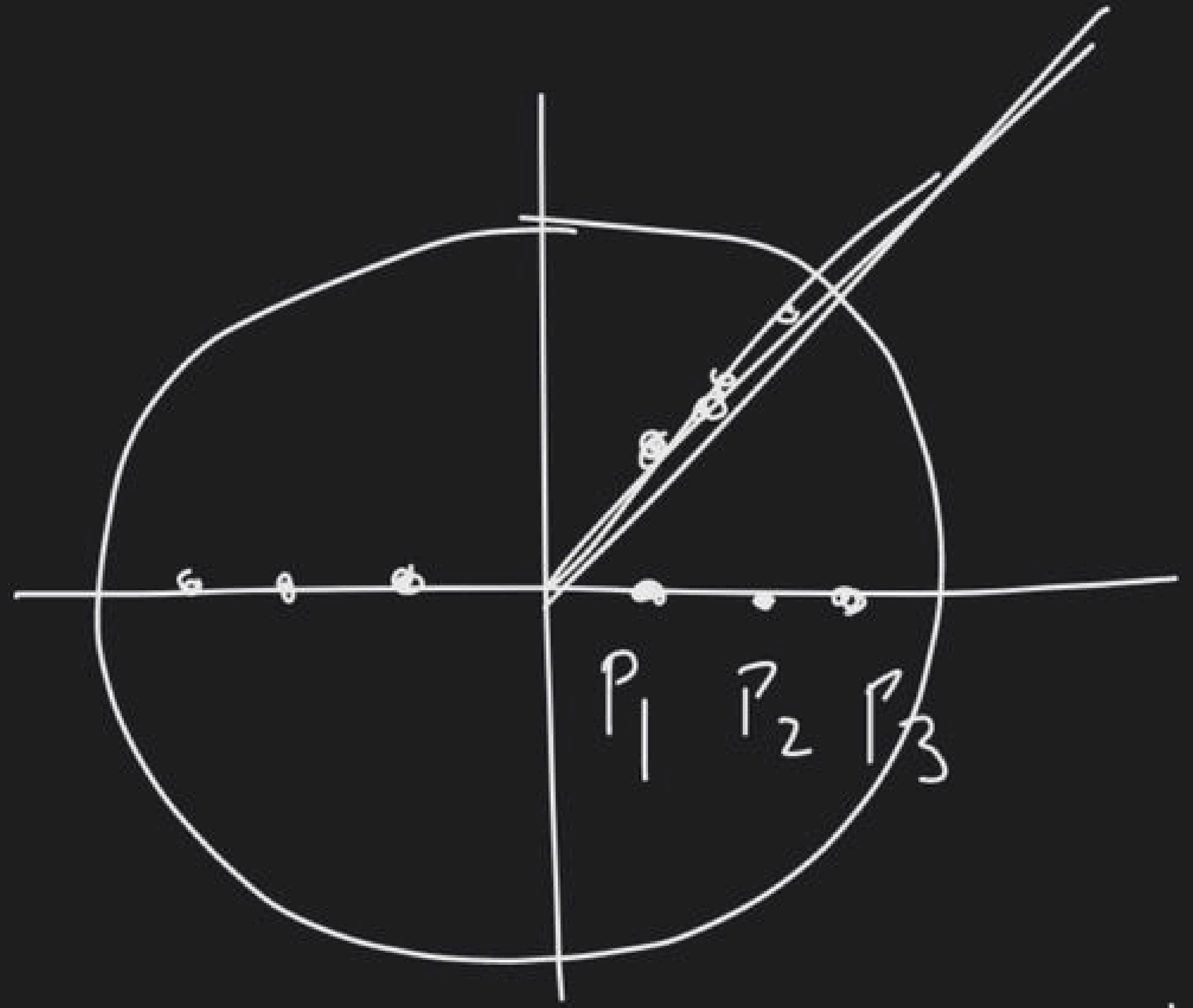
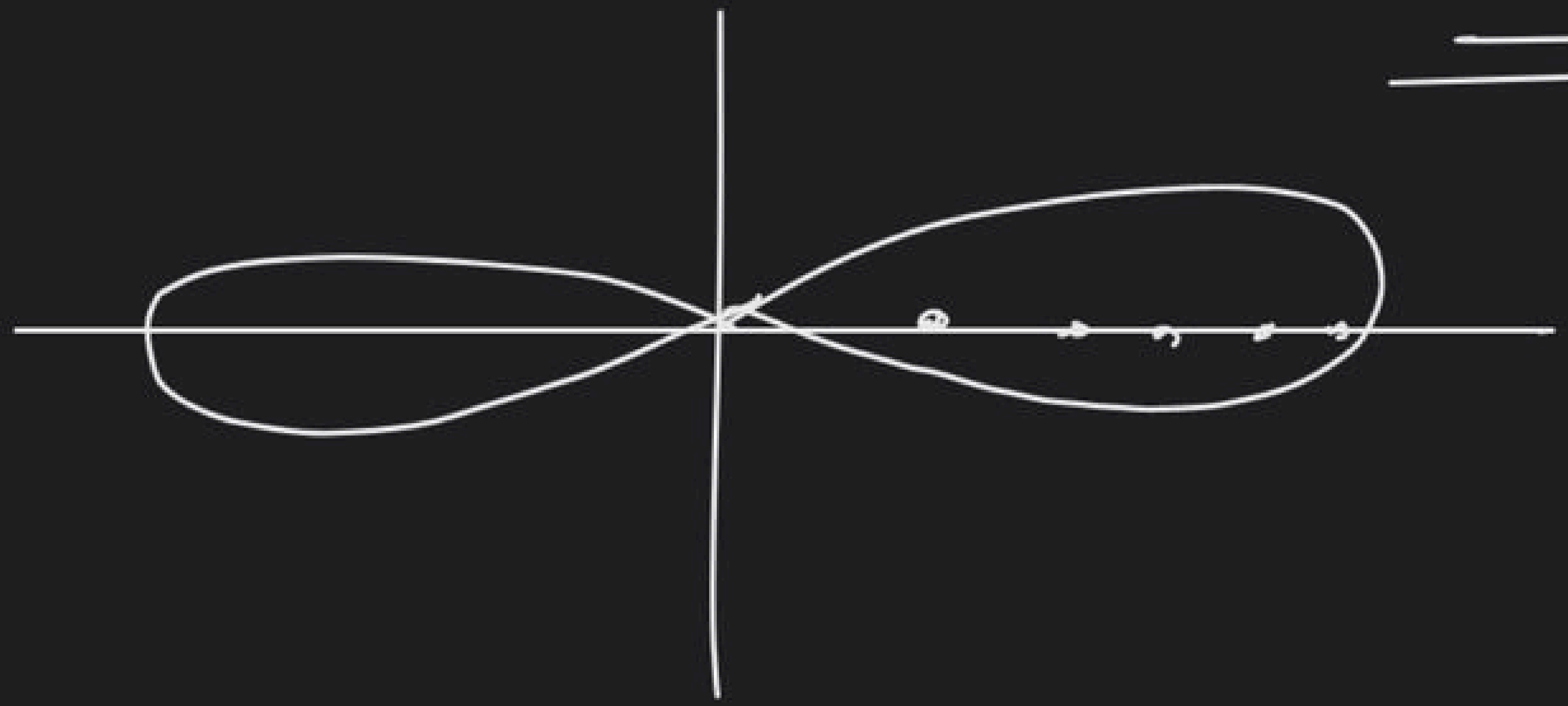
Schrodinger Equation

Course on Atomic Structure for Class XI

akhilesh • Lesson 13 • Sept 17, 2021





n, l, m

$$\Psi = f(r)(\theta, \phi)$$

$$\Psi = R(r)\,\Theta(\theta, \phi)$$

Varial of R(r) with r :→

$$R(r) = c\,\frac{1}{a_0^{3/2}} \cdot \sigma^{l} \cdot e^{-\sigma/2} \left(\begin{array}{c} \text{equation of 'r'} \\ \text{of order } n-l-1 \end{array} \right)$$

$$\sigma = \frac{2r}{n a_0}$$

$$\underline{\underline{R(r)_{1s}}} = \frac{2}{a_0^{3/2}} \cdot e^{-r/a_0}$$

$$\sigma = \frac{2r}{a_0}$$

$$n-l-1$$

$$1-0-1 = 0$$

$$R(r)_{2s} = \frac{1}{2\sqrt{2}} \frac{1}{a_0^{3/2}} e^{-\sigma/2}(2-\sigma)$$

$$\sigma = \frac{r}{a_0}$$

$$= \frac{1}{2\sqrt{2}} \frac{1}{a_0^{3/2}} e^{-r/2a_0}\left(2 - \frac{r}{a_0}\right)$$

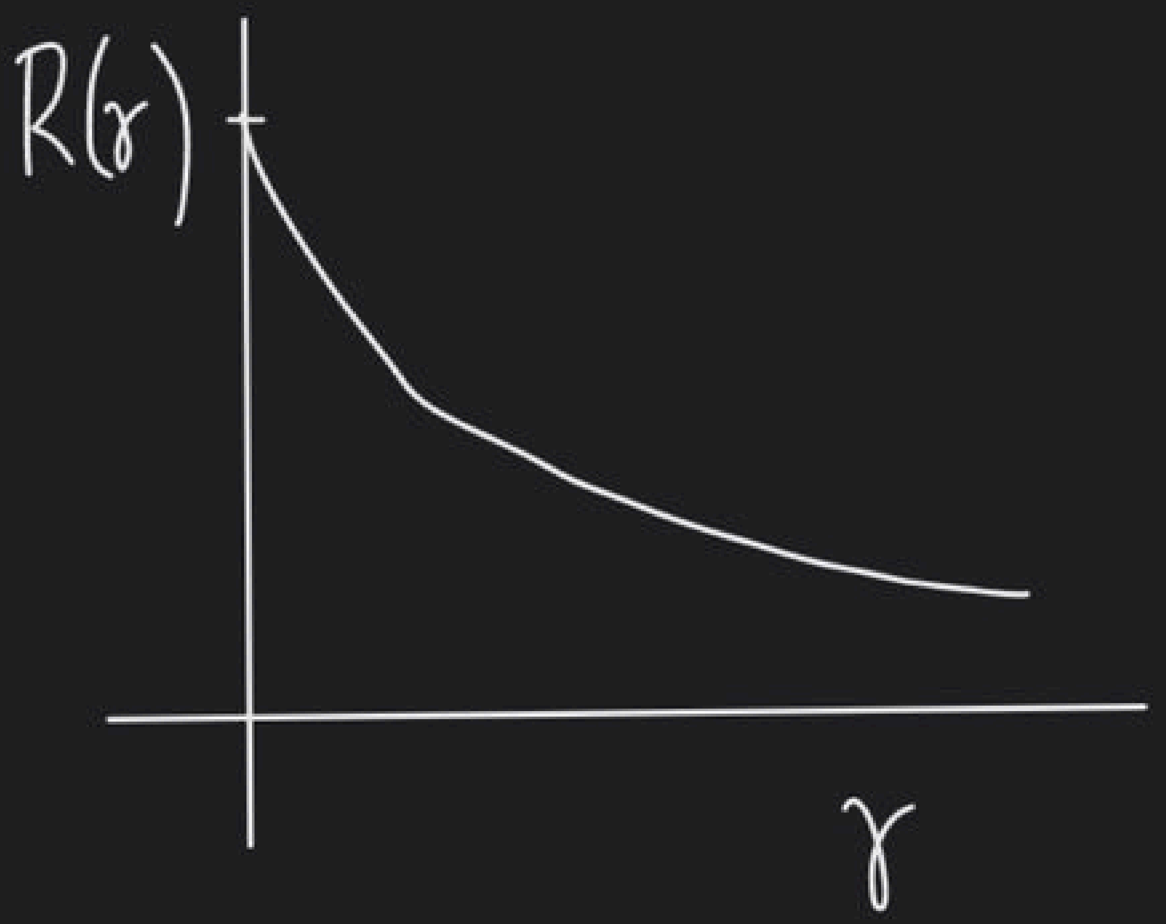
$$2-0-1=1$$

$$n-l-1$$

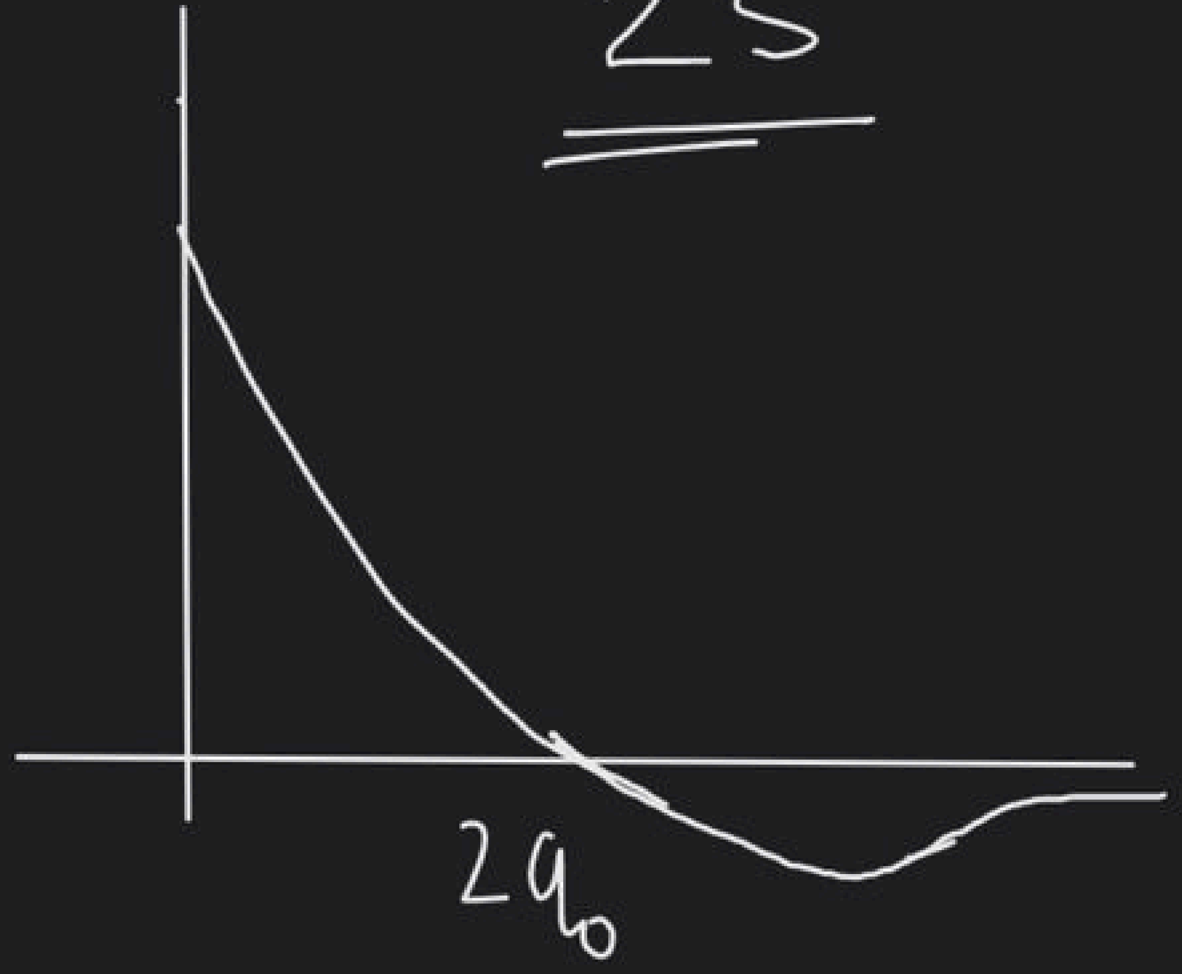
$$R(r)_{3s} = \frac{c}{a_0^{3/2}} e^{-\sigma/2}(\text{Quadratic})$$

$$R(r)_{4s} = \frac{c}{a_0^{3/2}} e^{-\sigma/2}(\text{Cubical})$$

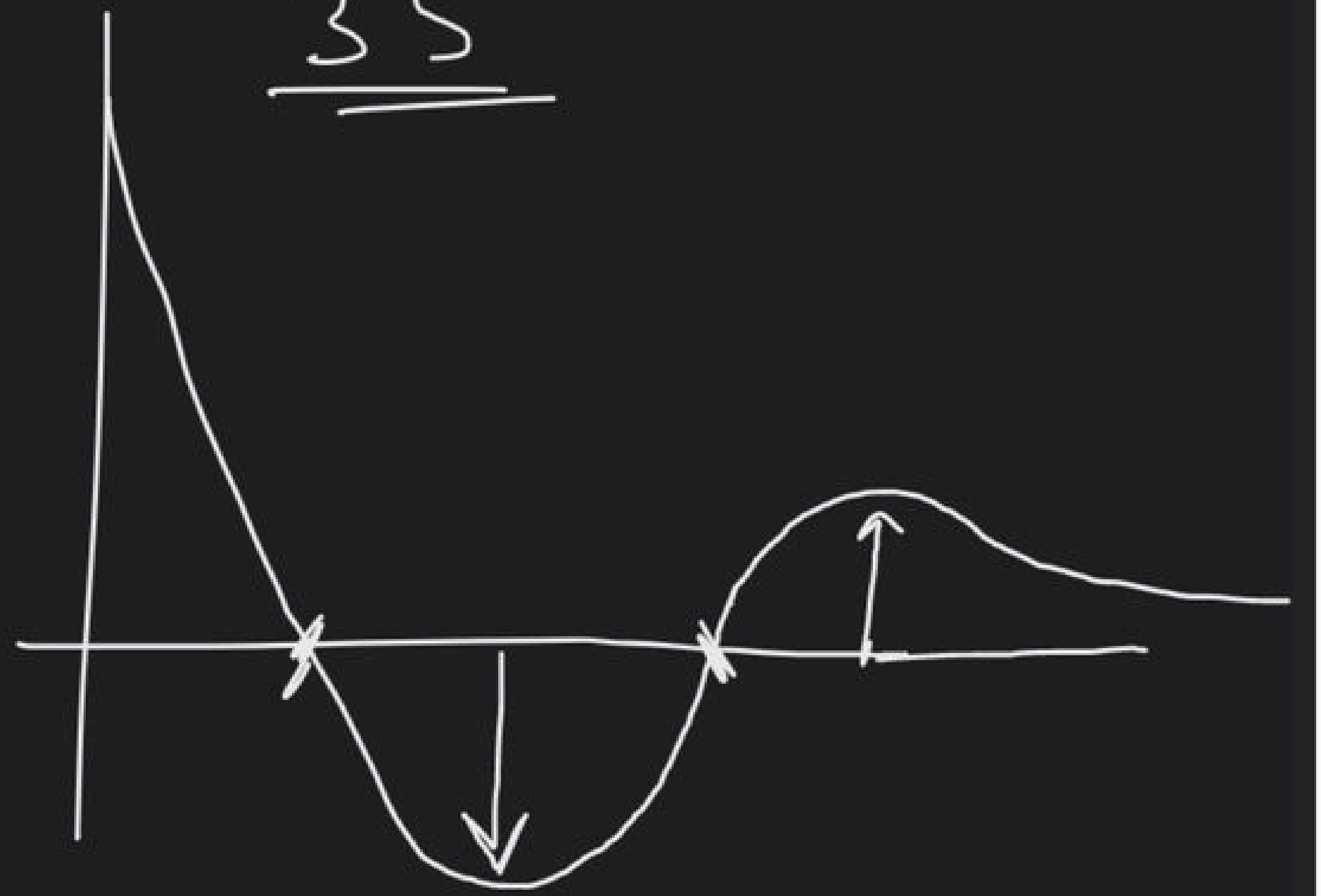
1s



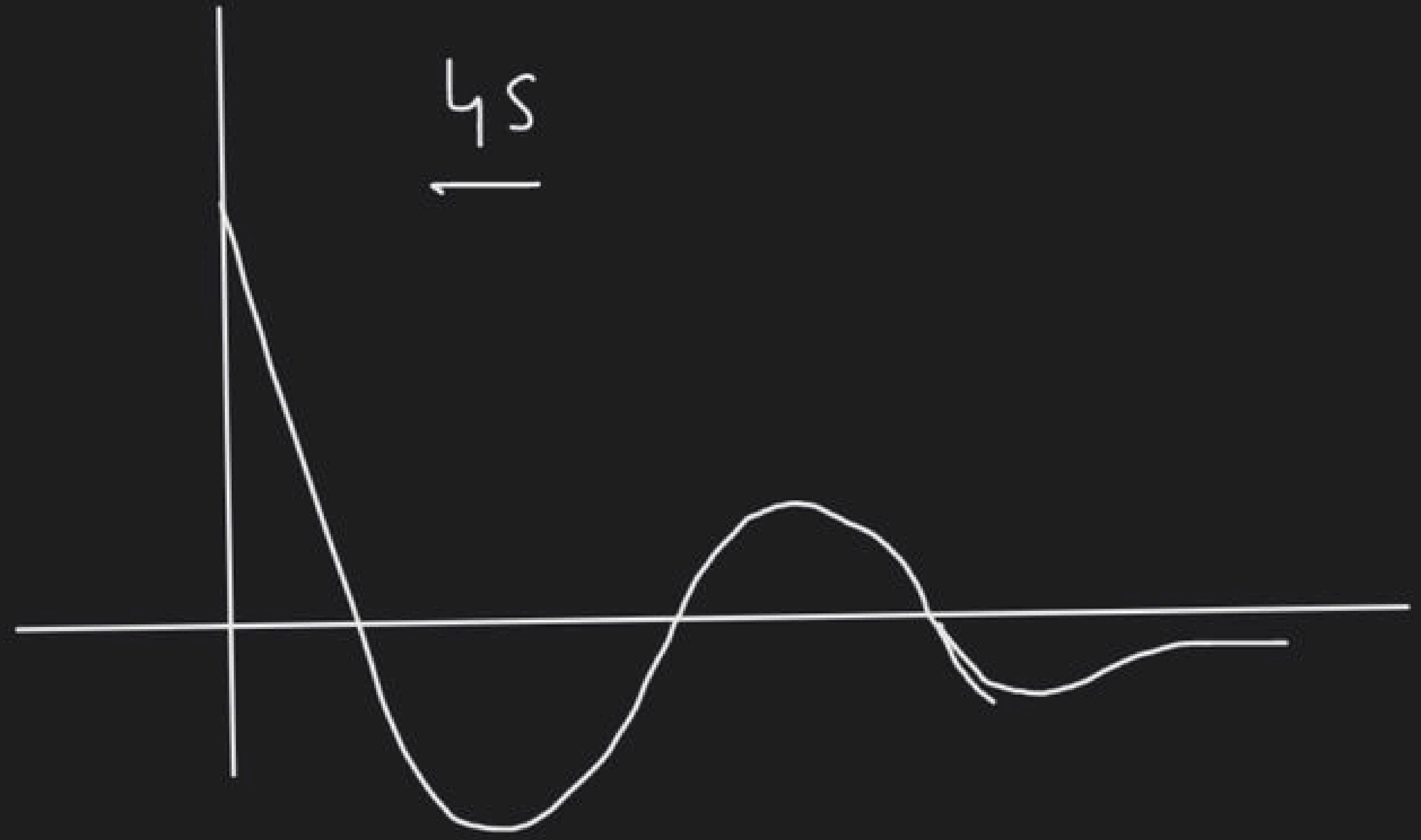
2s



3s



4s



$n - l - 1$

$$R(r)_{2p} = \frac{1}{2\sqrt{6}} \frac{1}{a_0^{3/2}} \sigma \cdot e^{-\sigma/2} \left(1 \right)$$

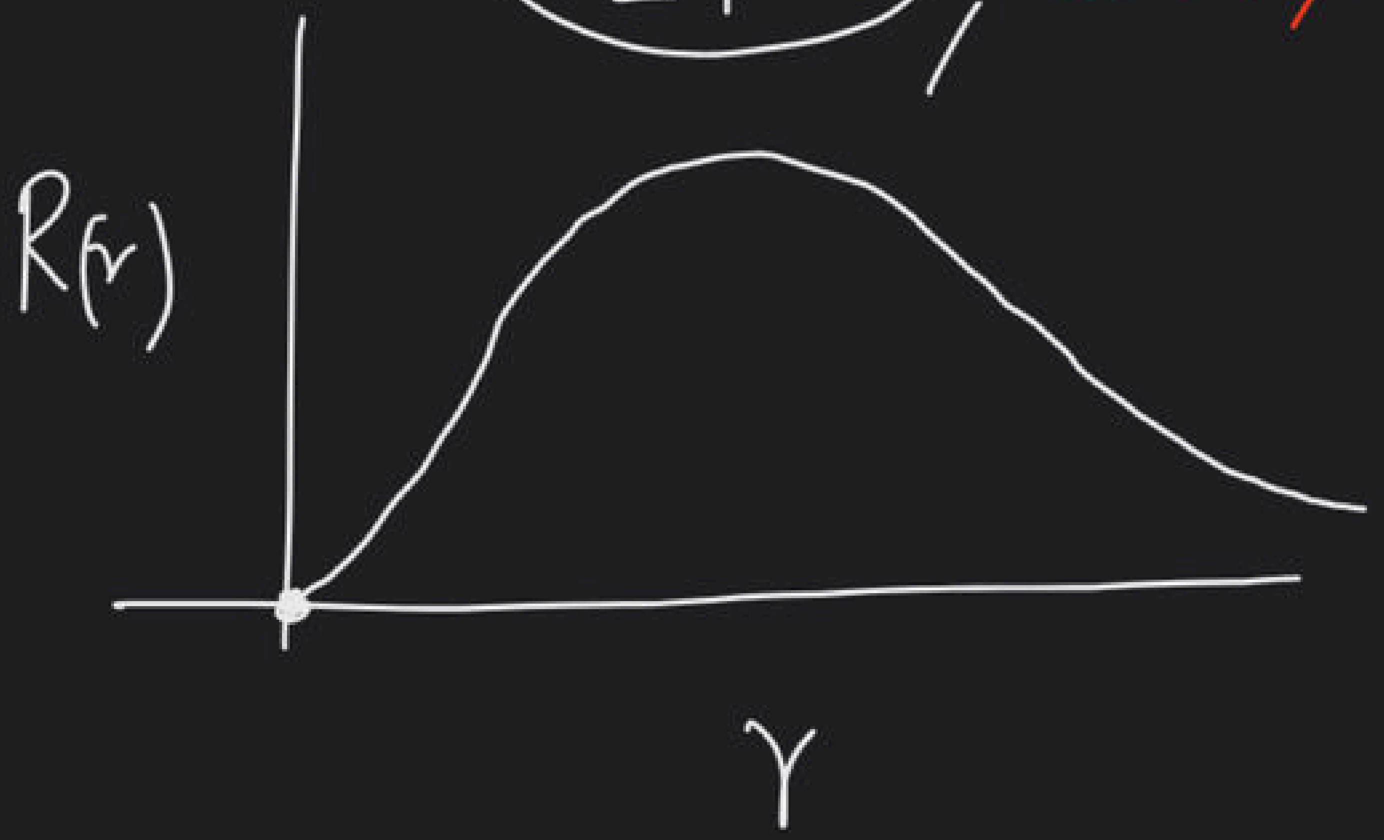
$$\sigma = \frac{r}{a_0}$$

$n - l - 1$

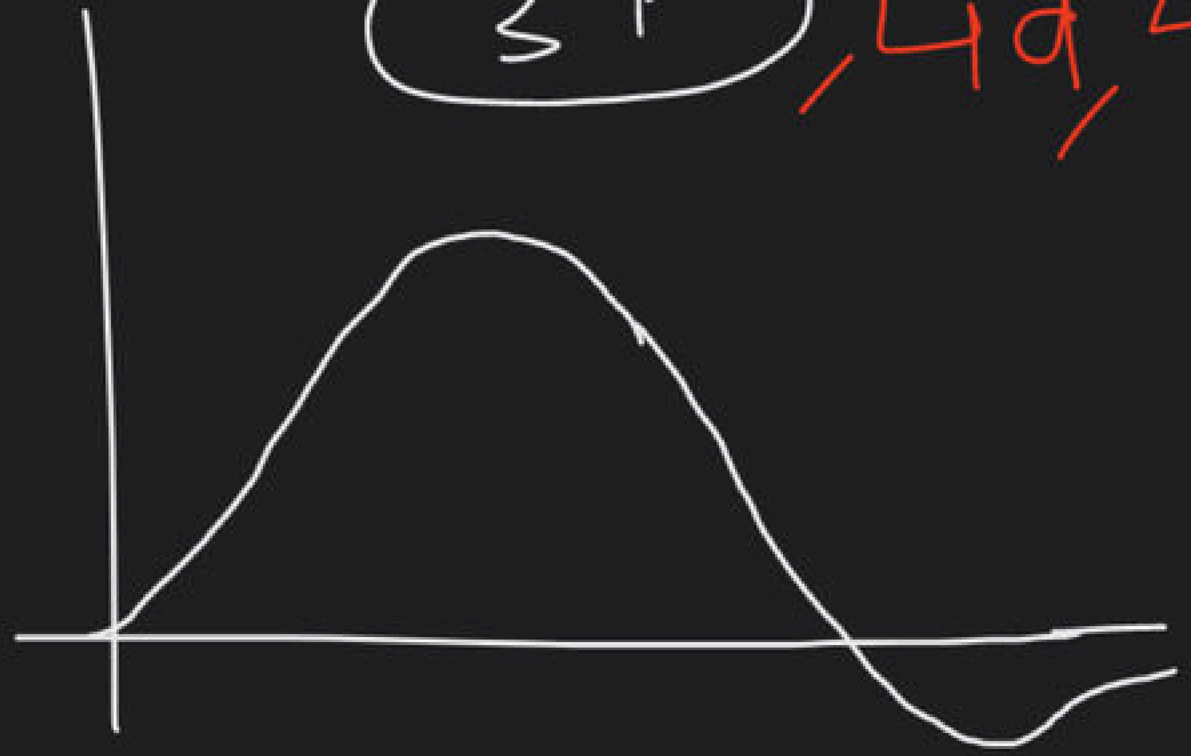
$2 - 1 - 1 = 0$

$$R(r)_{3p} = c \frac{1}{a_0^{3/2}} \sigma \cdot e^{-\sigma/2} \left(\text{linear} \right)$$

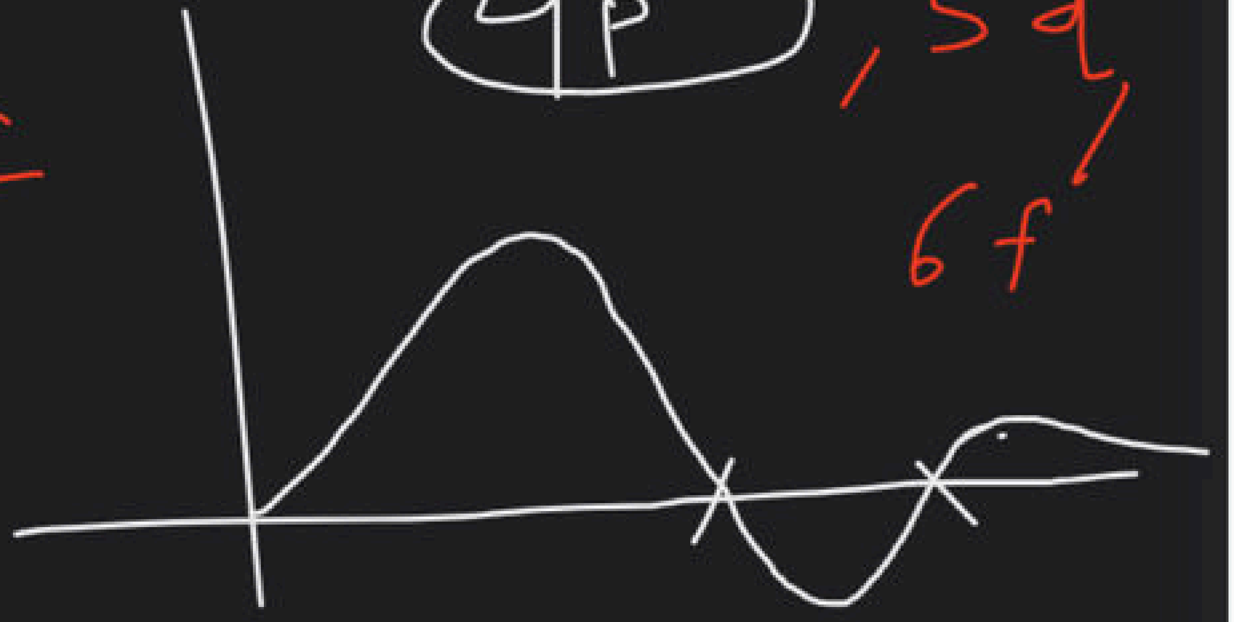
2p, 3d, 4f



3p, 4d, 5f



4p, 5d, 6f

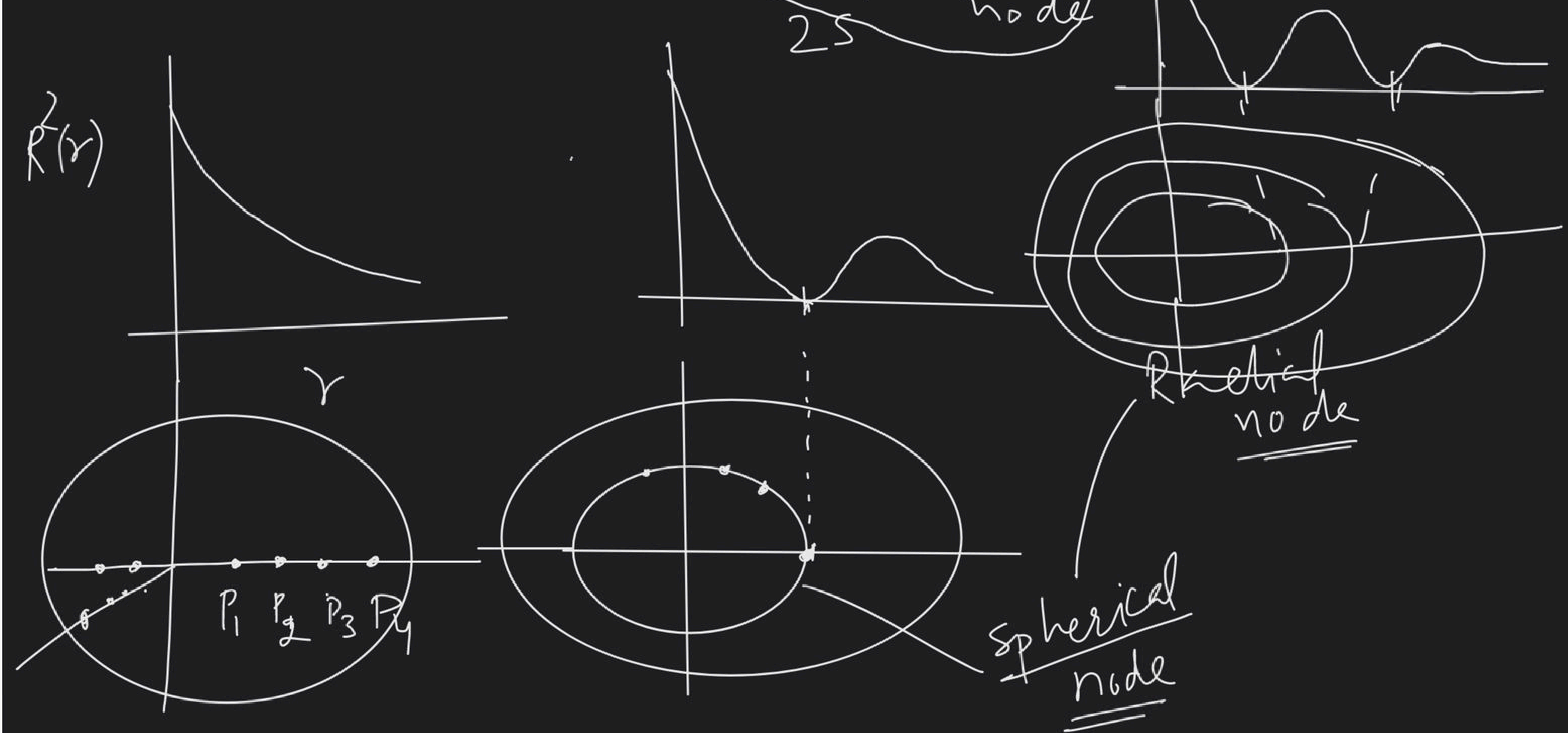


$$R(r)_{3d} = C \frac{1}{a_0^{3/2}} \sigma^2 e^{-\sigma/2} (1)$$

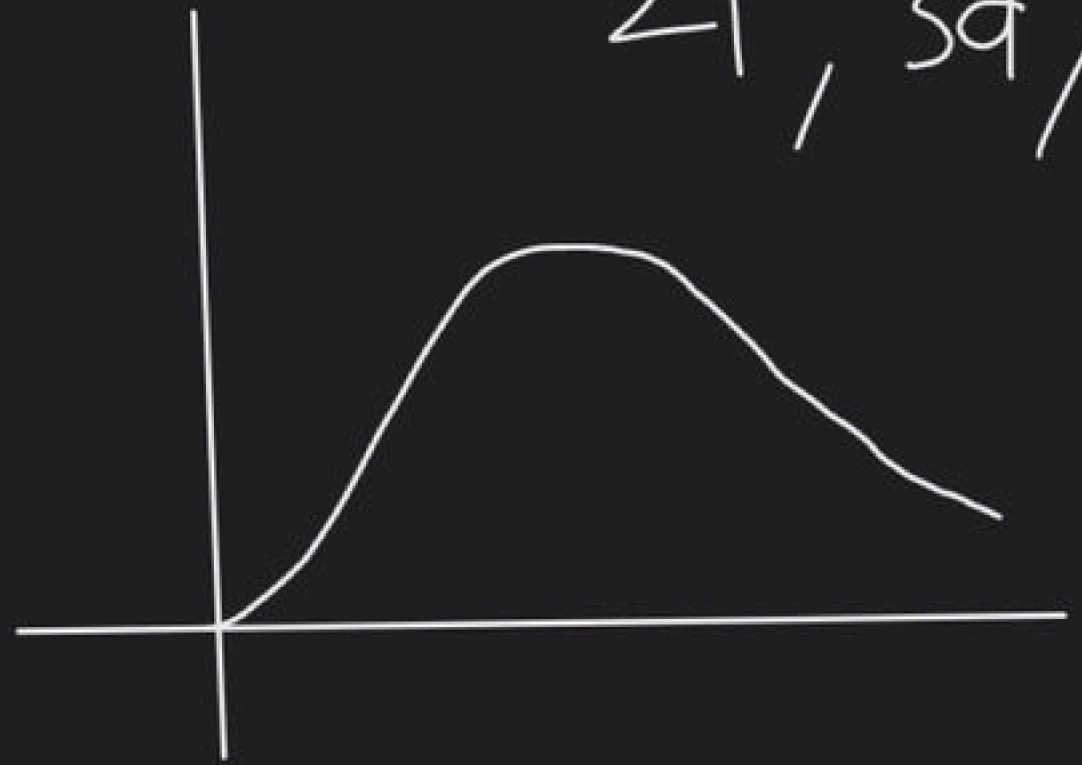
$$R(r)_{4d} = C \frac{1}{a_0^{3/2}} \sigma^2 e^{-\sigma/2} (\text{linear})$$

$R^2(r)$ vs r

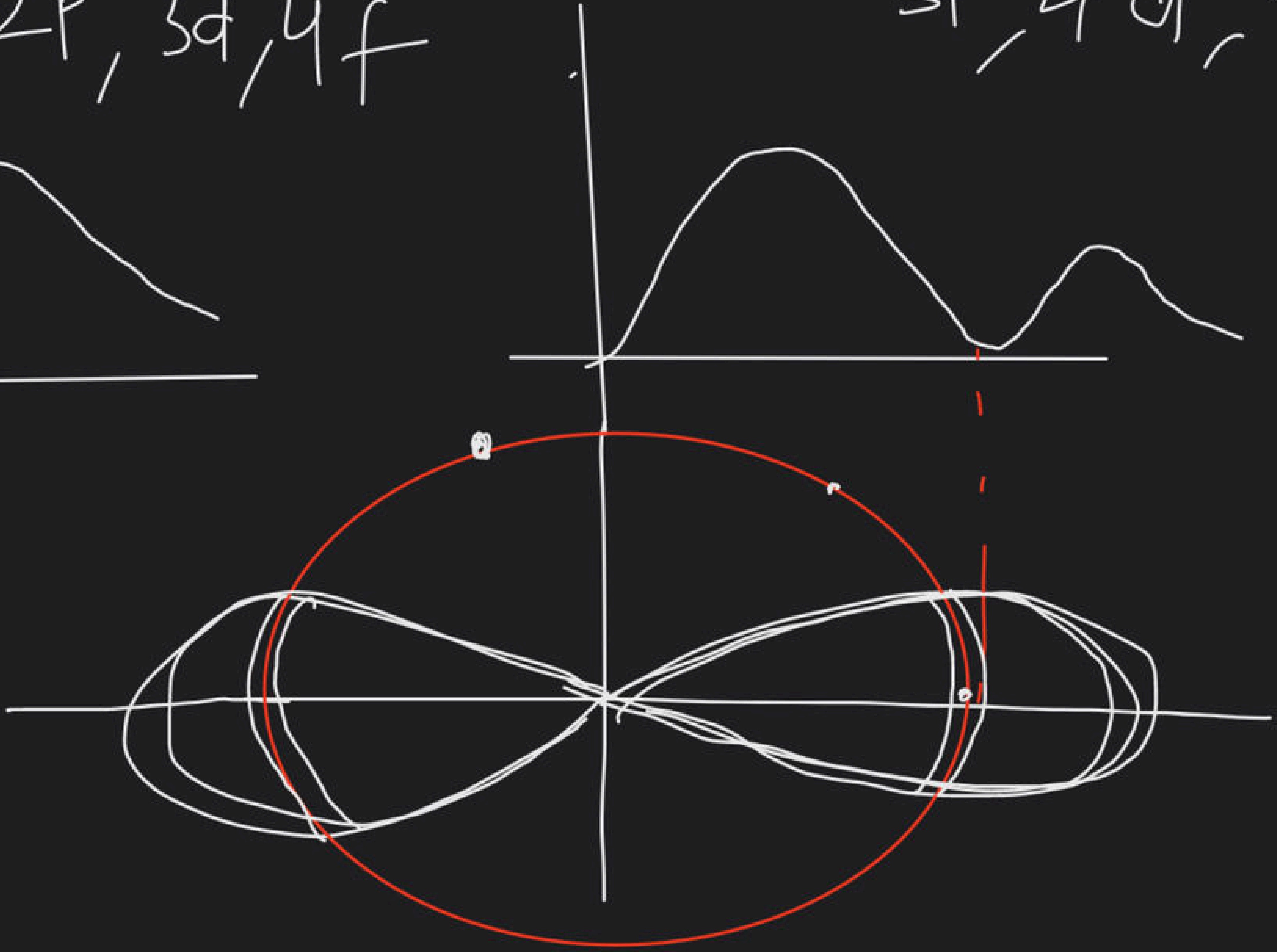
$n - l - 1 =$ no. of spherical node

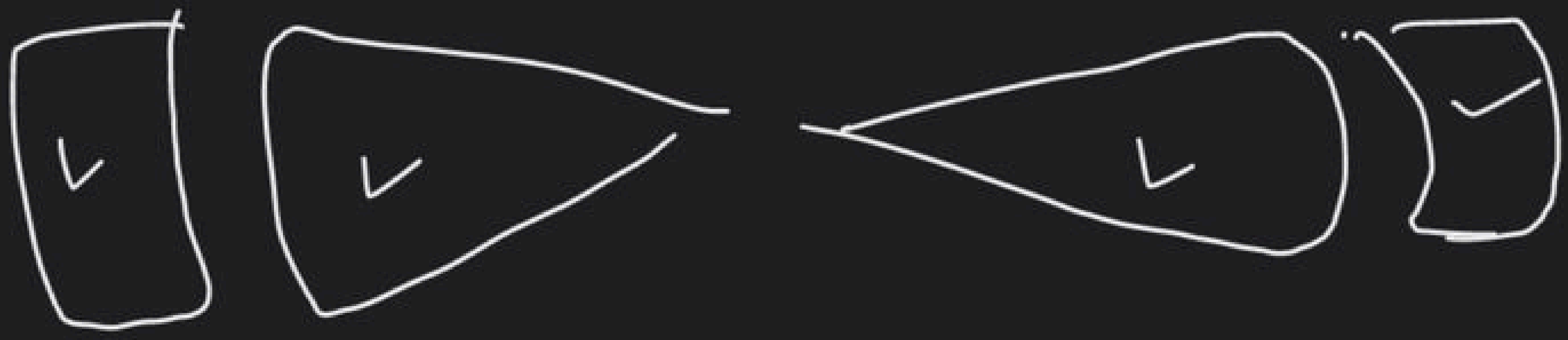


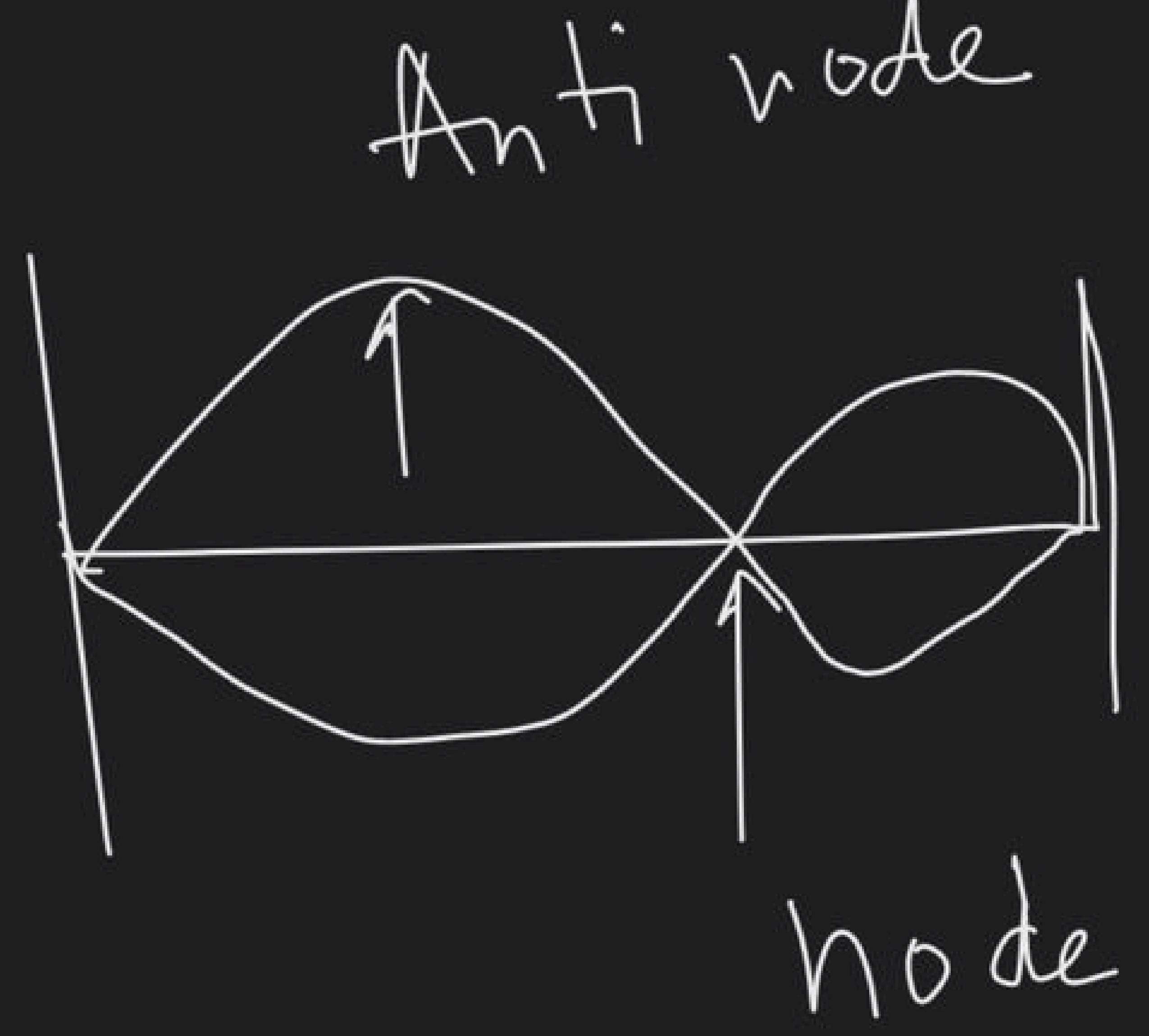
2p, 3d, 4f



3p, 4d, 5f

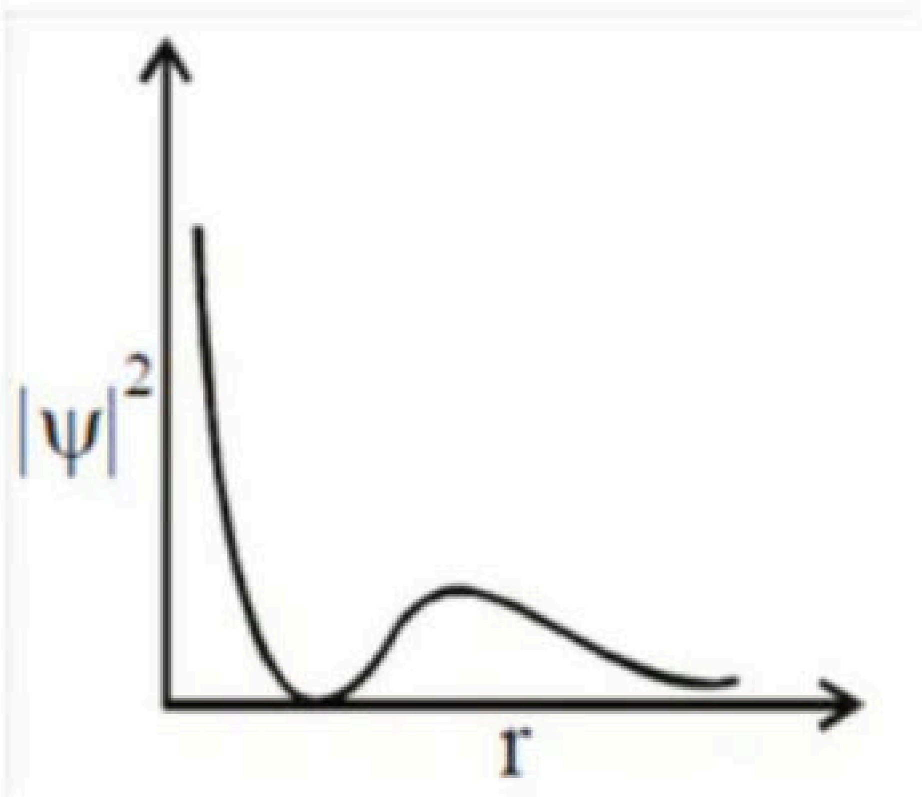





Anti node
node

45. The graph between $|\psi|^2$ and r(radial distance) is shown below. This represents:

[JEE Main (April) 2019]



(1) 1s orbital (2) 3s orbital (3) 2s orbital (4) 2p orbital

2S
3P
3S
3d
None

$$\frac{1}{9\sqrt{3}}\left(\frac{z}{a_0}\right)^{3/2}(6-6\sigma+\sigma^2)e^{-\sigma/2}$$

7. The correct statement about probability density (except at infinite distance from nucleus) is :

[Atomic Structure]

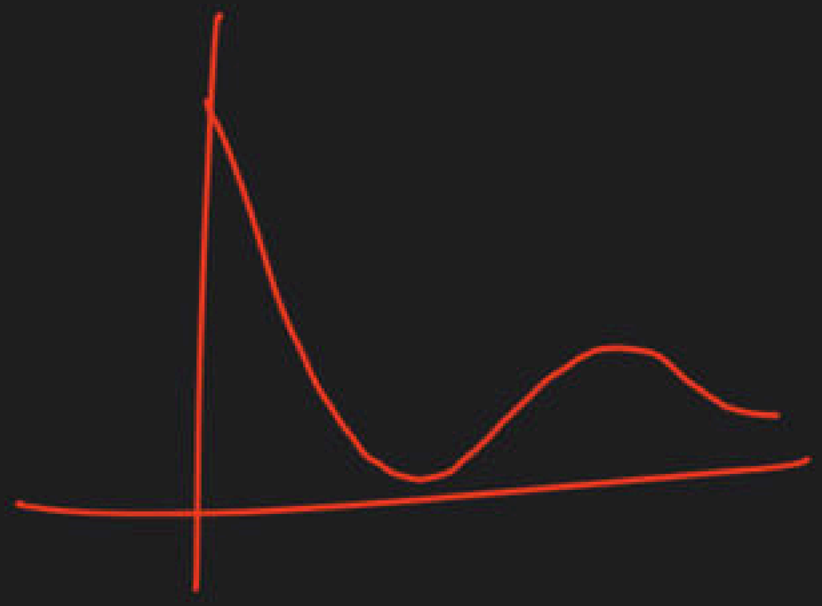
[Jee-Mains (Sep) 2020]

(1) It can negative for 2p orbital

(2) It can be zero for 1s orbital

(3) It can never be zero for 2s orbital

(4) It can be zero for 3p orbital



4f $\quad n, \quad l, \quad m_l \quad m_s$

0 $\qquad -3$

8. A certain orbital has n = 4 and $m_L = -3$. The number of radial nodes in this orbital is________. (Round off to the Nearest Integer)

[JEE Main 17, March 21 (Shift-1)]

1	0	s	
2	1	p	–1
3	2	d	–2
4	3	f	–3

2p 3p 4p

0 1 2

5. (a) The Schrodinger wave equation for hydrogen atom is [IIT-2004]

$$\psi_{2s} = \frac{1}{4(2\pi)^{1/2}}\left(\frac{1}{a_0}\right)^{3/2}\left(2-\frac{r_0}{a_0}\right)e^{-r/a} = 0$$

$\boxed{r_0 = 2a_0}$

3s
2p
3p
3d

Where a_0 is Bohr's radius. Let the radial node in 2s be at r_0. Then find r_0 in terms of a_0.

$$= \frac{1}{9\sqrt{30}} \left(\frac{z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/2}$$

σ^l

$n - l - 1$

$n - 2 - 1 = 0$

$n = 3$

3d

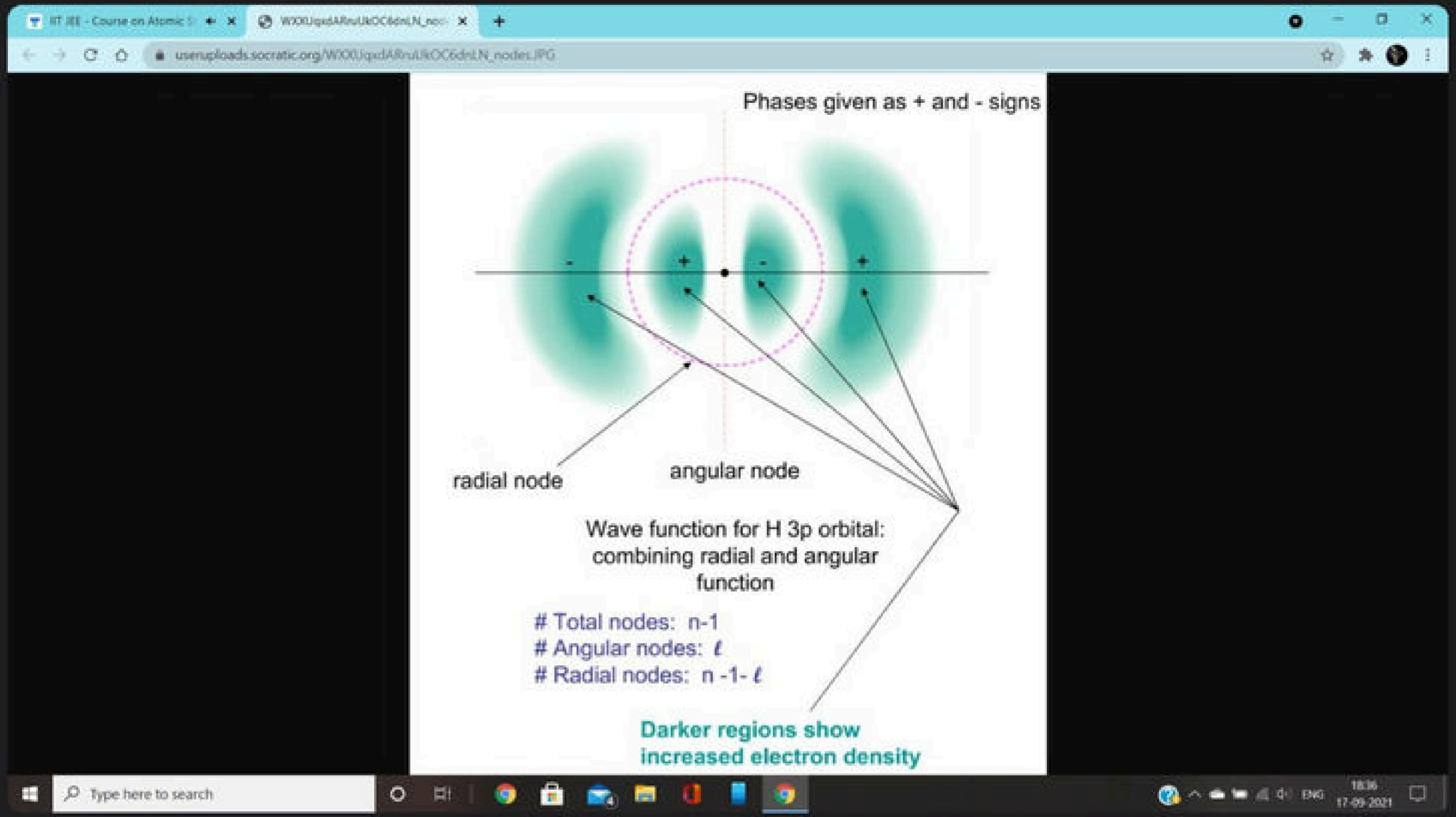
4d

4f

3P

▲ 8 • Asked by Arnavgupta

SIR YE RHA DIAGRAM



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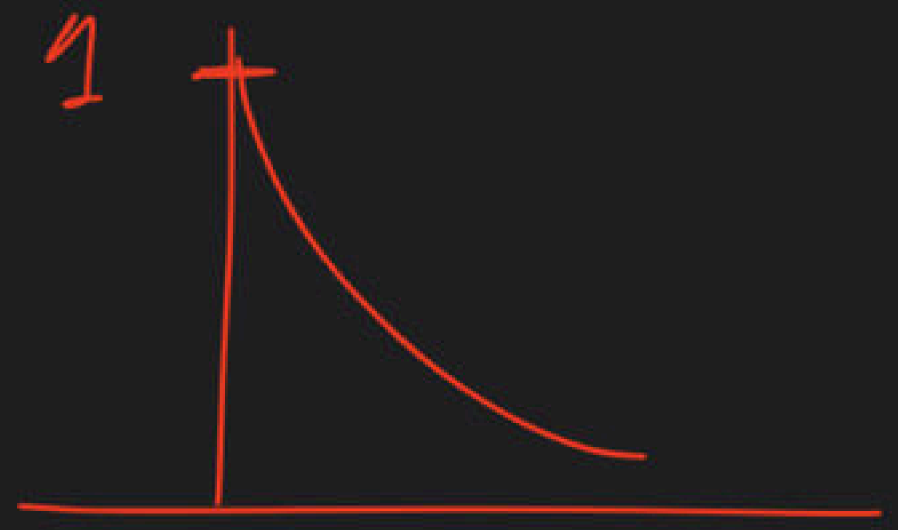
▲ 11 • Asked by Aaditya Ag...

sir agar iske mathematical part ko alag rakh de toh iska theoritical explanation kya hoga spherical node ka ??

SAURABHLUB... • 17:46

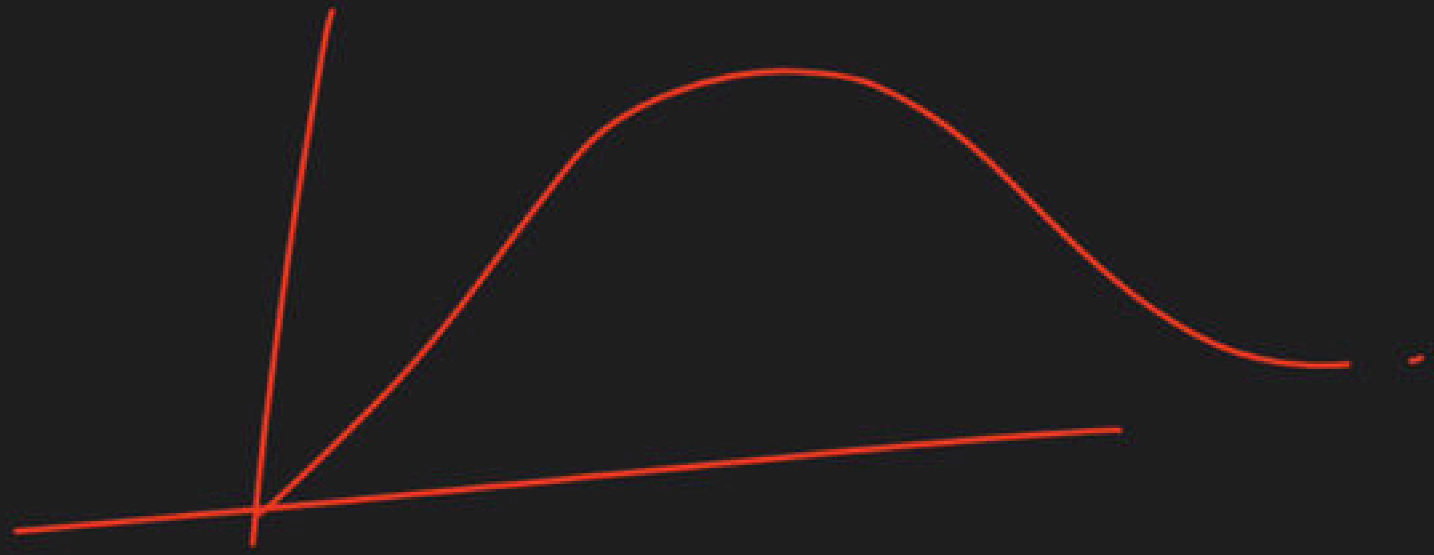
Sir aaj BDay pr gaana gaana chahta hoo m please VC Sir

$y = e^{-x}$



$y = e^{-2x}$

$y = x e^{-x}$



$$x - 1 = 0$$

$$x^2 - x - 2 = 0$$

$$\underline{x^3 - 3} = 0$$

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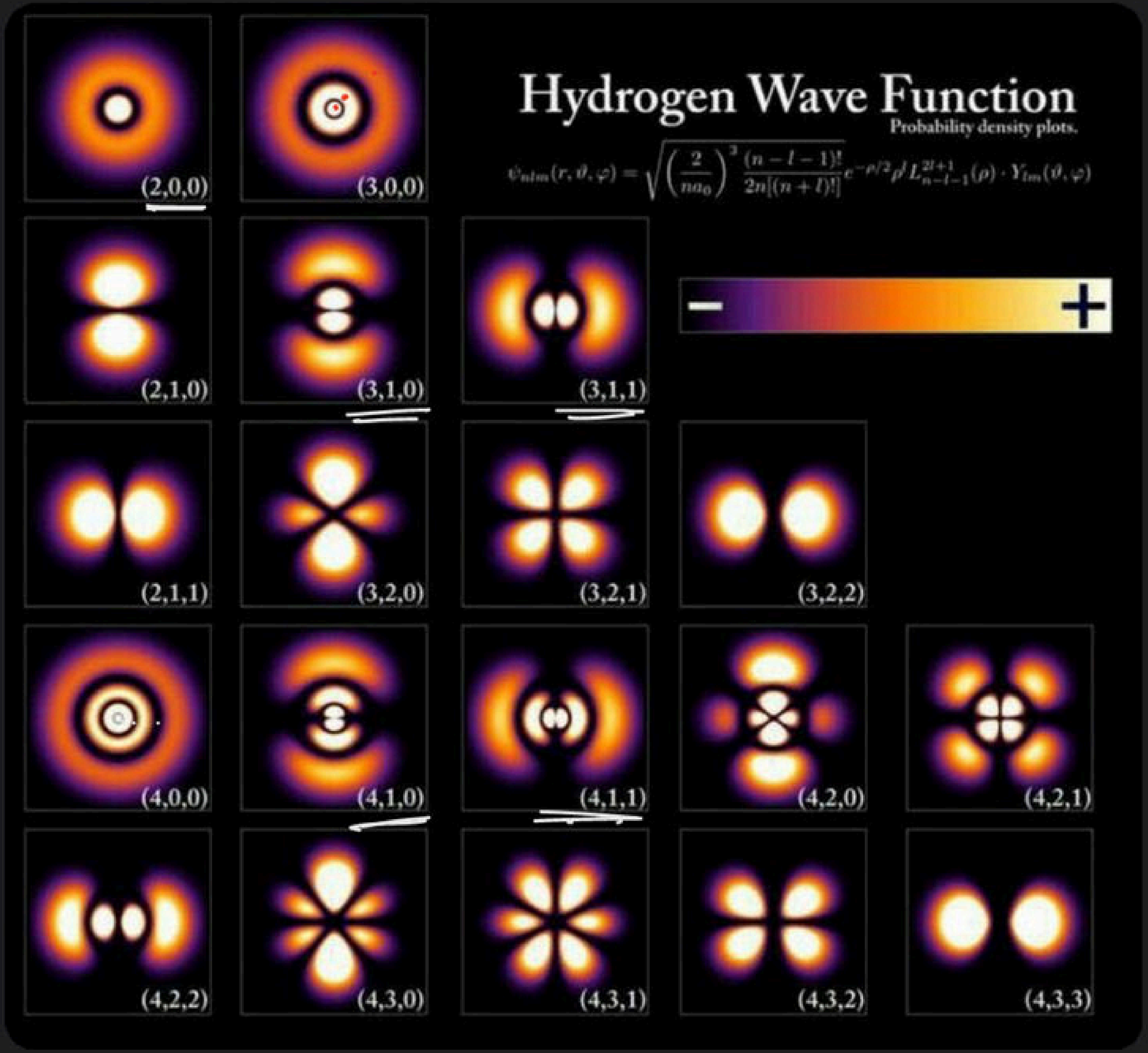
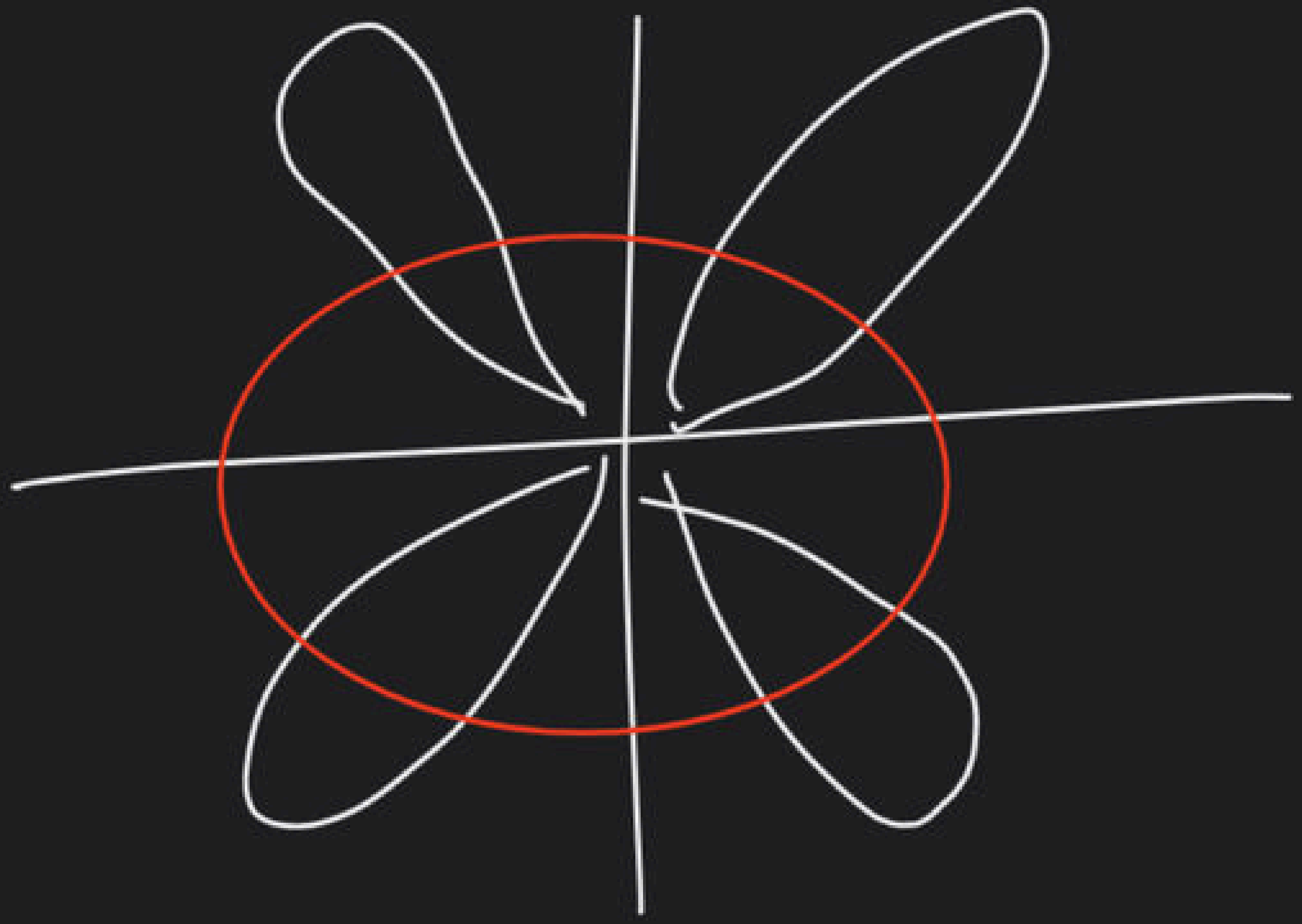
▲ 5 • Asked by Shreya

Please help me with this doubt





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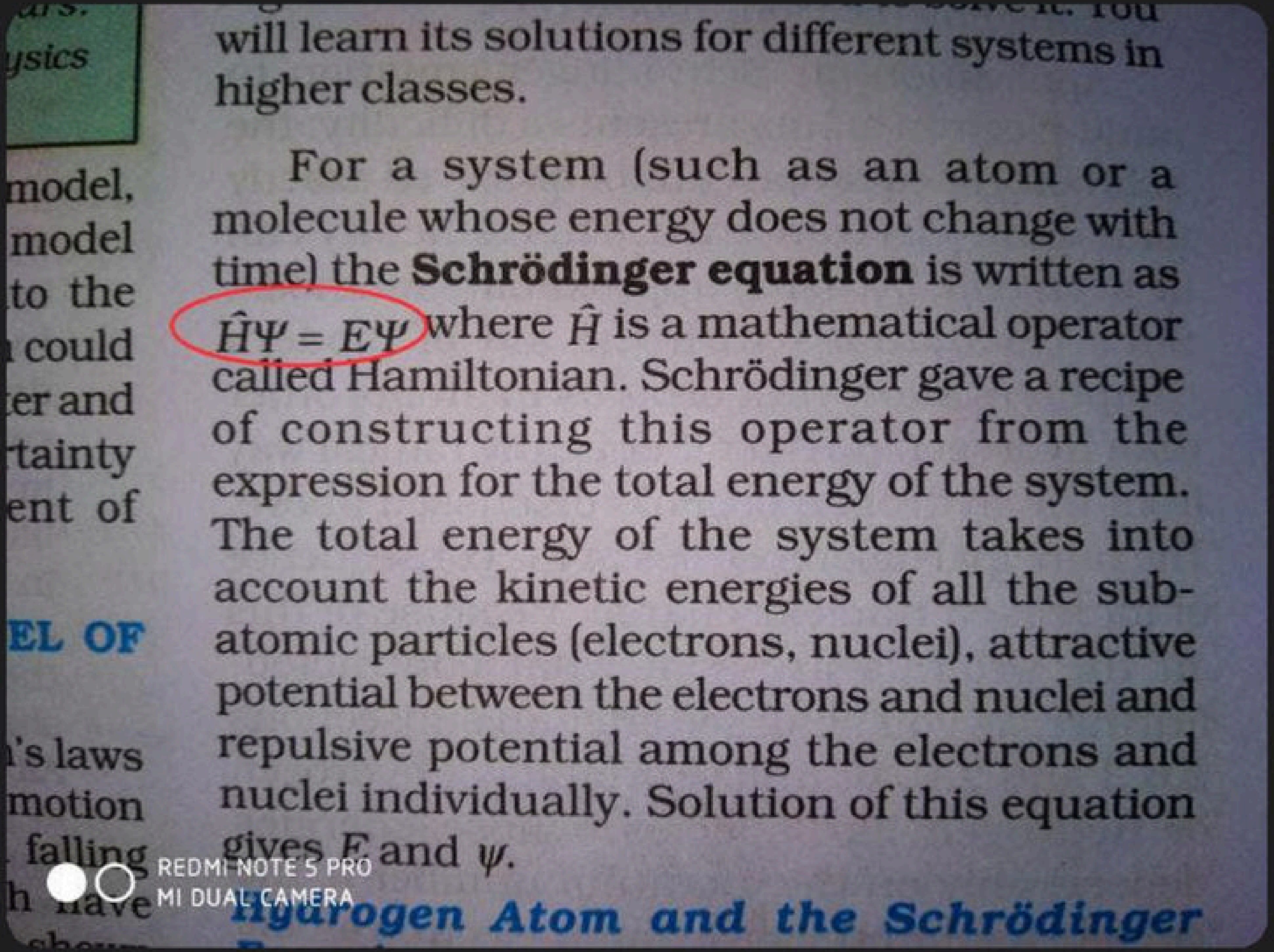
▲ 23 • Asked by Raviraj

Ncert saste mein niptaa Diya,, aapne sahi bola tha

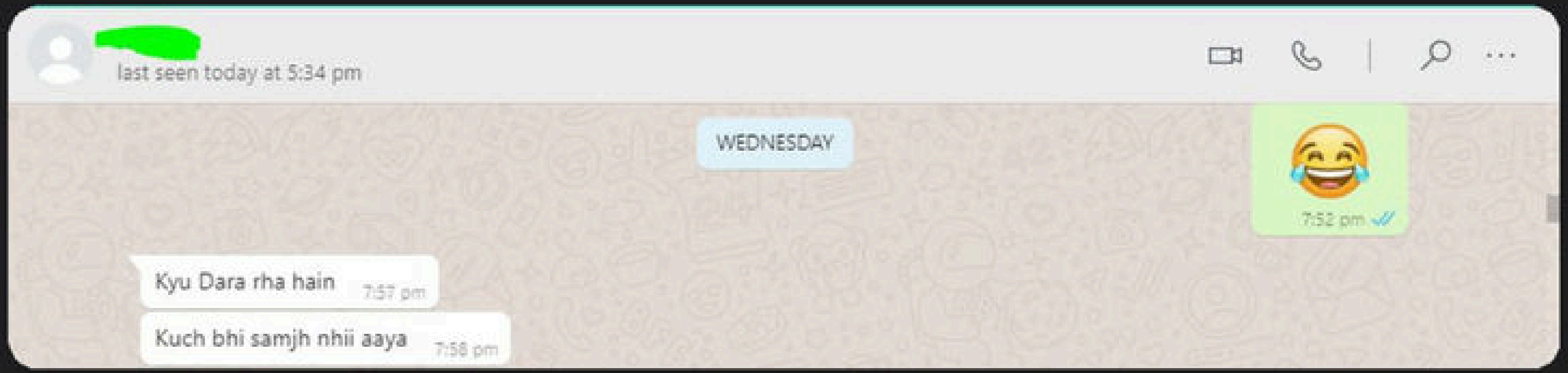

will learn its solutions for different systems in higher classes.

For a system (such as an atom or a molecule whose energy does not change with time) the **Schrödinger equation** is written as $\hat{H}\Psi = E\Psi$ where $\hat{H}$ is a mathematical operator called Hamiltonian. Schrödinger gave a recipe of constructing this operator from the expression for the total energy of the system. The total energy of the system takes into account the kinetic energies of all the sub-atomic particles (electrons, nuclei), attractive potential between the electrons and nuclei and repulsive potential among the electrons and nuclei individually. Solution of this equation gives E and ψ.

Hydrogen Atom and the Schrödinger

▲ 19 • Asked by Aaditya Ag...

Commerce wale friend ka reaction on Schrodinger's equation



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▲ 5 • Asked by Rachit

Sir yeh dekhiye xddd saaf image

$$\hat{U}(t) = \lim_{N\to\infty}\left[1 - \frac{i}{\hbar}\hat{H}\left(\frac{t}{N}\right)\right]^N = e^{-i\hat{H}t/\hbar} \tag{4.9}$$

where we have taken advantage of Problem 2.1. Then

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle \tag{4.10}$$

Thus in order to solve the equation of motion in quantum mechanics when $\hat{H}$ is time independent, all we need is to know the initial state of the system $|\psi(0)\rangle$ *and* to be able to work out the action of the operator (4.9) on this state.

What is the physical significance of the operator $\hat{H}$? Like the generator of rotations, $\hat{H}$ is a Hermitian operator. From (4.4) we see that the dimensions of $\hat{H}$ are those of Planck's constant divided by time—namely, energy. In addition, when $\hat{H}$ itself is time independent, the expectation value of the observable to which the operator $\hat{H}$ corresponds is also independent of time:

$$\langle\psi(t)|\hat{H}|\psi(t)\rangle = \langle\psi(0)|\hat{U}^\dagger(t)\hat{H}\hat{U}(t)|\psi(0)\rangle = \langle\psi(0)|\hat{H}|\psi(0)\rangle \tag{4.11}$$

since $\hat{H}$ commutes with $\hat{U}$.[3] All of these things suggest that we identify $\hat{H}$ as the energy operator, known as the **Hamiltonian**. Therefore

$$\langle E\rangle = \langle\psi|\hat{H}|\psi\rangle \tag{4.12}$$

The eigenstates of the Hamiltonian, which are the energy eigenstates satisfying

$$\hat{H}|E\rangle = E|E\rangle \tag{4.13}$$

play a special role in quantum mechanics. The action of the time-evolution operator $\hat{U}(t)$ on these states is easy to determine using the Taylor series for the exponential:

$$\begin{aligned} e^{-i\hat{H}t/\hbar}|E\rangle &= \left[1 - \frac{i\hat{H}t}{\hbar} + \frac{1}{2!}\left(-\frac{i\hat{H}t}{\hbar}\right)^2 + \cdots\right]|E\rangle \\ &= \left[1 - \frac{iEt}{\hbar} + \frac{1}{2!}\left(-\frac{iEt}{\hbar}\right)^2 + \cdots\right]|E\rangle = e^{-iEt/\hbar}|E\rangle \end{aligned} \tag{4.14}$$

The operator $\hat{H}$ in the exponent can simply be replaced by the energy eigenvalue *when* the time-evolution operator acts on an eigenstate of the Hamiltonian. Thus if the initial state of the system is an energy eigenstate, $|\psi(0)\rangle = |E\rangle$, then

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|E\rangle = e^{-iEt/\hbar}|E\rangle \tag{4.15}$$

[3] To establish that $\hat{H}$ commutes with $\hat{U}$, use the Taylor-series expansion for $\hat{U}$, as in (4.14).

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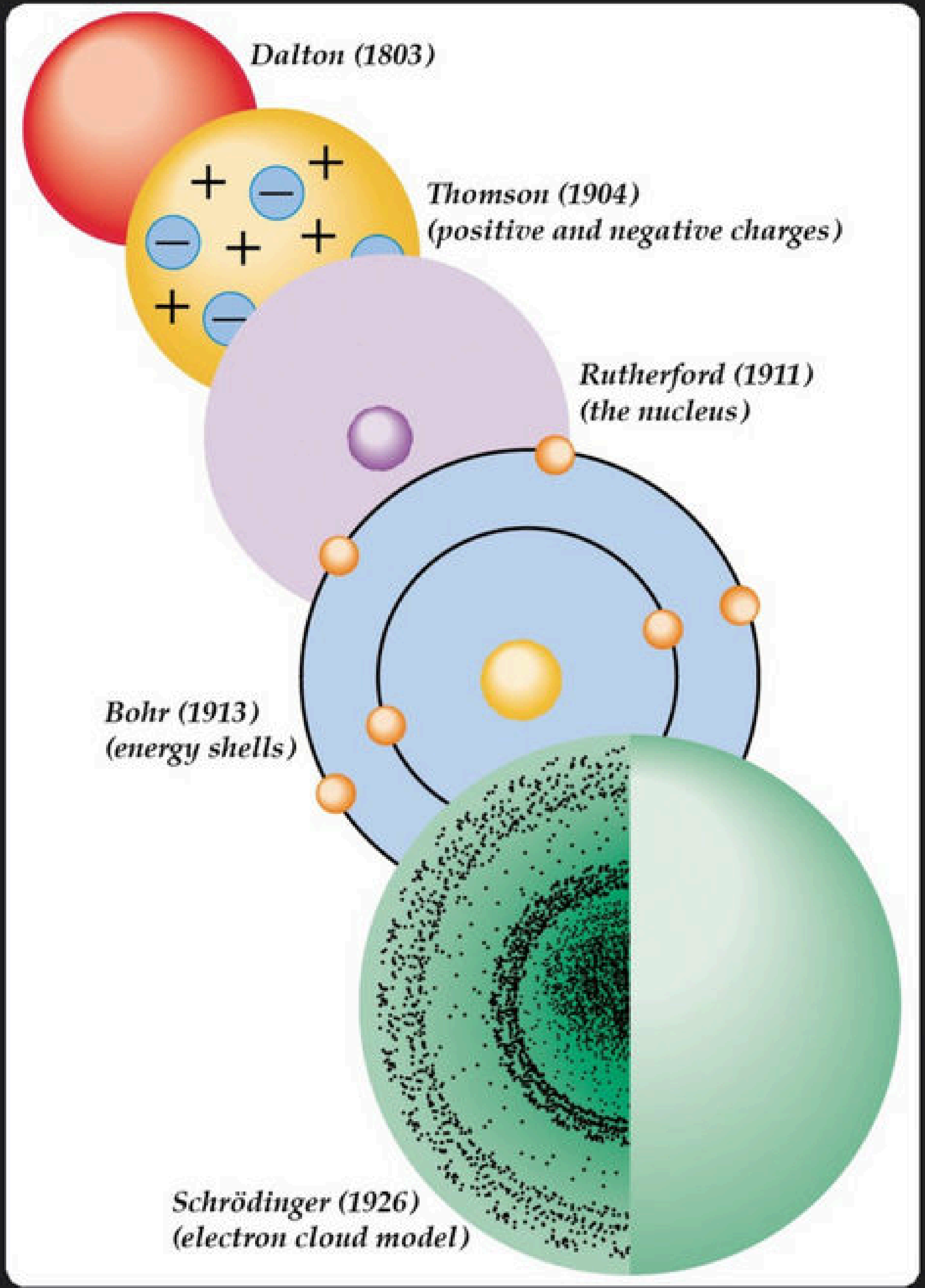
▲ 7 • Asked by Kavya

Models ka evolution



9 • Asked by Dhruv

Pls confirm this sir

functions pertaining to one-electron species are called one-electron systems. The probability of finding an electron at a point within an atom is proportional to the $|\psi|^2$ at that point. The quantum mechanical results

sir yahan pa bhi zie square dv ana chaiya na

$$\psi^2 dV$$

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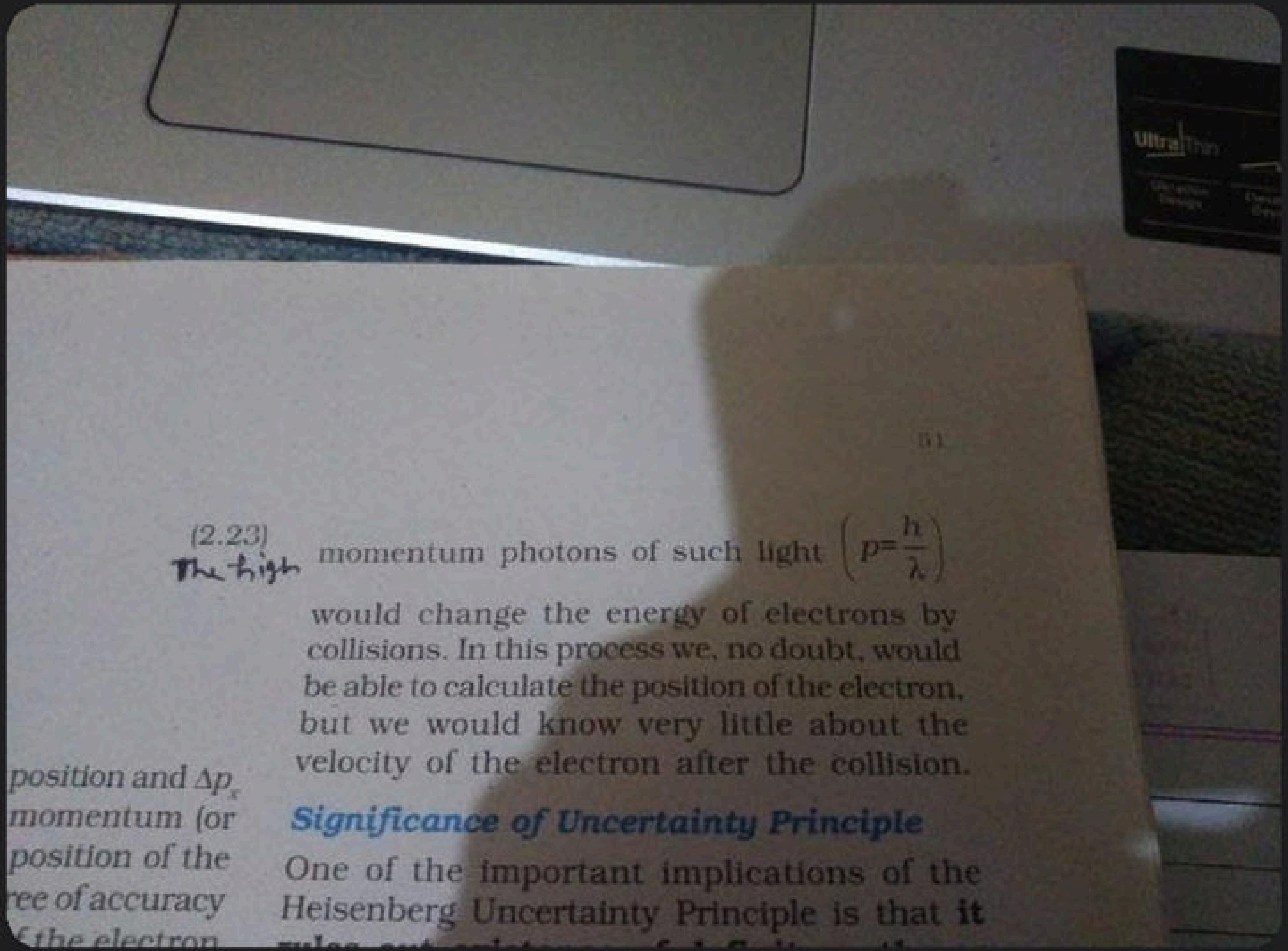
▲ 10 • Asked by Ritik

Sir why it has used this equation for photon but it is applicable for electron only



(2.23)

The high momentum photons of such light $\left(p=\frac{h}{\lambda}\right)$ would change the energy of electrons by collisions. In this process we, no doubt, would be able to calculate the position of the electron, but we would know very little about the velocity of the electron after the collision.

position and Δp_x
momentum (or
position of the
ee of accuracy

Significance of Uncertainty Principle

One of the important implications of the Heisenberg Uncertainty Principle is that **it**

mv

$p = \frac{h}{\lambda}$

$$= \underline{\underline{\psi^2 \, dv}}$$