Lecture-27

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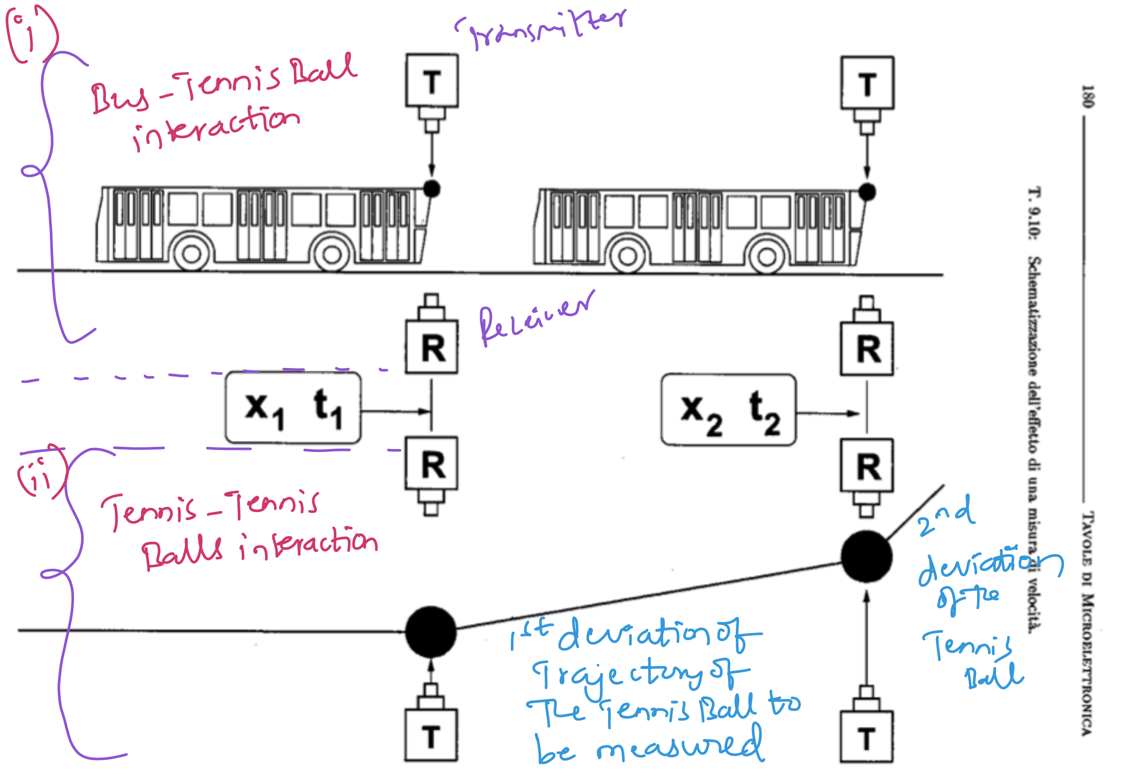

Q) What can we say about the Measurement of TennisBall-Tennis Ball (T.B) interaction?

Ans: The velocity of The Tennis Ball b/w x_1 & x_2

$$v = \frac{x_2 - x_1}{t_2 - t_1}$$

- However, we cannot deduce much about The Dynamics of The Tennis Ball before The 1st measurement.

Because The T.B was perturbed but we cannot do anything about The motion of The T.B after The 2nd measurement because again we have perturbed (deviation of T.B)

- The Perturbation is becoming essential part of the measurement. And we can little about The Dynamics of The T.B.

Q) Is There an easy way out to know about The Dynamics of T.B ?

Ans. The perturbation of T.B is because of The collisions b/w the T.B's and This calculation can be done using Classical Mechanics. Assuming one knows the Potential Energy of the Interaction b/w two particles.

- Another possible way out is to consider particles that are much much less than the size of Tennis Balls like (Bus against a T.B)

$\Updownarrow$

(T.B against an e^-) $\Rightarrow$ Here perturbation can be neglected

Q) But what if we want to measure Dynamics of an e^- ?

Ans

- Unfortunately there is nothing we can do because e^- is so small and to measure Dynamics of individual e^-s is Impossible.

- When we consider Microscopic objects to perform experiments then the Perturbation induced by a measurement is something that cannot be avoided and cannot be neglected.

- Another possibility of measuring Dynamics of microscopic particles is to use Light (photons) (May be this is a way out) i.e Measuring the position of e^- using light (collection of photons)

Monochromatic Light $\Rightarrow$ All photons have same Frequency.

$$E = h\nu$$

- if we take low frequencies, the energy of the photons is very less which will reduce the impact of photons on e^-s during the measurement. But there is a Drawback

if we $\downarrow$ frequency $\uparrow$ wavelength and the resolution

of the optical instruments depends on the wavelength
We cannot have resolution better than wavelength.
(Here We can grossly mistake the position of e^- using the photons of low frequencies)

We can see Position & Momentum are dual.

Q) Is it really true that in order to measure something we must interfere with object?

→ Ex: Tracing the Trajectory of the Moon.

(Big Bang Theory experiment - 3rd season episode 23 _ Lunar Excitation)

∴ it is impossible to measure something without interacting with the object to be measured.

∴ We must abandon the idea that is so convenient in Classical Mechanics is that, Motion of particles can be described by the Diff. Eq^n that provide us with full information at each time of position velocity, energy and all Dynamical quantities of these particles. & We must be content with the smaller information that is associated with the statistical distribution of the particles. if we're considering many particles. on to the Probability Distribution when we are localizing a particle in some Region of space.

- In this respect, we have already introduced Wavefunction that depends on Position & time and we have associated a physical meaning to the Wavefunction.

$$\boxed{\int_{\tau} |\psi|^2 d\tau \implies \text{provides the probability of finding an electron in that volume, provided wavefunction can be Normalized.}}$$

→ Then we also earlier studied to split the problem by considering only forces which are conservative! (Forces that are derivable from a potential energy)

If Total Energy of a particle is given then the angular frequency (ω) associated with the particle is also given

$$\omega = \frac{E}{\hbar}$$

* → In conservative forces case Wave function can be split into two functions one w.r.to Space (still to be found) & Time part. (exponential of $-j\omega t$)

** Now, we are left with the problem of finding a function for the Space part of a Wave function.

Qualitatively, we can state that this function will be a solution of a Differential Equation.

It is possible to derive such an Equation i.e Schrodinger Equation Independent of time

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T. 10.4: Condizioni al contorno e normalizzazione della parte spaziale della f. d'onda.

Time independent Schrodinger's Equation with unknown 'w' which is the space part of the wave function.

Properties of Schrödinger's Equation — I

Non-Relativistic form

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2 w + V w = E w}$$

- The time-independent Schrödinger equation is a linear, homogeneous partial differential equation (PDE) of the second order, with the zero-order coefficient depending on $\boldsymbol{r}$.
- The boundary conditions (BCs) for w are homogeneous as well. As a consequence, w is defined apart from a multiplicative constant.
- Diverging solutions must be discarded.
- The non-diverging solutions may be normalizeable ($\int_\infty |w|^2 \, d\tau < \infty$) or may not ($\int_\infty |w|^2 \, d\tau = \infty$); for example, $w = A \exp(j\boldsymbol{k} \bullet \boldsymbol{r})$ is not.
- The solution w is continuous; its first derivatives are continuous, unless the potential energy V has discontinuities of the second kind. The second derivatives are continuous if V is continuous.

$$\boxed{\frac{\hbar^2}{2m}\nabla^2 w + V w = E w}$$

if 'V' is a constant then this equation would be called Helmholtz Eq^n

$\therefore$ This eq^n is Linear & Homogeneous

The Boundary conditions of the Eq^n are also Homogeneous. $\therefore$ it is sufficient to say that the 'w' solution of the eq^n is defined apart from multiplicative constant

it may happen that some solutions of the eq^n might Diverge. These sol^ns cannot be accepted on physical grounds.

- Convergence or Divergence of Solution

- The non-diverging solutions may be normalizeable ($\int_\infty |w|^2 \, d\tau < \infty$) or may not ($\int_\infty |w|^2 \, d\tau = \infty$); for example, $w = A \exp(j\boldsymbol{k} \bullet \boldsymbol{r})$ is not.

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- Continuity of The Solution.

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T. 10.5: **Deduzione formale dell'operatore hamiltoniano dalla funzione hamiltoniana.**

Properties of Schrödinger's Equation — II

laplacian operator

multiplicative operator

- Defining the Hamiltonian operator

$$\mathcal{H} \doteq -\hbar^2/(2m)\,\nabla^2 + V$$

Schrödinger's equation takes the form

Compact form of the Schrödinger's eqn

$$\mathcal{H}w = Ew \qquad + \text{ BCs}$$

Boundary conditions

which is that of an eigenvalue equation, of eigenvalue E and eigenfuction w.

- $\mathcal{H}$ is linear: $\mathcal{H}(c_1 w_1 + c_2 w_2) = c_1 \mathcal{H} w_1 + c_2 \mathcal{H} w_2$.
- Schrödinger's equation has a formal similarity with the classical expression $H(\boldsymbol{p}, \boldsymbol{q}) = E$ of the total energy of a particle in a conservative field, where $H = T + V$ is the Hamiltonian function. By similarity, the classical kinetic energy $T = p^2/(2m)$ corresponds to the kinetic operator $\mathcal{T} \doteq -\hbar^2/(2m)\,\nabla^2$:

$$\frac{1}{2m}\left(p_1^2 + p_2^2 + p_3^2\right) \iff -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right)$$

- It follows that $H \Leftarrow \mathcal{H}$ if $p_i \Leftarrow \hat{p}_i \doteq -j\hbar\,\partial/\partial x_i$.

$$\boxed{Hw = Ew}$$

This looks like an Eigen value eqⁿ if we consider 'H' as a Matrix and 'ω' a vector.

'E' : Eigen value

'ω' : Eigen function

- $\mathcal{H}$ is linear: $\mathcal{H}(c_1 w_1 + c_2 w_2) = c_1 \mathcal{H} w_1 + c_2 \mathcal{H} w_2$.
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- It follows that $H \Leftarrow \mathcal{H}$ if $p_i \Leftarrow \hat{p}_i \doteq -j\hbar\,\partial/\partial x_i$.

$\hat{p}_i$ is the Quantum Momentum operator

→ Continuing analysis of The Time independent Schrodinger's equation

→ when we consider The classical mechanism conversative case The Total energy conserves be smaller than the P.E then K.E is -ve which is impossible

T. 10.6: Vincoli sugli autovalori dell'equazione di Schrödinger.

Properties of Schrödinger's Equation — III

- Schrödinger's equation written in the form $-\hbar^2/(2m)\,\nabla^2 w = (E - V)\,w$ yields, after multiplication by w^*, and integrate w.r.to the SPACE.

$$\boxed{-\int_\tau w^*\,\nabla^2 w\,\mathrm{d}\tau = \frac{2m}{\hbar^2}\int_\tau (E-V)\,|w|^2\,\mathrm{d}\tau\,.}$$

- Thanks to the identity $w^*\,\nabla^2 w = \operatorname{div}(w^*\,\operatorname{grad} w) - |\operatorname{grad} w|^2$, the above becomes

Gauss Divergence Theorem

$$\frac{2m}{\hbar^2}\int_\tau (E-V)\,|w|^2\,\mathrm{d}\tau = \int_\tau |\operatorname{grad} w|^2\,\mathrm{d}\tau - \int_{\partial\tau} w^*\,\frac{\partial w}{\partial \nu}\,\mathrm{d}\partial\tau\,.$$

- If w vanishes at the boundary it must be $\operatorname{grad} w \not\equiv 0$ since $w \not\equiv 0$. It follows

$$\int_\tau (E-V)\,|w|^2\,\mathrm{d}\tau > 0 \quad\Longrightarrow\quad E > \frac{\int_\tau V\,|w|^2\,\mathrm{d}\tau}{\int_\tau |w|^2\,\mathrm{d}\tau} \geq V_{\min}\,.$$

- If $V = 0$ it is $w = A\exp(j\boldsymbol{k}\bullet\boldsymbol{r})$, where $\boldsymbol{k}$ is any real vector. As a consequence, w does not vanish at the boundary. On the other hand it is $\nabla^2 w = -k^2 w$ whence $-\int_\tau w^*\,\nabla^2 w\,\mathrm{d}\tau = k^2|A|^2\tau$. In conclusion, for any volume τ it is found

$$k^2|A|^2\,\tau = \frac{2m}{\hbar^2}\,E|A|^2\tau \quad\Longrightarrow\quad E = \frac{\hbar^2 k^2}{2m} \geq 0\,.$$

Gauss Divergence Theorem $\Rightarrow$ $\displaystyle\int_T \operatorname{div}(w^*\operatorname{grad} w) = \int_{\partial T} w^*\,\frac{\partial w}{\partial \nu}\,d\,\partial T$

Integral over the surface of the volume of the Normal derivative of the argument of the Divergence.

$w^* \frac{\partial w}{\partial \nu}$ is the Normal derivative

'ν' is the unit vector Normal to the Boundary and pointing in the Normal Direction.

$\partial \tau$ is the Boundary of τ

→ Now we let τ go to infinity and we assume that function with 'w' is Normalizable

If the function is Normalizable, then Necessarily it goes to zero when we extend the Boundary to infinity.

$$\text{if } w \to 0 \quad \text{at } \infty$$

$$\Rightarrow w^* \to 0 \quad \text{at } \infty$$

$$\therefore \int_{\partial \tau} w^* \frac{\partial w}{\partial \nu} \, d\partial\tau \Rightarrow 0 \quad \text{at } \infty$$

→ instead $\int_\tau |\text{grad } w|^2 d\tau$ cannot be zero

because 'w' is by hypothesis one of the possible Eigen functions of the eqn & Eigenfunctions are Non zero. we now only seek for nonzero solutions.

- $w \neq 0$ inside the volume

$w = 0$ at the Boundary

Then the grad $w \neq 0$ inside the volume

$\therefore \int_\tau |\text{grad } w|^2 d\tau$ is strictly +ve

& $\therefore \int_\tau (E-V)|w|^2 d\tau > 0$

- If w vanishes at the boundary it must be grad $w \neq 0$ since $w \neq 0$. It follows

$$\int_\tau (E-V)\,|w|^2\,\mathrm{d}\tau > 0 \quad \Longrightarrow \quad \boxed{E > \frac{\int_\tau V\,|w|^2\,\mathrm{d}\tau}{\int_\tau |w|^2\,\mathrm{d}\tau} \geq V_{\min}}\,.$$

if wavefunction is Normalizable

- If $V = 0$ it is $w = A\exp(j\boldsymbol{k} \bullet \boldsymbol{r})$, where $\boldsymbol{k}$ is any real vector. As a consequence, w does not vanish at the boundary. On the other hand it is $\nabla^2 w = -k^2 w$ whence $-\int_\tau w^* \nabla^2 w\,\mathrm{d}\tau = k^2|A|^2\tau$. In conclusion, for any volume τ it is found

$$k^2|A|^2\tau = \frac{2m}{\hbar^2}E|A|^2\tau \quad \Longrightarrow \quad E = \frac{\hbar^2 k^2}{2m} \geq 0\,.$$

→ Instead if wave function is Not Normalizable then we can exploit the property of 'w' vanishing at the Boundary. ex: free particle

in this case $E \simeq V$

→ **Schrödinger Equation for a Free Particle**

Letting $V = \text{const} = 0$, a linear uniform motion of the particle is obtained, and the Schrödinger eq. reads $\nabla^2 w = -(2mE/\hbar^2)\, w$. As the above can be solved by separation, it is sufficient to consider here only the one-dimensional case

$$\boxed{\frac{d^2 w}{dx^2} = -\frac{2mE}{\hbar^2}\, w\,.}$$

- The case $E < 0$ must be discarded as it gives rise to divergent solutions, which are not acceptable from the physical standpoint.
- The case $E = 0$ yields $w = a_1 x + a_2$, where a_1 must be set to zero to prevent w from diverging. Finally, the case $E > 0$ yields

Solution for $E > 0$ →

- $$\boxed{w = c_1 \exp(jkx) + c_2 \exp(-jkx)}\,, \qquad k \doteq \sqrt{2mE/\hbar^2} = p/\hbar\,,$$

for $x = \pm\infty$ the solutions would Diverge so we discard those values

where c_1, c_2 are indetermined constants. The time-dependent, monochromatic wave function $\psi = w \exp(-j\omega t)$ reads

- $$\psi = c_1 \exp[j(kx - \omega t)] + c_2 \exp[-j(kx + \omega t)]\,, \qquad \omega = E/\hbar\,.$$

One sees that E and p are fully determined, and no constraint is imposed on the total energy apart from $E \geq 0$.

C_1, C_2 are undetermined coefficients because we don't have Boundary conditions to determine them.

So, it is non Normalizable!

→ But we can reconstruct the full Time dependent

Schrodingers Eq^n then we have

$$\boxed{\Psi = c_1 \exp[j(kx-\omega t)] + c_2 \exp[-j(kx+\omega t)]}$$

- This is a Planar Monochromatic wave with wave vector 'k' & Angular frequency 'ω' it propogates along the x-axis in the +ve direction.

- $c_2 \exp[-j(kx-\omega t)]$ propogats in '$-x$' direction.

Conclusion: The wavefunction is the Superposition of Two planar Monochromatic waves

& The Total Energy > 0

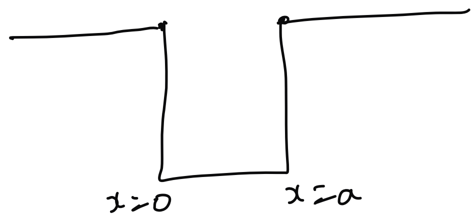
So we have full knowledge of 'p' $= \hbar k$

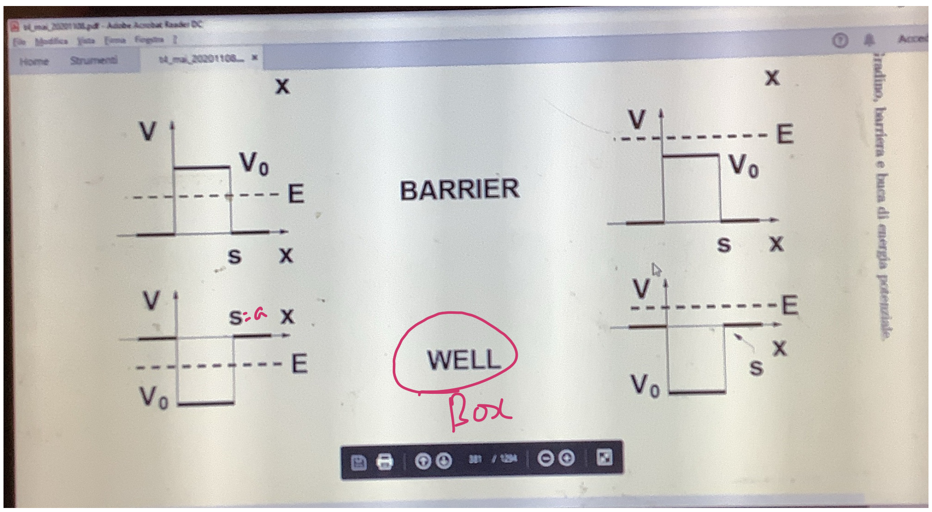
offcourse we have No information about the Position

& we also have No information about the Direction of Momentum

→ let's consider the ==problem of a particle in a Box==

- particle in a Box is s.t we can consider an interval $x=0$ to $x=a$ in which P.E $=0$ and $x=0$ & $x=a$ P.E becomes finite with Discontinuity





The solution for particle in a Box is not easy, but if we consider two sides of the well go up to infinity.

So P.E on two sides becomes infinitely large and in conclusion this makes impossible for the wave function of the particle to be different from zero to the left & right of the Box.

Schrödinger Equation for a Particle in a Box — I

Taking again the one-dimensional case

$$\boxed{\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} = -\frac{2m}{\hbar^2}(E - V)\,w\,,} \qquad V = V(x)\,,$$

let $V = \mathrm{const} = 0$ for $x \in [0, a]$, and $V = V_0 > 0$ elsewhere. It can be shown that, if $V_0 \to \infty$, then w vanishes identically outside the interval $[0, a]$. Continuity yields $w(0) = w(a) = 0$. From the general properties it follows $E > V_{\min} = 0$, whence in $x \in [0, a]$ it is again

Here we have Boundary conditions

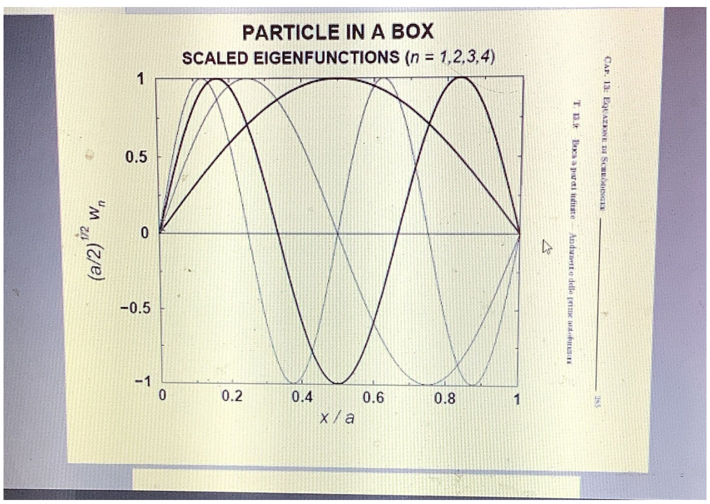
$$\boxed{w = c_1 \exp(jkx) + c_2 \exp(-jkx)\,, \quad k \doteq \sqrt{2mE/\hbar^2}\,.}$$

Letting $w(0) = 0$ yields $\boxed{c_1 + c_2 = 0}$ and $\boxed{w = 2jc_1\,\sin(kx)}$. Then, $w(a) = 0$ yields $ka = n\pi$ with n an integer, whence

we have a Relation involving an Integer ∴ we have Quantization.

$$E = E_n = \frac{\hbar^2\pi^2}{2ma^2}\,n^2\,, \qquad w = w_n = 2jc_1\,\sin\left(\frac{n\pi}{a}\,x\right).$$

The case $n = 0$ is to be excluded as $w_0 \equiv 0$. Similarly, the negative indices are to be excluded as $|w_{-n}|^2 = |w_n|^2$. In conclusion, $n = 1, 2, \ldots$



Q) How to interpret these solutions?

Ans ∵ w is zero outside the Box the probability of finding the particle outside the Box is zero.

→ Now we are left with problem of finding the constant c_1

$$w = w_n = 2j c_1 \sin\left(\frac{n\pi}{a} x\right)$$

Schrödinger Equation for a Particle in a Box — II

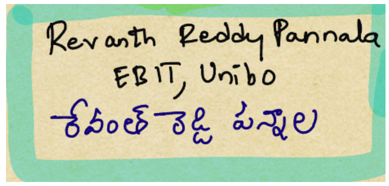
- In conclusion, the Schrödinger equation for a particle in a box yields the eigenvalues E_n and the eigenfunctions w_n. The energy is thus quantized. One eigenfunction corresponds to each eigenvalue. The eigenfunctions are normalizeable:

$$\int_0^a |w_n|^2 \, dx = 4|c_1|^2 \int_0^a \sin^2\left(\frac{n\pi}{a} x\right) \, dx =$$

$$= \frac{4|c_1|^2 a}{n\pi} \int_0^{n\pi} \sin^2(y) \, dy .$$

- Integration by parts shows that the last integral equals $n\pi/2$, hence the normalization condition $\int_0^a |w_n|^2 \, dx = 1$ yields $4|c_1|^2 = 2/a$. Choosing $2c_1 = -j\sqrt{2/a}$ provides the eigenfunctions

$$\boxed{w_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) .}$$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