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ASSIGNMENT - 2

ENGINEERING PHYSICS

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Q1. what do you understand by the wavefunction ψ of a moving particle? what does one calculate from wave function.

WAVE FUNCTION

- A wavefunction is a mathematical description of the quantum state of an isolated quantum system. The wave function is a complex valued probability amplitude, and the probabilities ~~of~~ for the possible results of measurement made on the system can be derived from it.

- WAVES are associated with quantities that vary periodically. In case of matter waves associated with a moving particle, the quantity that varies periodically is wavefunction.

- ψ itself has no physical interpretation as it is not an observable quantity however it is useful in calculating

  (i) The square of absolute magnitude of ψ wavefunction of a moving body evaluated at a particular time at a particular location is PROPORTIONAL to the probability of finding the particle at that place at that instant.

  (ii) The linear momentum, angular momentum, energy of a body can be established from a wave function.

Q2. What is normalisation condition? The wavefunction of a particle is given by $\psi(x) = C\exp(-\alpha^2 x^2)$, C and α are constants, over the domain $-\infty \le x \le \infty$. Calculate the probability of finding the particle in region $0 < x < \infty$

- Normalisation condition : $\int_{-\infty}^{\infty} |\psi|^2 dV = 1$

which implies particle is found completely in all space.

- $$\psi(x) = C\exp(-\alpha^2 x^2)$$

Applying normalisation condition,

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \qquad (1D \therefore dV \rightarrow dx)$$

$$\int_{-\infty}^{\infty} C^2 \exp(-2\alpha^2 x^2)\, dx = 1.$$

$$\boxed{\text{using } \int_{-\infty}^{\infty} e^{-\alpha x^2 + \beta x} dx = \sqrt{\frac{\pi}{\alpha}}\, e^{-\beta^2/4\alpha}}$$

$$C^2 \sqrt{\frac{\pi}{2\alpha^2}} = 1 \rightarrow C^2 = \sqrt{\frac{2}{\pi}}\,\alpha.$$

- Finding probability of finding part. in given domain $0 < x < \infty$.

$$P = \int_{0}^{\infty} |\psi(x)|^2 dx$$

$$= \int_{0}^{\infty} C^2 e^{-2\alpha^2 x^2} dx$$

$$= \int_{0}^{\infty} \sqrt{\frac{2}{\pi}}\,\alpha\, e^{-2\alpha^2 x^2} dx$$

$$= \sqrt{\frac{2}{\pi}}\,\alpha \int_{0}^{\infty} e^{-2\alpha^2 x^2} dx.$$

$$\boxed{\begin{array}{l} \text{since } e^{-\alpha x^2} \text{ is symmetric about } y\text{-axis} \\ \therefore \int_{0}^{\infty} e^{-2\alpha^2 x^2} = \frac{1}{2}\int_{-\infty}^{\infty} e^{-2\alpha^2 x^2} = \frac{1}{2}\sqrt{\frac{\pi}{2\alpha^2}} \end{array}}$$

$$= \sqrt{\frac{\cancel{2}}{\cancel{\pi}}}\,\cancel{\alpha} \times \frac{1}{2}\sqrt{\frac{\cancel{\pi}}{\cancel{2}}} \times \frac{1}{\cancel{\alpha}}$$

$$\boxed{P = 1/2}$$

Q3. Starting from the wave equation and introducing energy and momentum operators, obtain an expression for three dimensional shrödinger's eqⁿ in time dependent form.

A ~~unidirectional~~ 1D wave can be modelled by a second order linear partial differential equation as

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}$$ where v is the velocity of wave.

Solution to this eqⁿ is given by,

$$y = Ae^{-i\omega(t - x/v)}$$ $\omega = 2\pi\nu$; $v = \nu\lambda$; $k = 2\pi/\lambda$

which can be written as for a free particle moving along the x dir.

$$\psi(x,t) = Ae^{+i(kx-\omega t)} \quad - ①$$

As per de-broglie's relation,

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \times \frac{2\pi}{\lambda} = \hbar k \rightsquigarrow k = \frac{p}{\hbar} \quad - ②$$

As per einstein's equation,

$$E = h\nu = \frac{h}{2\pi} \times 2\pi\nu = \hbar\omega \rightsquigarrow \omega = \frac{E}{\hbar} \quad - ③$$

substituting ②, ③ in ①

$$\psi(x,t) = Ae^{i/\hbar (px - Et)} \quad - ④$$

This is a heuristic (non-rigourous) derivation of shrödinger's equation

Differentiate ④ wrt x & multiply by $-i\hbar$

$$-i\hbar\frac{\partial\psi}{\partial x} = -i\hbar\cdot\frac{ip}{\hbar}\psi(x,t) = p\psi \Rightarrow p \Leftrightarrow -i\hbar\frac{\partial}{\partial x}$$

Momentum opertor

Differentiate again wrt x & multiply by $-i\hbar$

$$(-i\hbar)^2\frac{\partial^2\psi}{\partial x^2} = p^2\psi$$

Divide by $2m$ where m is mass of particle,

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{p^2}{2m}\psi. \quad - ⑤$$

Differentiate ④ wrt t & multiply by $i\hbar$

$$i\hbar\frac{\partial\psi}{\partial t} = i\hbar\left(-\frac{iE}{\hbar}\right)\psi = E\psi \Rightarrow E \Leftrightarrow i\hbar\frac{\partial}{\partial t} \quad - ⑥$$

Energy operator

for a free particle, total energy is kinetic energy

$$\therefore \quad E = p^2/2m$$

$\therefore$ RHS of eqns (5), (6) become equal $\rightarrow$ LHS is also equal.

$$\therefore \quad i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} \quad — (7)$$

If the particle is not free (ie in a potential field), total energy is

$$E = p^2/2m + \underbrace{V(x)}_{\text{pot}^n\text{ energy}}$$

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

Hence
$$E\psi = \left[\frac{p^2}{2m} + V(x)\right]\psi(x,t)$$

Now,
$$i\hbar \frac{\partial \psi}{\partial t} = \underbrace{\left[\frac{p^2}{2m} + V(x)\right]}_{\boxed{\text{Hamiltonian operator}}}\psi(x,t)$$

similarly, in 3D,

$$i\hbar \frac{\partial \psi(x,y,z,t)}{\partial t} = \frac{-\hbar^2}{2m}\overbrace{\left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2}{\partial y^2}\psi + \frac{\partial^2 \psi}{\partial z^2}\right]}^{\boxed{\text{Del operator}^2}} + V(x)\psi$$

$$\therefore \quad \boxed{i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2 \psi + V(x)\psi = H\psi}$$

3D Time dependent schrödinger eqn for a particle in a potential field.

Q4 Obtain three dimensional time independent schrödinger's equation from time dependent schrödinger's equation.

Schrödinger in 1D for a particle is.

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t) \quad -(1)$$

solving the partial diffn eqn by variable separable method

Assume soln to be of form

$$\psi(x,t) = X(x)\,T(t) \quad -(2)$$

put (2) in (1)

$$-\frac{\hbar^2}{2m} T X'' + V X T = i\hbar X T'$$

Dividing both sides by XT

$$-\frac{\hbar^2}{2m} \frac{\cancel{T} X''}{X \cancel{T}} + \frac{V \cancel{XT}}{\cancel{XT}} = i\hbar \frac{\cancel{X} T'}{\cancel{X} T}$$

$$-\frac{\hbar^2}{2m} \frac{X''}{X} + V = i\hbar \frac{T'}{T}$$

since x, t are independent variables, LHS & RHS can be equal if equal to a constant, say A.

$$+V -\frac{\hbar^2}{2m} \frac{X''}{X} = A \quad -(3) \qquad ; \qquad i\hbar \frac{T'}{T} = A \quad -(4)$$

~~$\psi(t) = \exp\left[\frac{-iAt}{\hbar}\right]$~~

~~$i\hbar T' - AT = 0$.~~

~~Auxillary equation~~

~~$i\hbar m - A = 0$.~~

~~$m = A/i\hbar$~~

~~$\therefore$ sol^n is.~~

~~$T = c_1 e^{A/i\hbar \, t} = c_1 e^{-iAt/\hbar}$~~

E

$$i\hbar \frac{\partial \phi(t)}{\partial t} = E \phi(t)$$

compare with (4), we get $A = E$

$\therefore$ (3) becomes.

$$-\frac{\hbar^2}{2m} X'' + V X = E X.$$

$$X'' - \frac{2m}{\hbar^2}\left[V X - E X\right] = 0$$

$$X'' + \frac{2m}{\hbar^2}\left[E - V\right] X = 0.$$

ie $$\boxed{\frac{d^2 X}{dx} + \frac{2m}{\hbar^2}\left[E - V\right] X = 0}$$

Time independent schrödinger eq^n.

Q5. In a certain one dimensional problem, the quantum mechanical behaviour of particle of mass m, is described by the wave function

$$\psi(x,t) = A e^{-\alpha x^2} e^{-i\omega t}$$

where A is the normalisation constant ; α is real +ive const and $\omega = E/\hbar$. Normalise the given function.

Passage of time has no effect on normalis^n.

$\therefore$ Applying normalisation condition to $\psi(x,t)$.

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

$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1.$$

$$\psi = A e^{-\alpha x^2 - i\omega t} \sim \psi^* = A e^{-\alpha x^2 + i\omega t}$$

$$\int_{-\infty}^{\infty} A e^{-\alpha x^2 - \cancel{i\omega t}} \cdot A e^{-\alpha x^2 + \cancel{i\omega t}} \, dx = 1.$$

$$\int_{-\infty}^{\infty} A^2 e^{-2\alpha x^2} \, dx = 1.$$

using std integral

$$\int_{-\infty}^{\infty} e^{-\alpha t^2 + \beta t} = \sqrt{\frac{\pi}{\alpha}} \, e^{\beta^2/4\alpha} \quad \text{here } \beta = 0$$

$$\int_{-\infty}^{\infty} A^2 e^{-2\alpha x^2 + 0x} = 1$$

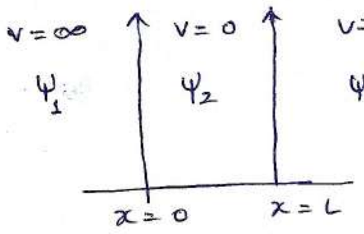
$$A^2 \sqrt{\frac{\pi}{2\alpha}} = 1.$$

$$A^2 = \sqrt{\frac{2\alpha}{\pi}}$$

$$\boxed{A = \left[\frac{2\alpha}{\pi}\right]^{1/4}}$$

Q6. Calculate the energy eigen values and eigenfunction, the expectation values of position $\langle x \rangle$ and momentum $\langle p_x \rangle$ of a particle trapped in potential

$$V(x) = 0 \quad \text{for} \quad 0 \le x \le a$$
$$V(x) = \infty \quad \text{for} \quad \text{otherwise}$$



∞ potn well

since $V = \infty$ for $x \notin [0, a]$,

$$\psi_1 = \psi_3 = 0 \quad - (1)$$

Time indep. shrodinger eqn.

$$\frac{\partial^2 \psi_2}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi_2 = 0$$

$V = 0$

$$\therefore \frac{\partial^2 \psi_2}{\partial x^2} + \underbrace{\frac{2mE}{\hbar^2}}_{k^2} \psi_2 = 0$$

$$\therefore \frac{\partial^2 \psi_2}{\partial x^2} + k^2 \psi_2 = 0. \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$(2) \quad - \quad E = \frac{\hbar^2 k^2}{2m}$$

soln of this eqn is (simple harmonic)

$$\psi_2 = A \sin kx + B \cos kx \quad - (3)$$

at $x = 0$ Boundary condn 1.

$$\psi_2 = \psi_1 = 0$$
$$A \sin 0 + B \cos 0 = 0$$
$$0 + B = 0$$
$$B = 0$$
$$\therefore \psi_2 = A \sin kx \quad - (4)$$

at $x = L$ boundary condn in (4)

$$\psi_2 = \psi_3 = 0.$$
$$A \sin kL = 0$$
$$\sin kL = 0$$

Trivial

$$kL = n\pi \quad n = \cancel{0}, \pm 1, \pm 2, \ldots$$
$$k = \frac{n\pi}{L} \quad - (5)$$

put (5) in (2)

$$E = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad - (6)$$

put (5) in (4)

$$\psi_2 = A \sin \frac{n\pi}{L} x$$

Normalising ψ_2,

$$\int_{-\infty}^{\infty} \psi_2^* \psi_2 \, dx = 1$$

$$\int_0^L A \sin \frac{n\pi}{L} x \,.\, A \sin \frac{n\pi}{L} x \, dx = 1$$

$$\int_0^L \frac{A^2}{2}\left[1 - \cos \frac{2n\pi x}{L}\right] dx = 1.$$

$$\frac{A^2}{2}\int_0^L dx - \frac{A^2}{2}\int_0^L \cancel{\cos\frac{2n\pi x}{L}}^{\,0}\,dx = 1$$

$$\frac{A^2}{2}L = 1 \rightsquigarrow A = \sqrt{\frac{2}{L}}$$

$$\therefore \boxed{\psi_2 = \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x}$$

for energy

$$\therefore \boxed{\begin{array}{ll}\text{Eigen func}^n & \psi_x = \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x \\ \text{Eigen val.} & E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}\end{array}}$$

Expectation value from position operator

$$\langle x\rangle = \int_{-\infty}^{\infty}\psi^* x\,\psi\,dx$$

$$= \int_0^L \frac{2}{L}x\sin^2\frac{n\pi x}{L}dx.$$

$$= \int_0^L \frac{\cancel{2}}{L}\left(\frac{x}{\cancel{2}}\right)\left(1-\cos\frac{2n\pi x}{L}\right)dx.$$

$$= \frac{1}{L}\left(\int_0^L x\,dx - \int_0^L x\cos\frac{2n\pi x}{L}dx\right)$$

$$\boxed{\begin{array}{l} - \int x\cos ax\,dx = \frac{1}{a^2}\cos ax + \frac{x}{a}\sin ax \\ - \text{consider } n=1\end{array}}$$

$$= \frac{1}{L}\left(\int_0^L x\,dx - \left[\frac{L^2}{4\pi^2}\cos\frac{2\pi}{L}x + \frac{xL}{2\pi}\sin\frac{2\pi}{L}x\right]_0^L\right)$$

$$= \frac{1}{L}\left(\left[\frac{x^2}{2}\right]_0^L - \left[\frac{L^2}{4\pi^2}\cancel{\cos 2\pi}^{\,-1} + \frac{L^2}{2\pi}\cancel{\sin 2\pi}^{\,0} - \frac{L^2}{4\pi^2}\cancel{\cos 0}^{\,1} + 0\right]\right)$$

$$= \frac{1}{L}\left(\frac{L^2}{2} - \frac{L^2}{4\pi^2} - \frac{L^2}{4\pi^2}\right) = \boxed{L\left[\frac{1}{2}-\frac{1}{2\pi^2}\right]} \quad \text{for } n=1.$$

Expectation value from momentum operator

$$\langle p\rangle = \int_{-\infty}^{\infty}\psi^*\hat{p}\,\psi\,dx = i\hbar\int_{-\infty}^{\infty}\psi^*\frac{\partial}{\partial x}\psi\,dx$$

$$= \int_0^L \frac{2}{L}\sin\frac{\pi x}{L}\frac{\partial}{\partial x}\sin\frac{\pi x}{L}dx$$

$$= \int_0^L \frac{2}{L}\sin\frac{\pi x}{L}\cdot\frac{\pi}{L}\cos\frac{\pi x}{L}dx$$

$$= \int_0^L \frac{\pi}{L^2} \sin\frac{2\pi x}{L}$$

$$= \frac{\cancel{\pi}}{L^{\cancel{2}}} \left[\cos\frac{2\pi x}{L}\right]_0^L = \frac{1}{2L}(\cos 2\pi - \cos 0) = \boxed{0}$$

$$\frac{\cancel{4\pi}}{\cancel{L}}$$

Q7 The wave function of a particle confined in a two dimensional box of side L is given by

$$\psi(x,y) = \frac{2}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)$$

calculate the pblity of finding the particle in region

$$0 \le x \le L/2 \;;\; 0 \le y \le L/2$$

probability of finding particle in the given boundaries

$$P = \int_{L=0}^{L/2}\int_0^{L/2} \frac{4}{L} \sin^2\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{\pi y}{L}\right) dx\,dy.$$

$$= \frac{\cancel{4}^2}{L^2}\int_0^{L/2}\int_0^{L/2} \frac{1}{\cancel{2}}\left[1-\cos\frac{2\pi x}{L}\right]\left(\sin^2\frac{\pi y}{L}\right)dx\,dy.$$

$$= \frac{2}{L^2}\int_0^{L/2}\left[x + \frac{L}{2\pi}\sin\frac{2\pi x}{L}\right]_0^{L/2} \sin^2\left(\frac{\pi y}{L}\right) dy$$

$$= \frac{2}{L^2}\int_0^{L/2}\left[\frac{L}{2} + \frac{L}{2\pi}\cancel{\sin}\overset{0}{\pi} - 0 - 0\right] \sin^2\left(\frac{\pi y}{L}\right) dy$$

$$= \frac{\cancel{2}}{\cancel{L}^2}\int_0^{L/2} \frac{\cancel{L}}{\cancel{2}} \sin^2\left(\frac{\pi y}{L}\right) dy.$$

$$= \int_0^{L/2} \frac{1}{L}\left[1-\cos\frac{2\pi y}{L}\right] dy$$

$$= \frac{1}{2L}\left[y + \frac{L}{2\pi}\sin\frac{2\pi y}{L}\right]_0^{L/2}$$

$$= \frac{1}{2L}\left[\frac{L}{2} + \frac{L}{2\pi}\sin\frac{\cancel{2}\pi \cancel{L}}{\cancel{2L}}\right]$$

$$= \boxed{\frac{1}{4}}$$

Q8. An electron is bound in a one dimensional potential box which has a width 2.5×10^{-10} m. Assuming the height of box is infinite, calculate the lowest two permitted values of electron.

Energy in a given quantum no. is given by

$$E_n = \frac{n^2 h^2}{8 m a^2}$$

for $n = 1$,

$$E_1 = \frac{1^2 \times (6.626 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (2.5 \times 10^{-10})^2}$$

$$= \frac{43.9 \times 10^{-68}}{455 \times 10^{-51}}$$

$$\simeq 0.0965 \times 10^{-68+51}$$

$$\approx \boxed{9.65 \times 10^{-19}\ \text{J}}$$

for $n = 2$

$$E_2 = \frac{2^2 \times (6.626 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (2.5 \times 10^{-10})^2} = 4E_1$$

$$\simeq \boxed{3.86 \times 10^{-18}\ \text{J}}$$

Q9. A particle described by the wavefunction

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

confined to the region $0 < x < L$. The particle is in the first excited state. Then find the maximum probability of finding the particle.

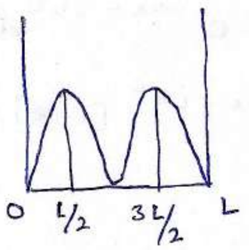
For position with maximum probability of finding electron,

$$\frac{\partial}{\partial x} |\psi|^2 = 0$$

for $n = 2$ (first excited state);

$$\frac{\partial}{\partial x} \frac{2}{L} \sin^2 \frac{2\pi x}{L} = 0.$$

$$\frac{2}{L}\, 2 \sin\frac{2\pi x}{L} \cdot \cos\frac{2\pi x}{L} \cdot \frac{2\pi}{L} = 0$$



$$\frac{4\pi}{L^2} \sin\frac{4\pi x}{L} = 0$$

$$\therefore \sin\frac{4\pi x}{L} = 0$$

for $0 < \frac{4\pi x}{L} < \cancel{L}$; corresponding to 2π

$$\frac{\pi x}{L} = \frac{\pi}{4} \; ; \; \frac{3\pi}{4}.$$

$$\therefore \boxed{x = \frac{L}{4}, \frac{3L}{4}}$$

Q10. The normalised wave function of a particle is $\psi(x,t) = A\exp(iax - ibt)$, where A, a, b are constants. Evaluate the uncertainty in its momentum

using
$$\langle p \rangle = i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial}{\partial x} \psi(x)\, dx$$

&
$$\langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi^* \frac{\partial^2}{\partial x^2} \psi(x)\, dx$$

&
$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \; ;$$

$$\psi(x,t) = A e^{iax - ibt}$$

Normalising the function

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

$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$$

$$\int_{-\infty}^{\infty} A e^{-iax+ibt} \cdot A e^{iax-ibt} dx = 1$$

$$\int_{-\infty}^{\infty} A^2 dx = 1$$

$$\langle p \rangle = i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial}{\partial x} \psi \, dx$$

$$= i\hbar \int_{-\infty}^{\infty} A e^{-iax+ibt} \cdot \frac{\partial}{\partial x} \cdot A e^{iax-ibt} dx$$

$$= i\hbar \int_{-\infty}^{\infty} A e^{-iax+ibt} \cdot A e^{iax-ibt} [ia] \, dx$$

$$= i\hbar \int_{-\infty}^{\infty} A^2 \cdot ia \, dx$$

$$= i\hbar \cdot ia \cancel{\int_{-\infty}^{\infty} A^2 dx}^{\,1}$$

$$= -\hbar a$$

$$\langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi^* \frac{\partial^2}{\partial x^2} \psi \, dx$$

$$= -\hbar^2 \int_{-\infty}^{\infty} A e^{-iax+ibt} \cdot A e^{iax-ibt} [ia]^2 dx$$

$$= -\hbar^2 \int_{-\infty}^{\infty} A^2 \times (-a) \, dx$$

$$= \hbar^2 a^2 \cancel{\int_{-\infty}^{\infty} A^2 dx}^{\,1}$$

$$= h^2 a^2.$$

$$\therefore \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

$$= \sqrt{h^2 a^2 - (-ha)^2}$$

$$= \boxed{0}$$

———— x ————

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