple term for "Hermitian Conjugation transpose & compl. conjugation". The $\sqrt{\langle v|v\rangle}$ equals to taking the norm, such as $\langle \Psi|\Psi\rangle=1$

2.2.3 Orhonormal basis

Are a set of basis such as $\langle i|j\rangle = \delta_{ij}$ such as it is equal to 1 if i=j or 0 if $i\neq j$. This means that the components v_i is given by $v_i = \langle i|v\rangle$

2.2.4 Hilbert space

It is a complex vector space with a complex scalar product, with some rules:

- States of quantum system are vectors in a Hilbert space with unit norm. $|\Psi\rangle$ and $|\Psi\rangle e^{i\phi}$ represent <u>SAME</u> state.
- This means that \hat{A} applied to $|v\rangle$ is equal to $\hat{A}|v\rangle$ and also $\hat{A}(a|v\rangle + b|w\rangle) = a\hat{A}|v\rangle + b\hat{A}|w\rangle$
- Note that \hat{A} can be represented by a matrix. So an equivalent writing should be $\langle i|\hat{A}|j\rangle \equiv A_{ij}$
- \hat{A} is hermitian if $\hat{A} = \hat{A}^{\dagger}$ and $(A^{\dagger})_{ij} = (A_{ji})^*$

2.2.5 Hermitian operators properties

- Diagonalizable: $\hat{A}|e_i\rangle = \lambda_i|e_i\rangle$ where $|e_i\rangle$ is an eigenvector and λ_i is an eigenvalues
- Can choose an orthon basis of eigenvalues.
- There's a proof that the eigenvalues are Real numbers.

2.3 [X] Exercise

$$|1\rangle = (0\ 1)\ |2\rangle = (1\ 0)$$

• Verify that $|1\rangle$ and $|2\rangle$ form an orthonormal basis

$$|1\rangle = \begin{bmatrix} 1\\i \end{bmatrix} \frac{1}{\sqrt{2}}$$

$$|2\rangle = \begin{bmatrix} 1 \\ -i \end{bmatrix} \frac{1}{\sqrt{2}}$$

• Verify that $|1\rangle$ and $|2\rangle$ form an orthonormal basis

• Write
$$|v\rangle = \begin{bmatrix} 5+i\\7-i \end{bmatrix}$$
 as $|v\rangle = v_1 |1\rangle + v_2 |2\rangle$ and $|v\rangle = v_1' |1'\rangle + v_2' |2'\rangle$

• Given this: $\hat{A} |1\rangle = |2\rangle$

• And this: $\hat{A}\left|2\right\rangle = \left|1\right\rangle$

$3 \quad 4/10/24 ightarrow ext{Skipped}$

Something about the eigenvalues and properties of Hermitian Operators and initial superposition conditions.

An eigenvector can be seen as a state where a system can collapse. If you can collapse a state and describe it with 2 operators simultaneously it means that the operators can commute.

$4 \quad 9/10/24$

4.1 $[\checkmark]$ Operators and uncertanty

The operators might or might not commute, this can occour only if the operators commute: $[A, B] = AB - BA \rightarrow [\hat{\vec{x}}, \hat{\vec{p}}] = 0$. Let's try it.

Example 1D:

$$\left[x,p_x\right]f(x) = \left[x,-i\hbar\frac{\partial}{\partial x}\right]f(x) = x\left(-i\hbar\frac{\partial f}{\partial x}\right) - \left(-i\hbar\frac{\partial}{\partial x}(xf)\right) = i\hbar x\frac{\partial f}{\partial x} - \left[-i\hbar f - i\hbar x\frac{\partial f}{\partial x}\right] = i\hbar f$$

This is true for all f. Where A = x and $B = \left(-i\hbar \frac{\partial}{\partial x}\right)$

2D case: Remember that when using more variables (x,y) you need to remember that when applying $\frac{\partial}{\partial y}$ on position x it doesn't interfere therefore it **COMMUTE**, otherwise it does not. This means that 2 operators can commute when they are linearly indipendent. Physically it means that you can measure 2 different attributes together. Also known as the *Canonical Commutation Relations*:

$$[\hat{x_i}, \hat{p_i}] = i\hbar I \delta_{ii}$$

Heisenberg's uncertanty principle and the consequences of $[\hat{x}, \hat{p_x}] \neq 0$: Let's introduce 2 operators:

- $\Delta \hat{x} \equiv \hat{x} \langle \Psi | \hat{x} | \Psi \rangle$ (the second term indicates the mean value of an attribute across Ψ)
- $\Delta \hat{p_x} \equiv \hat{p_x} \langle \Psi | \hat{p_x} | \Psi \rangle$

The $\langle \Psi | (\Delta \hat{x})^2 | \Psi \rangle = \langle \Psi | \hat{x}^2 | \Psi \rangle - (\langle \Psi | \hat{x} | \Psi \rangle)^2 = (\Delta x)^2$ is the variance of x.

The $\langle \Psi | (\Delta \hat{p_x})^2 | \Psi \rangle = \langle \Psi | \hat{p_x}^2 | \Psi \rangle - (\langle \Psi | \hat{p_x} | \Psi \rangle)^2 = (\Delta p_x)^2$ is the variance of p_x .

The result is that $(\Delta x)^2 (\Delta p_x)^2 \ge \frac{1}{4} |\langle \Psi | [\hat{x}, \hat{p_x}] | \Psi \rangle|^2$. If they commute, the uncertanty can reach 0. Only in this case.

Which leads to Heisenberg's uncertanty principle: $\Delta x \Delta p_x \geq \frac{\hbar}{2}$

4.2 [X] Probability current density

Charge case:

$$\rho(\vec{x},t)$$
 conserved $\rightarrow \vec{J}(\vec{x},t)$

They satisfy the continuity equation:

$$\frac{\partial \rho(\vec{x},t)}{\partial t} = -\vec{\nabla} \vec{J}(\vec{x},t)$$



Figure 5: Diagram of the continuity equation and charge conservation

General case: In general if there's the conservation of "mass" or whatever is moving, the continuity equation is satisfied.

QM case: We have a $\rho(\vec{x},t) = |\Psi(\vec{x},t)|^2$, so what is the probability corresponding to the $J(\vec{x},t)$?

From $i\hbar \frac{\partial}{\partial t}\Psi = H\Psi$ we take the conjugate $i\hbar \frac{\partial}{\partial t}\Psi^* = H\Psi^*$

Which we use to obtain the equivalent of ρ which is: $\frac{\partial}{\partial t}\rho \equiv \frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}\Psi^*\Psi = (\frac{\partial\Psi^*}{\partial t})\Psi + \Psi^*\frac{\partial\Psi}{\partial t} = -\frac{1}{i\hbar}(H\Psi^*)\Psi + \Psi^*(\frac{1}{i\hbar}H\Psi)$

Assuming that $H = \frac{\hat{p}^2}{2m} + V(\vec{x})$, we can finally obtain the result substituting H in the equation.

$$\frac{\partial \rho}{\partial t} = \frac{\hbar}{2mi} [\Psi \nabla^2 \Psi^* - \Psi^* \nabla^2 \Psi] + \frac{\hbar}{2mi} [\vec{\nabla} \Psi \vec{\nabla} \Psi^* - \vec{\nabla} \Psi \vec{\nabla} \Psi^*]$$

The second term of the right term equals to 0, we add it just to rewrite it and combining it in a more fancy way. "We just use it to make it more cute" [Francesca].

$$\frac{\partial \rho}{\partial t} \equiv \frac{\hbar}{2mi} \vec{\nabla} (\Psi \vec{\nabla} \Psi^* - \Psi^* \vec{\nabla} \Psi) \equiv - \vec{\nabla} \vec{J}$$

with $\vec{J} = \frac{\hbar}{2mi} (\Psi^* \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^*)$

4.3 $[\checkmark]$ 1D potential barrier (Dispense UCCIRATI)

4.3.1 Revised

Conditions:

- Ψ and Ψ' continuous to avoid infinite spikes in Ψ' and Ψ'' . Imposed by: $\Psi_L(a) = \Psi_R(a)$ and $\Psi'_L(a) = \Psi'_R(a)$
- Potential of region I = 0
- Potential of region II = V

Cases:

- $E > V_0$
- $E < V_0$

C'è la continuazione ma non la seguo. Una cosa che fa in più è il controllo se effettivamente il risultato ottenuto è un'onda nella forma di una autofunzione. $\hat{p}Ae^{ikx}=-i\hbar\frac{\partial}{\partial x}Ae^{ikx}=-i\hbar(ik)Ae^{ikx}=+\hbar kAe^{ikx}$ this confirms that the function found is an eigen function, since the function remains the same, just scaled by a real factor.

The demonstration goes on by imposing the conditions to the test functions. obtaining the amount of particles reflected and how many can get through. Given an A you can obtain B/A and C/A.

Magari disegnino della funzione prima e dopo la barriera?

Viene fatto un confronto in cui la soluzione è usata come Ψ dentro all'equazione, questa è nella regione I e poi ci sarà l'equivalente ma per la regione II: $J=\frac{\hbar}{2mi}(\Psi^*\frac{\partial}{\partial x}\Psi-\Psi\frac{\partial}{\partial x}\Psi^*)=\frac{\hbar}{2mi}ik\left[2|A|^2-2|B|^2\right]=\frac{\hbar k}{m}\left[|A|^2-|B|^2\right]$, where the term with the A is the J_{in} and the B is the J_{refl} . Finally computing the trasmitted we obtain for C the J_{trans} .

There will be also the case where the energy of the wave will be greater than the potential energy. This means that the reflected amount goes nearly to 0, while transmission to 1.

In the classical example it will be ALWAYS true or false, while in QM it's a range of possibilities. And when the energy is less then the potential it might penetrate a little (n/g) but it will always be reflected at the end.

- $5 \quad 11/10/24$
- $5.1 \quad [\checkmark]$ Effetto tunnel (UCCIRATI)

6 11/10/24 TUTORATO

6.1 $[\checkmark]$ Esercizio 1

Given
$$|e_1\rangle=\begin{bmatrix}1\\0\end{bmatrix}$$
 and $|e_2\rangle=\begin{bmatrix}0\\1\end{bmatrix}$
$$\vec{e_1}^\dagger\vec{e_2}=\begin{bmatrix}1\ 0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix}=0+0=0$$

$$|\vec{e_1}|^2=\langle e_1|e_1\rangle=\begin{bmatrix}1\ 0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix}=1+0=1$$

The most important thing to remember is $\langle e_i | e_j \rangle = \delta_{ij}$

6.2 [✓] Esercizio 2

Given
$$|e_1\rangle = \begin{bmatrix} 1\\i \end{bmatrix} \frac{1}{\sqrt{2}}$$
 and $|e_2\rangle = \begin{bmatrix} 1\\-i \end{bmatrix} \frac{1}{\sqrt{2}}$

$$\langle e_1|e_2\rangle = \frac{1}{2}[1 - i] \begin{bmatrix} 1\\-i \end{bmatrix} = \frac{1}{2}(1 + i^2) = 0$$

The reason for [1 - i] is caused but he complex conjugate.

$$|\vec{e_1}|^2 = \langle e_1 | e_1 \rangle = \frac{1}{2} [1 - i] \begin{bmatrix} 1 \\ i \end{bmatrix} = \frac{1}{2} (1 - i^2) = 1$$

6.3 $\lceil \checkmark \rceil$ Esercizio 3

Write
$$|v\rangle = \begin{bmatrix} 5+i\\ 7-i \end{bmatrix}$$
 as components of $|e_1\rangle = \begin{bmatrix} 1\\ 0 \end{bmatrix}$ and $|e_2\rangle = \begin{bmatrix} 0\\ 1 \end{bmatrix}$ $\langle e_1|v\rangle = v_1$ and $\langle e_2|v\rangle = v_2$ is used to obtain components v_1 and v_2 .

6.4 $[\checkmark]$ Esercizio 4

- Given this: $\hat{A}|1\rangle = |2\rangle$
- And this: $\hat{A}|2\rangle = |1\rangle$
- Write \hat{A} as a matrix
- Prove it's Hermitian

 $A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, and it's obtained by stacking the vectors horizontally to prove it's Hermitian you need to take the "Trasposta" it and taking the complex conjugate.

6.5 $\ [\checkmark]$ Esercizio 5

Prove that $\langle \Psi | \Delta \hat{x}^2 | \Psi \rangle = \langle \Psi | \Delta x^2 | \Psi \rangle - \langle \Psi | \Delta \hat{x} | \Psi \rangle$: DONE (Maybe).

7 14/10/24

$\lceil \checkmark \rceil$ Continuazione effetto tunnel

The transmission coefficient is equal to the ratio between Ψ before the wall and the Ψ after the wall and it's equal to: $e^{-2\beta L}$

In the general case where there's a generic potential and not a well defined wall. The claim is that

 $\Psi(x) = \Psi(x_1)e^{-\int_{x_1}^x dx' K(x')}$ is an approx. solution to Schrodinger's equation. To do this we just need to check if $\Psi'(x) = -K(x)\Psi(x)$ and $\Psi''(x) = K^2(x)\Psi(x) - K'(x)\Psi(x)$. Whenever i can neglect the term $-K'\Psi$ with respect to $K^2\Psi''$, than the claim is true. This is named as WKB approximation.

Immagine sul caso generale della barriera.

What does that mean? The smoother the potential varies, the more accurate we can approximate the tunnel effect.

WKB approximation: So what is the tunnelling rate is $t(E) = \frac{|\Psi(x_2)|^2}{|\Psi(x_1)|^2}$, so it's the exponential part:

$$e^{-2\int_{x_1}^{x_2} dx \frac{\sqrt{2m(V(x)-E)}}{\hbar}}$$

In the special case where $V(x) = V_0$ and $x_2 - x_1 = L$ then $t(E) = e^{-2\frac{\sqrt{2m(V_0 - E)}}{\hbar}L}$

$[\checkmark]$ APPLICATION 1: α - decay

Immagine sul decadimento α .

Facciamo il calcolo, shall we?

Definisco:

$$t(E) = exp \left[-2\frac{\sqrt{2m}}{\hbar} \int_{x_1}^{x_2} dx \sqrt{V(x) - E} \right]$$
$$m = m_{\alpha} \sim 4m_p$$
$$x_1 = R$$
$$x_2 = \frac{Z_1 Z_2 e^2}{4\pi \varepsilon_0 E} \longrightarrow V(x_2) = E$$

Max height of the potential $E_c = V(R) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 R}$

$$\beta \equiv \frac{R}{\hbar} \sqrt{E_c m} = \left(\frac{Z_1 Z_2 e^2 mR}{4\pi \varepsilon_0 R}\right)^{1/2}$$

Sostituendo:

$$t(E) = \exp\left[-2\sqrt{2}\beta \int_{1}^{E_{c}/E} dy \left(\frac{1}{y} - \frac{E}{E_{c}}\right)^{1/2}\right]$$

if $E_{c} \gg E \to t(E) \sim \exp\left[-2\sqrt{2}\beta \left(\frac{\pi}{2}\sqrt{\frac{E_{c}}{E}} - 2\right)\right]$

The mean lifetime of mother nucleous τ is $\propto \frac{1}{t(E)}$, meaning that $ln(\tau) \propto \alpha - ln(t(E))$. We also remember that:

- $R \propto Z_1^{1/3}$
- $E_c = \frac{Z_1}{R} = \frac{Z_1}{Z_1^{1/3}} = Z_1^{2/3}$

So we can conclude that:

$$\beta \propto R\sqrt{E_c} \propto Z_1^{1/3} Z_1^{1/3} = Z_1^{2/3}$$

WHICH MEANS THAT:

$$ln(\tau) \propto \beta \left(\frac{\pi}{2} \sqrt{\frac{E_c}{E}} - 2\right) \propto Z_1^{2/3} \left(\frac{\pi}{2} \frac{Z_1^{1/3}}{\sqrt{E}} - 2\right)$$
$$ln(\tau) \propto \left(\frac{Z_1}{E} - Z_1^{1/3}\right) \longrightarrow \text{Geiger - Nutall, 1928}$$

This explains the fusion of an atom or the α - decay. (inverse processes), β controls the energy required to fusion for example hydrogen. This is why they use light materials, to minimize β , diminuishing the energy required.

7.3 $[\checkmark]$ APPLICATION 2: Cold emission of electrons

Considering for example a material like a metal.

Immagine sulla cold emission.

$8 \quad 17/10/24$

8.1 $\lceil \checkmark \rceil$ Continuazione effetto tunnel 2

Calculation tunnelling rate in WKB approx. (case cold emission):

$$t(E) = exp \left[-2 \int_{x_1}^{x_2} dx \frac{\sqrt{sm(V(x) - E)}}{\hbar} \right]$$

Where x_2 is obtained in such a way that $\Phi + E - |e| \varepsilon x_2 = E \to x_2 = \frac{\Phi}{|e|\varepsilon}$.

We finally obtain: $t(E) = exp\left[-\frac{4\sqrt{2}}{3}\sqrt{m}\frac{\Phi^{\frac{3}{2}}}{\hbar|e|\varepsilon}\right]$. Remember that Φ is the work function.

Conclusions: Given ε we obtain that when ε goes to 0 there's no probability of tunnelling. When ε goes to ∞ , the t(E) is 1 (probability of 100%).

8.2 [✓] Scanning Tunnelling Microscope (STM)

Immagine sulla STM.

8.3 [✓] Potential Well (UCCIRATI)

We start by defining what happens in the region with 0 potential and V_0 potential.

- $\Psi'' = -\frac{2m}{\hbar^2} E \Psi$ namely $-\frac{2m}{\hbar^2} E \equiv K^2$
- $\Psi'' = \frac{2m}{\hbar^2} (V_0 E) \Psi$ namely $-\frac{2m}{\hbar^2} (V_0 E) \equiv g^2$

Since: V(x) = V(-x) and $|\Psi(x)|^2 = |\Psi(-x)|^2$ so $\Psi(x) = \pm \Psi(-x)$, so we are look onely for even or odd functions (sins and cosines).

Even function inside: $|x| \le L/2 \to \Psi^{even}(x) = Acos(kx)$ we can write it like that because it's a real exponent and we take only the even part

Even function outside: $|x| > L/2 \to \Psi^{even}(x) = Be^{-g|x|}$ here we report the even part but from the general form $(\Psi = Ae^{gx} + Be^{-gx})$ Consideriamo la parte negativa, perchè delle 2 possibili soluzioni è l'unica che rispetta le condizioni al contorno (non FUCKING esplodere all' ∞).

Continuity: Ψ and Ψ' continuous at $x = \pm L/2$ so

$$A\cos\left(K\frac{L}{2}\right) = Be^{-gL/2} \text{ For } \Psi$$

$$AK\cos\left(K\frac{L}{2}\right) = -gBe^{-gL/2}$$
 For Ψ'

Their ratio equals to: $-K \tan{(KL/2)} = -g \rightarrow \tan{(KL/2)} = g/K$. This means that this term ζ DOESN'T depend on the E: $\frac{\sqrt{\zeta^2 - (KL/2)^2}}{(KL/2)}$, so only certain values of E depending on K (quantization of energy). The number of intersections depend on ζ , which depends on the V_0 . $(\zeta = \frac{\sqrt{2mV_0}L}{2\hbar})$.

- 8.4 [\checkmark] Potential Well (Case with ∞ wall) (UCCIRATI)
- 8.5 [✓] Potential Well (Case with 3D) (UCCIRATI)
- 8.6 $[\checkmark]$ Kroenig Penney

$9 \quad 21/10/24$

9.1 [\checkmark] Periodic δ - Potential (Kronig - Penney)

9.1.1 Math base model:

Starting with:

$$V(x) = -LV_0 \sum_{n=-\infty}^{\infty} \delta(x - nL)$$

We want to find the states of the electron with positive energy E > 0, so:

$$(n-1)L < x < nL \longrightarrow \Psi_n'' = -\frac{2mE}{\hbar^2}\Psi_n$$

$$\Psi_n(x) = a_n e^{ikx} + b_n e^{-ikx}$$
 with $K = \sqrt{2mE/\hbar}$

This means that increasing n nothing changes, because it is periodic. This helps us, because we only care resolving the equation in a limited range (L).

Introducing: $\Theta(a < x < b)$, (Immagine di una funzione quadra, ovvero tutti 0 fuori dal range e 1 nel range)

$$\Psi(x) = \sum_{n = -\infty}^{\infty} \Psi_n(x)\Theta((n-1)L < x < nL)$$

Which means that the V(x+L)=V(x) and $|\Psi(x+L)|^2=|\Psi(x)|^2$. We can write the most general equation as $\Psi(x+L)=e^{i\alpha}\Psi(x)$

We can combine the functions by rewriting one range in function of the other, so we can substitute the 2 expression with each other. Fa un sacco di trucchetti continuando a cambiare nome tra i, j e n fino ad arrivare a:

$$\Psi(x+L) = \sum_{n=-\infty}^{\infty} \Psi_{n+1}(x+L)\Theta((n-1)L < x < nL)$$

To conlcude we can rewrite the original Ψ in using the progressive and regressive wave with the increasing coefficients.

$$\Psi_n(x+L) = a_n e^{ikx} e^{ikL} + b_n e^{-ikx} e^{-ikL}$$

9.1.2 Physics impositions:

Continuity in
$$x = nL \to \Psi_n(nL) = \Psi_{n+1}(nL) \to (a_n - a_{n+1})e^{iknL} = (b_{n+1} - b_n)e^{-iknL}$$
.

Remember that there's the periodicity, continuity of Ψ and discontinuity of Ψ' .

9.1.3 The final agglomerate:

$$\cos(\alpha) = \cos(KL) - \frac{mV_0L}{K\hbar^2}\sin(KL)$$

10 [\checkmark] (INTRO) Angular momentum λ

It is usually a vector:

$$\vec{L} = \hat{\vec{x}} \times \hat{\vec{p}} \rightarrow -i\hbar \vec{x} \times \vec{\nabla} = L_x \text{ for example: } -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$[\vec{x}_i, \vec{p}_j] = i\hbar \delta_{i,j} \rightarrow [L_x, L_y] = i\hbar L_z$$

We can also verify that:

$$\left[L_i, \hat{\vec{x}}^2\right] = \left[L_i, \hat{\vec{p}}^2\right] = \left[L_i, \vec{L}^2\right] = 0$$

$11 \quad 23/10/24$

12 [\checkmark] Angular momentum λ

Simultaneous eigenstates: These are the simultaneous eigenstates of $\vec{L^2}$ and $\hat{L_z}$.

$$\hat{L_z} \left| \beta, m \right\rangle = \hbar m \left| \beta, m \right\rangle$$

$$\vec{L^2} |\beta, m\rangle = \hbar^2 \beta |\beta, m\rangle$$

Operator $\hat{L_+}$ and $\hat{L_-}$: Remember that they are NOT observable.

$$\hat{L_+} = \hat{L_x} + i\hat{L_y}$$

$$\hat{L}_{-} = \hat{L}_{x} - i\hat{L}_{y}$$

$$\hat{L_+^\dagger} = \hat{L_-}$$

Combining operators: We need to verify that:

$$\left[\hat{L_z}, \hat{L_+}\right] = \hbar \hat{L_+}$$

Proof: Controlla dispense

Another verify:

$$\hat{L}_{+}|\beta,m\rangle \propto |\beta,m+1\rangle$$

Relation between β and m: Controlla dispense

$13 \quad 25/10/24$

14 [\checkmark] Angular momentum λ 2.0 (chapter 4.3 dispense)

Rewriting of the previous solution in polar coordinates: single particle \rightarrow spherical harmonics. ASK FRA for typical question: quantum number bound to angular momentum formula how thy influence the equation.

- $15 \quad 30/10/24$
- $\ [\checkmark]$ Continuazione esercizio: 29/10/24

$17 \quad 4/11/24$

18 $[\checkmark]$ Addition of angular momentum

We can consider a binary system of e^- , where the spins are commutable $[S_{1i}, S_{2j}] = 0$. This means they are indipendent and can be measured together. We can define $\vec{S} = \vec{S_1} + \vec{S_2}$ (total spin of the system), and we want to find the state that satisfies $S^2 | S, M \rangle = \hbar^2 S(S+1) | S, M \rangle$ and $S_Z | S, M \rangle = \hbar M | S, M \rangle$.

For starters we only have the states of the single electrons indipendent from each other (the 4 combinations of states of the electron) $|++\rangle (|+\rangle |+\rangle), |+-\rangle, |-+\rangle, |--\rangle$, and we want to build $|S, M\rangle$ as combinations of the previous 4 possibilities.

We can say that S^2 commutes with S_1^2 , S_2^2 and S_Z but not with S_{1Z} and S_{2Z} , so they are not a good set of basis (the 4 combinations), because they do not commute, so we can't describe one using the other.

We now should try to understand the action of S_Z on $|++\rangle \dots |--\rangle$ and

$$S_Z |++\rangle = (S_{1Z} |+\rangle) |+\rangle + |+\rangle (S_{2Z} |+\rangle)$$

$$\left(\frac{\hbar}{2}\left|+\right\rangle\right)\left|+\right\rangle+\left|+\right\rangle\left(\frac{\hbar}{2}\left|+\right\rangle\right)=\hbar\left|++\right\rangle$$

This means that S_Z can commute and reppresent all the states correctly. It will be now our new basis (all the 4 combinations are eigen values of S_Z). Let's check if we can compute S^2 with this setup by computing the action of S^2 on $|++\rangle$:

$$S^2 = S_1^2 + S_2^2 + 2S_{1X}S_{2X} + 2S_{1Y}S_{2Y}$$

Where we use the $S_{1\pm} = S_{1X} \pm i S_{1Y}$ (Ladder operator). Let's start computing:

$$S^{2} |+-\rangle = (S_{1}^{2} |+\rangle) |-\rangle + |+\rangle (S_{2}^{2} |-\rangle)$$

Soluzione nelle dispense, in pratica espande l'equazione ed elimina molti termini (L'operatore S+ va ad aumentare di uno stato lo spin, ma se lo applico a spin UP il risultato è 0 eliminando il termine). Poi a prendere roba fatta prima: $S_{\pm}|s,m\rangle$ risolve tutto ed ottiene:

$$S^2 \left| +- \right\rangle = \hbar^2 (\left| +- \right\rangle + \left| -+ \right\rangle)$$

Which is NOT and eigenstate, since it uses 2 different basis. This is because S^2 do NOT commute with S_Z .

We then find that:

$$|++\rangle \equiv |S=1, M=1\rangle$$

$$|--\rangle \equiv |S=1, M=-1\rangle$$

This means that i can find the value of one basis set (S=1, M=0, ecc.) in terms of another basis set (++, -, ecc.), finding the value of all the others combinations.

To check if everything works: $S^2[...] = 2\hbar^2[...]$ and $S_Z[...] = 0$ and you should see that everything is proportional and written in terms of one base (eigen - something).

We then find that:

$$\frac{1}{\sqrt{2}}(|+-\rangle+|-+\rangle)\equiv |S=1,M=0\rangle$$

And now for the last one: we must engineer the coefficients of the other 3 solutions to create a 4th solution orthogonal to all the others. Which is:

$$\frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \rightarrow |S=0, M=0\rangle$$

Which is spin singlet, while the other 3 are the spin triplet.

18.1 Sum of \vec{L} and \vec{S}

Consider $\vec{J} = \vec{L} + \vec{S}$ and let's contrusct a basis $|J,M\rangle$ such that $\vec{J}^2 |J,M\rangle = \hbar^2 J(J+1) |J,M\rangle$ and $J_Z |J,M\rangle = \hbar M |J,M\rangle$.

As a starting point let's use $|l,m\rangle$ basis for \vec{L}^2 and L_Z and $|+-\rangle$ as a basis for \vec{S}^2 and S_Z . So we now start from $|l,m,+\rangle$ and $|l,m,-\rangle$.

$19 \quad 6/11/24$

20 $[\checkmark]$ Addition of angular momentum 2.0

Now we consider just one electron, but we use the orbital component and the spin as $\vec{J} = \vec{L} + \vec{S}$, i want to find linear combinations of the states that are eigenstates of J^2 and J_Z . So i want to find:

$$J^{2} |J, M\rangle = \hbar^{2} J(J+1) |J, M\rangle$$
$$J_{Z} |J, M\rangle = \hbar M |J, M\rangle$$

Immagino che la descrizione sia nelle dispense, in pratica parte da $J_Z | l, l, + \rangle$ e arriva a $J_Z = \hbar(l+\frac{1}{2}) | l, l, + \rangle$ per il primo, mentre per J^2 ottiene la versione espansa del quadrato (quadrato di un binomio (L+S))

21 [✓ Perturbation theory]

Given an hamiltonian H_0 and we know eigen states and values:

$$H_0 |n^0\rangle = E_n^0 |n^0\rangle$$

We can add an "perturbation" to the "unperturbed hamiltonian" $H=H_0+\lambda H_1$ and try to solve the new problem and finding the new energy levels: $H|n\rangle=E_n|n\rangle$

$22 \quad 11/11/24$

The important thing that these are relativistic correction, derived from the fact that the particle is moving AND that there's a magnetic field applied.

24 [X] Anomalous Zeeman effect

- 25 13/11/24
- $[\checkmark]$ MASCHIO

$27 \quad 13/11/24$

28 [✓] MASCHIO 2.0

28.1 Operators & Slater determinants

Let's start from the $\hat{H}\Psi = E\Psi$, and then introduce the ORBITAL approximation, which is a mono electronic function of 1 electron.

$$\chi(\mathbf{x}) = \chi(\mathbf{r}; \omega) = \psi(\mathbf{r})\sigma(\omega)$$

We assume to have these SPINORBITALS, how do we handle them? What properties do they have to need? They needs to be ORTHONORMALS. Once we have them, we can separate them into a product of spinorbitals.

28.2 Determinante di Slater

Rappresenta una matrice, in cui ogna colonna rappresenta l'elettrone in uno degli spin-orbitali, mentre ogni colonna rappresenta uno scambio tra gli elettroni: ogni colonna rappresenta tutti i possibili spin-orbitali, ogni riga rappresenta ogni possibile elettrone.

è un modo per rappresentare tutte le possibile configurazioni degli elettroni in un modo comodo. Il determinante è la funzione d'onda che rappresenta questo stato. Questo perchè il modo in cui calcoli il determinante, va a prendere tutti i contributi di un elettrone in tutti gli orbitali, che corrisponde a considerare la sovrapposizione dei vari orbitali.