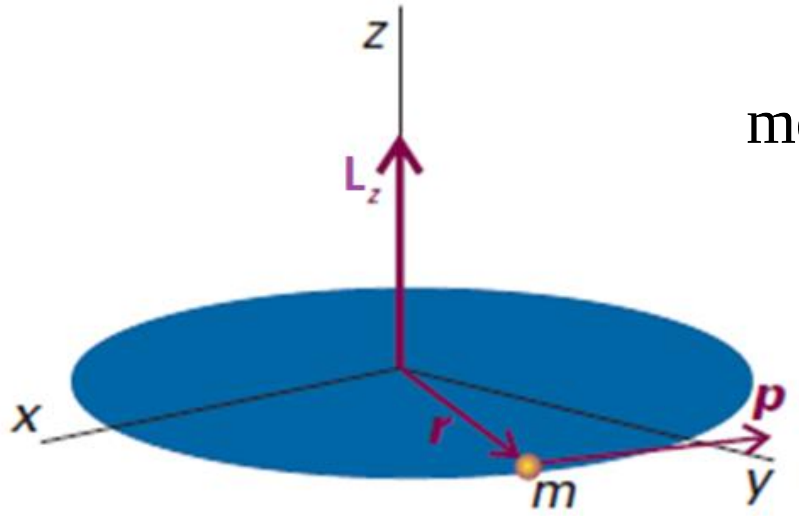
Erwin Schrödinger (1887-1961)

Annalen der Physik **79**, 361 (1926)

" In this communication I wish to show that the usual rules of quantization can be replaced by another postulate (the Schrödinger equation) in which there occurs no mention of whole numbers. Instead, the introduction of integers numbers arises in the same natural way as, for example, in a vibrating string, for which the number of nodes is integral. The new conception can be generalized, and I believe that it penetrates deeply into the true nature of the quantum rules."

Observable		Operator	
Name	Symbol	Symbol	Operation
Position	x	$\hat{X}$	Multiply by x
Momentum	p_x	$\hat{P}_x$	$-i\hbar \dfrac{\partial}{\partial x}$



momento angular

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

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componentes de **L** clássico → operadores

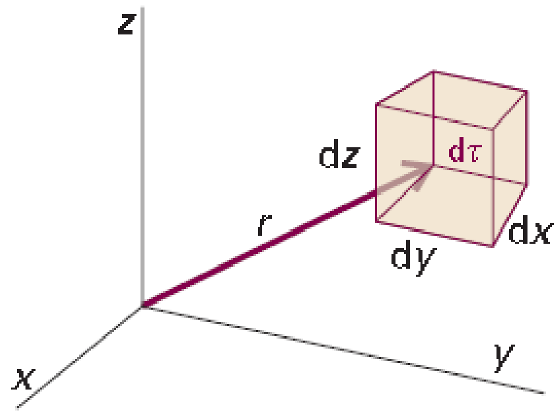
$$L_x = yp_z - zp_y \qquad \hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$L_y = zp_x - xp_z \quad \Rightarrow \quad \hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$L_z = xp_y - yp_x \qquad \hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

Postulados da Mecânica Quântica

O estado do sistema é descrito pela função de onda $\Psi(\mathbf{R},t)$. O produto $\Psi^*(\mathbf{R},t).\Psi(\mathbf{R},t)d\mathbf{R}$ é a probabilidade de encontrar a partícula no intervalo entre $\mathbf{R}$ e $\mathbf{R} + d\mathbf{R}$.



ψ^* complexo conjugado

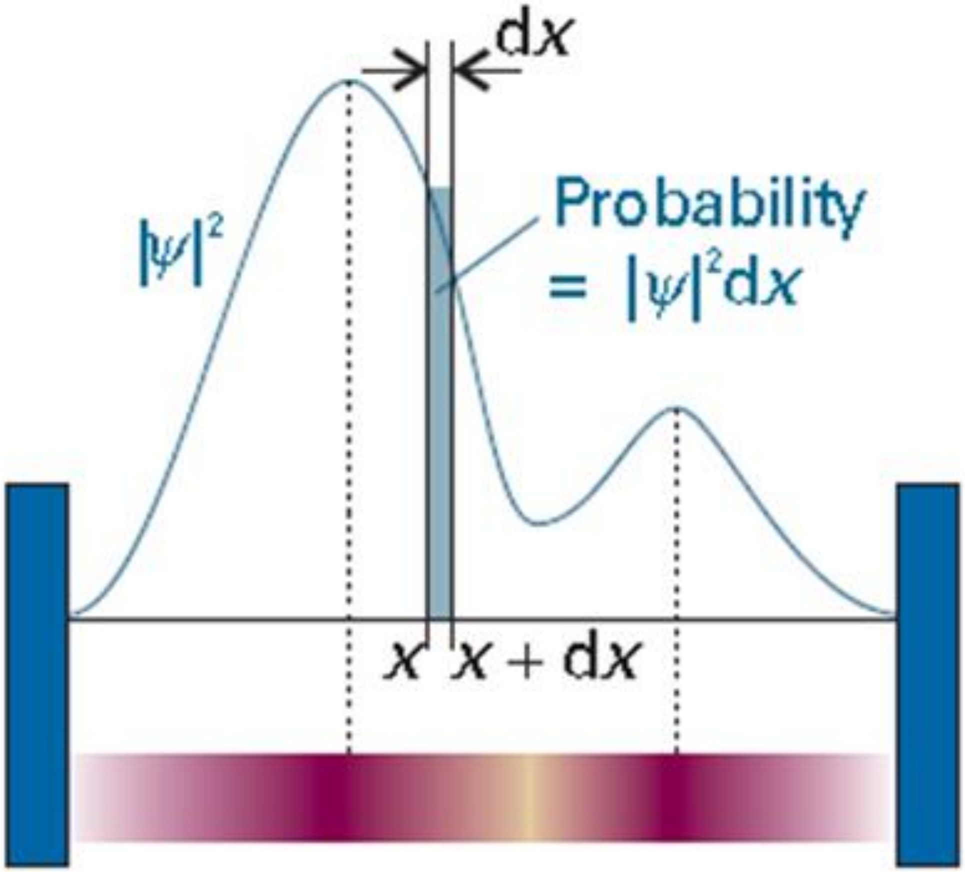


Fig. 8.19 The wavefunction ψ is a probability amplitude in the sense that its square modulus ($\psi^*\psi$ or $|\psi|^2$) is a probability density. The probability of finding a particle in the region dx located at x is proportional to $|\psi|^2 dx$. We represent the probability density by the density of shading in the superimposed band.

$$\int_{\text{all space}} \psi^*(x)\psi(x)dx = 1$$

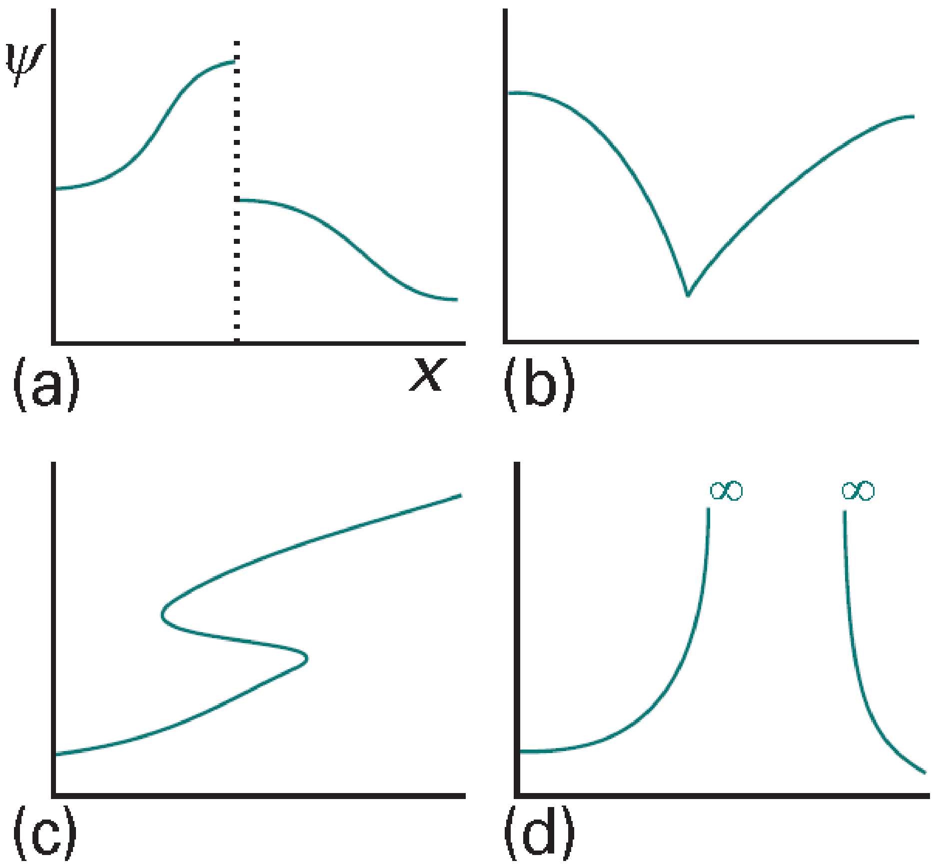
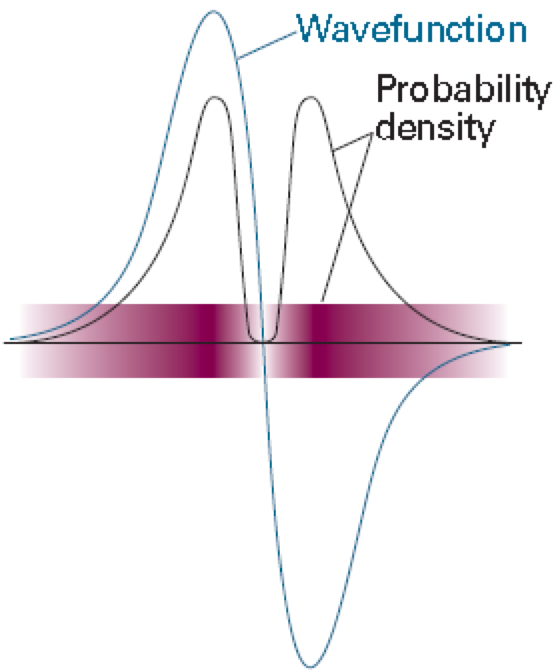
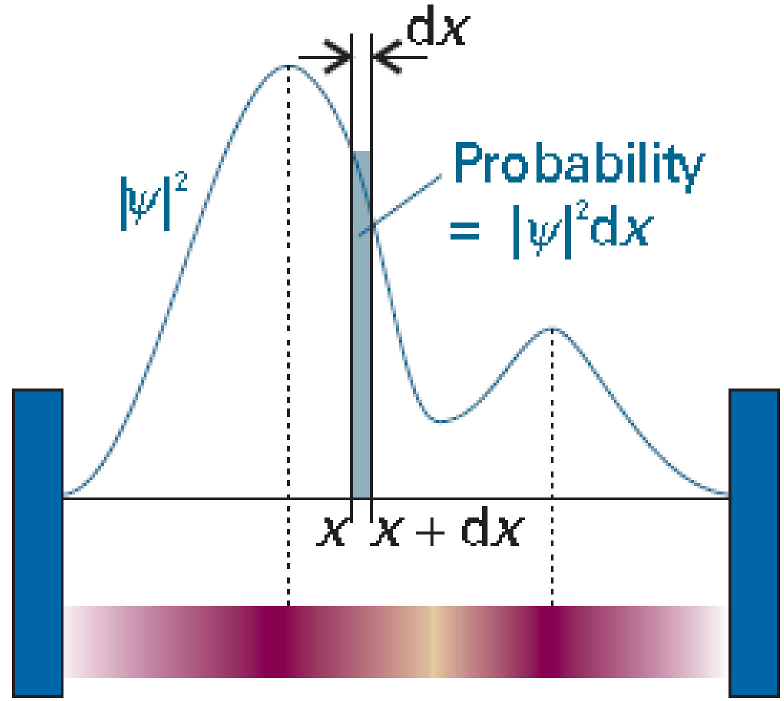


Fig. 8.24 The wavefunction must satisfy stringent conditions for it to be acceptable. (a) Unacceptable because it is not continuous; (b) unacceptable because its slope is discontinuous; (c) unacceptable because it is not single-valued; (d) unacceptable because it is infinite over a finite region.





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Postulados da Mecânica Quântica

A cada observável em Mecânica Clássica, corresponde um operador em Mecânica Quântica.

Observable		Operator	
Name	Symbol	Symbol	Operation
Position	x	$\hat{X}$	Multiply by x
Momentum	p_x	$\hat{P}_x$	$-i\hbar \frac{\partial}{\partial x}$

Observable		Operator	
Name	Symbol	Symbol	Operation
Position	x	$\hat{X}$	Multiply by x
	$\mathbf{r}$	$\hat{\mathbf{R}}$	Multiply by $\mathbf{r}$
Momentum	p_x	$\hat{P}_x$	$-i\hbar\frac{\partial}{\partial x}$
	$\mathbf{p}$	$\hat{\mathbf{P}}$	$-i\hbar\left(\mathbf{i}\frac{\partial}{\partial x}+\mathbf{j}\frac{\partial}{\partial y}+\mathbf{k}\frac{\partial}{\partial z}\right)$
Kinetic energy	K_x	$\hat{K}_x$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
	K	$\hat{K}$	$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$ $=-\frac{\hbar^2}{2m}\nabla^2$
Potential energy	$V(x)$	$\hat{V}(\hat{x})$	Multiply by $V(x)$
	$V(x, y, z)$	$\hat{V}(\hat{x}, \hat{y}, \hat{z})$	Multiply by $V(x, y, z)$
Total energy	E	$\hat{H}$	$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$ $+V(x, y, z)$ $=-\frac{\hbar^2}{2m}\nabla^2+V(x, y, z)$

Postulados da Mecânica Quântica

A função de onda evolui de acordo com a equação de Schrödinger:

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

Se *H* não depende do tempo:

$$\hat{H}\psi(x) = E\psi(x)$$

Postulados da Mecânica Quântica

Valores obtidos em uma medida de um observável associado ao operador $\hat{A}$ são os autovalores que satisfazem a equação de autovalor, $\hat{A}\psi_n = a\psi_n$.

Se um sistema é descrito por uma função de onda normalizada ψ, então o valor médio do observável correspondente a $\hat{A}$ é dado por:

$$\langle a \rangle = \int \psi^* \hat{A} \psi \, d\tau$$