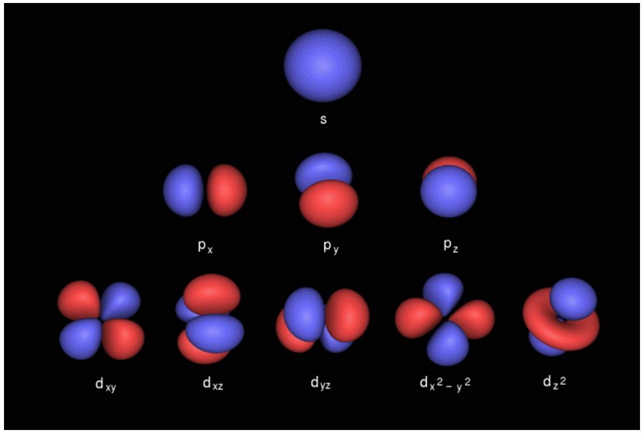
“Revisão de Física Moderna”

- **A equação de Schrödinger:**
  - **Fundamentos.**
  - **Exemplos:**
    - **Partículas livres.**
    - **Poço infinito de potencial.**
    - **Elétrons livres em metais.**
    - **Tunelamento de barreiras.**
    - **Átomo de hidrogênio.**



Alguns problemas e experimentos históricos

Séculos XIX-XX

- Radiação térmica: catástrofe do ultravioleta, modelo de Planck.
- Fótons: efeito fotoelétrico, modelo de Einstein, experimentos de Millikan; efeito Compton.
- Ondas de matéria: hipótese de de Broglie, experimento de Davisson-Germer, difração de elétrons.
- Modelos atômicos: espectros de raias; modelos de Rutherford, Bohr, Sommerfeld; átomo de hidrogênio; equação de Schrödinger.
- Spin do elétron: experimento de Stern-Gerlach, efeito Zeeman, átomos multieletrônicos.
- Calor específico dos sólidos: lei de Dulong-Petit, modelo de Einstein, modelo de Debye.

Analogia com o eletromagnetismo

- **Lei de Coulomb, Lei de Gauss.**
- **Lei de Ampère. Lei de Biot-Savart.**
- **Lei de Faraday. Lei de Lenz.**
- **Experimentos de Hertz.**
- **Experimentos de Young, Fresnel, Fraunhofer.**
- **(...)**

Equações de Maxwell

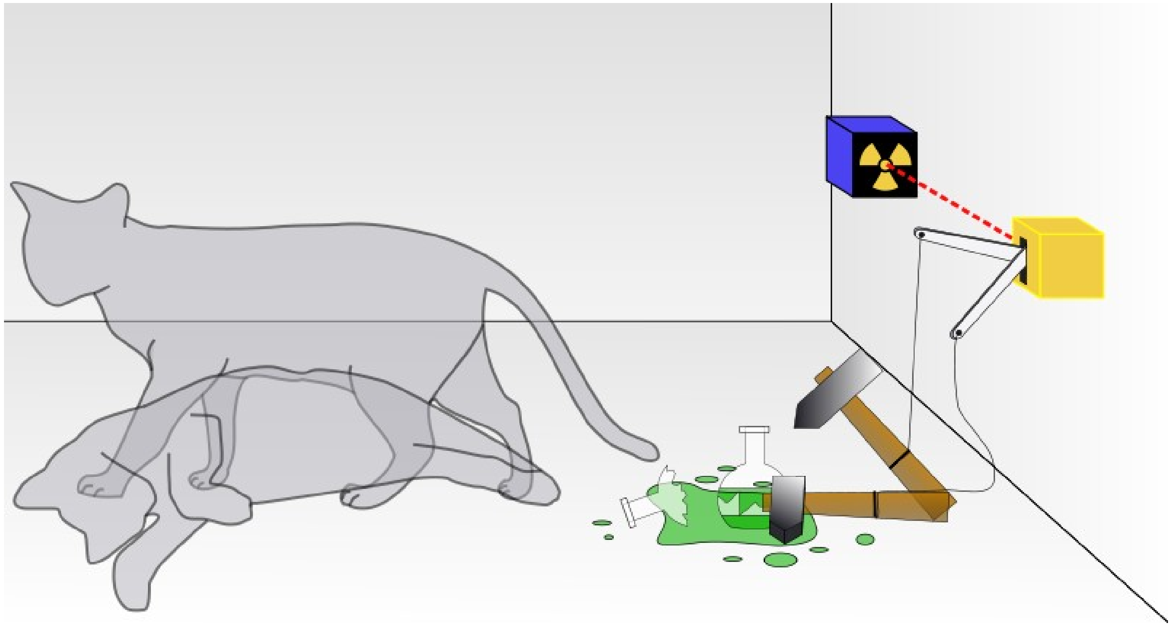
$\Downarrow$

Unificação do Eletromagnetismo / Ótica

$$
\begin{aligned}
\nabla\cdot\vec{D} &= \rho \\
\nabla\times\vec{E} &= -\frac{\partial\vec{B}}{\partial t} \\
\nabla\cdot\vec{B} &= 0 \\
\nabla\times\vec{H} &= \vec{J}+\frac{\partial\vec{D}}{\partial t}
\end{aligned}
$$

A equação de Schrödinger

Schrödinger e o paradoxo do gato:



Erwin Schrödinger (1887-1961)
Nobel de Física 1933

http://en.wikipedia.org/wiki/Schr%C3%B6dinger's_cat

A equação de Schrödinger

Função de onda: $\Psi(\vec{r},t)$ $\Rightarrow$ *Estado do sistema*

Energia potencial: $V(\vec{r},t)$

Erwin Schrödinger (1887-1961)
Nobel de Física 1933

Equação em 1 dimensão:

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

$\hbar = h/2\pi$

$m \rightarrow$ massa da partícula

Equação em 3 dimensões:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(r,t)\Psi(r,t)=i\hbar\frac{\partial\Psi(r,t)}{\partial t}$$

Analogia com o eletromagnetismo

Função de onda: $\vec{E}(\vec{r},t)\ ;\ \vec{B}(\vec{r},t)$

Equação de uma onda eletromagnética no vácuo: $$\nabla^2\vec{E}(\vec{r},t)-\frac{1}{c^2}\frac{\partial^2\vec{E}}{\partial t^2}=0$$

Soluções de ondas planas monocromáticas:

$$\vec{E}(\vec{r},t)=\vec{E}_0 e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

$$\vec{B}(\vec{r},t)=\vec{B}_0 e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

Intensidade média da onda: $I \propto \left|\vec{E}_0\right|^2$

A equação de Schrödinger

Interpretação probabilística da função de onda (1D):

$$P(x,t) = \Psi^*(x,t)\Psi(x,t) = \left|\Psi(x,t)\right|^2$$

$$dP = P(x,t)dx$$

Probabilidade de localizar a partícula entre ***x*** e ***x* + *dx*** no instante ***t***.

Condição de normalização:

$$\int_{-\infty}^{\infty} P(x,t)dx = \int_{-\infty}^{\infty} \left|\Psi(x,t)\right|^2 dx = 1$$

A equação de Schrödinger

Interpretação probabilística da função de onda (1D):

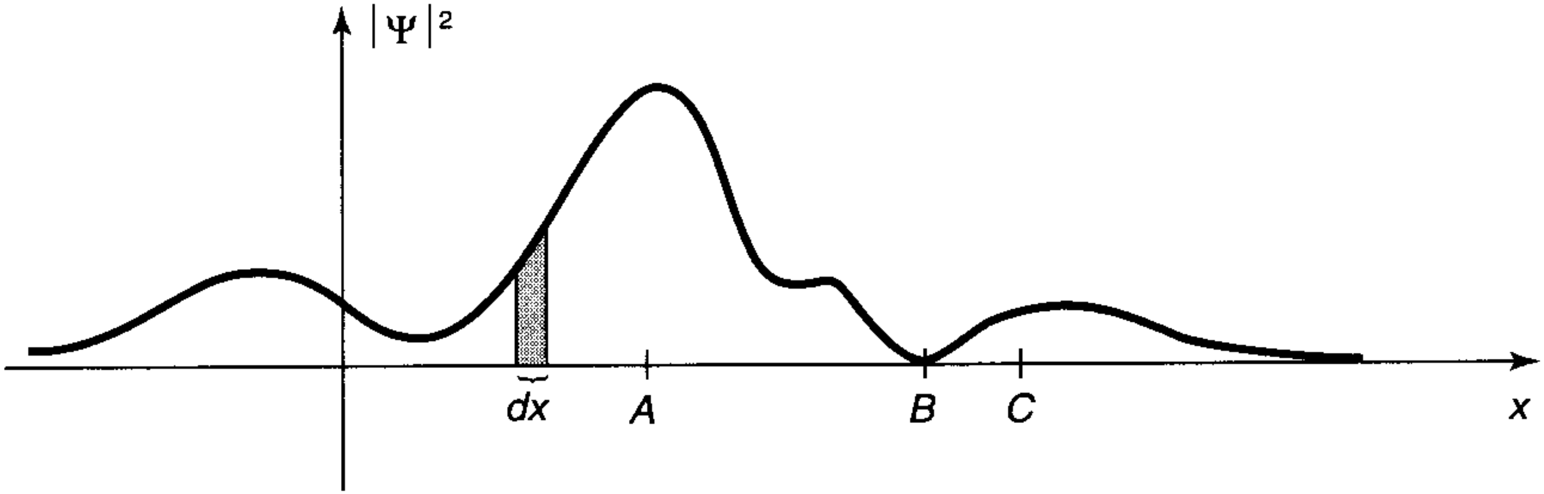


Figure 1.2: A typical wave function. The particle would be relatively likely to be found near A, and unlikely to be found near B. The shaded area represents the probability of finding the particle in the range dx.

Introduction to Quantum Mechanics, Griffiths, 1995.

A equação de Schrödinger independente do tempo

Energia potencial independente do tempo: $V(\vec{r},t) = V(\vec{r})$

Separação de variáveis: $\Psi(\vec{r},t) = \psi(\vec{r})\phi(t)$

$$E = \hbar\omega$$

$$\phi(t) = e^{-iEt/\hbar} = e^{-i\omega t}$$

$E \rightarrow$ energia total da partícula

Estados estacionários com energia *E*:

$$\left|\Psi(x,t)\right|^2 = \left|\psi(x)\phi(t)\right|^2 = \left|\psi(x)\right|^2$$

$P(x,t) = P(x) \rightarrow$ independente do tempo

A equação de Schrödinger independente do tempo

Estados estacionários com energia *E*: $\Psi(\vec{r},t) = \psi(\vec{r})e^{-iEt/\hbar}$

Equação em 1 dimensão:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$$

Equação em 3 dimensões:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

A equação de Schrödinger independente do tempo

Operadores associados a grandezas físicas – Observáveis:

Grandeza Clássica	Operador Quântico
x	x
$\vec{r}$	$\vec{r}$
p_x	$-i\hbar\partial/\partial x$
$\vec{p}$	$-i\hbar\nabla$
E	$i\hbar\partial/\partial t$
T	$-(\hbar^2/2m)\nabla^2$
$\vec{L}$	$-i\hbar\vec{r}\times\nabla$

$$Q_{op}\,\Psi(\vec{r},t) = Q\,\Psi(\vec{r},t)$$

Operador

Resultado (autovalor)

Valor esperado: $$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi^* Q_{op} \Psi \, dx$$

Operador associado à energia total – Hamiltoniano:

$$H = \frac{p^2}{2m} + V(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$$

$$H\,\psi(\vec{r}) = E\psi(\vec{r})$$

Materiais e Dispositivos Eletrônicos, Sérgio M. Rezende, 2004.

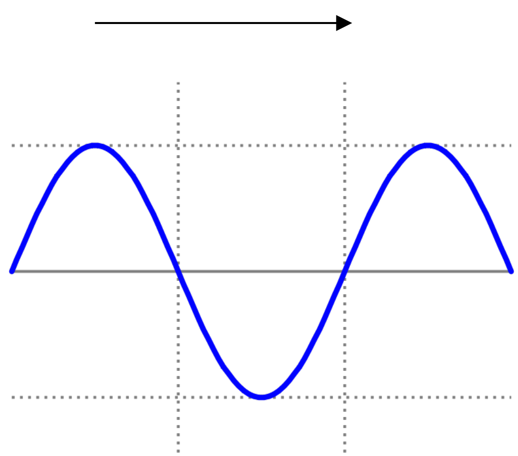
Partículas livres

Ausência de forças / potenciais: $$V(\vec{r},t) = 0$$

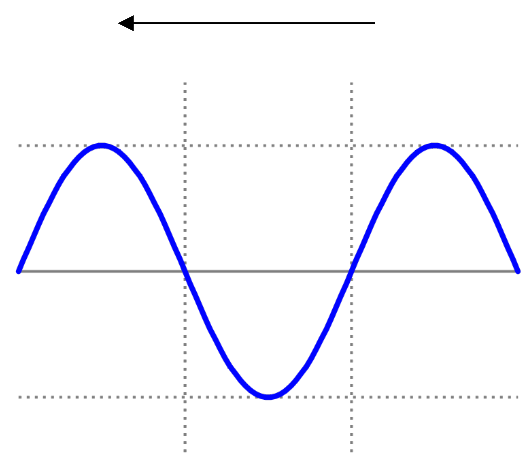
Soluções de onda plana: $$\Psi(\vec{r},t) = Ae^{i\vec{k}\cdot\vec{r}}e^{-iEt/\hbar} = Ae^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

Momento linear: $$\vec{p} = \hbar\vec{k} \qquad \lambda = \frac{2\pi}{k} = \frac{h}{p}$$

A: constante de normalização – depende do volume da região ocupada pela partícula



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

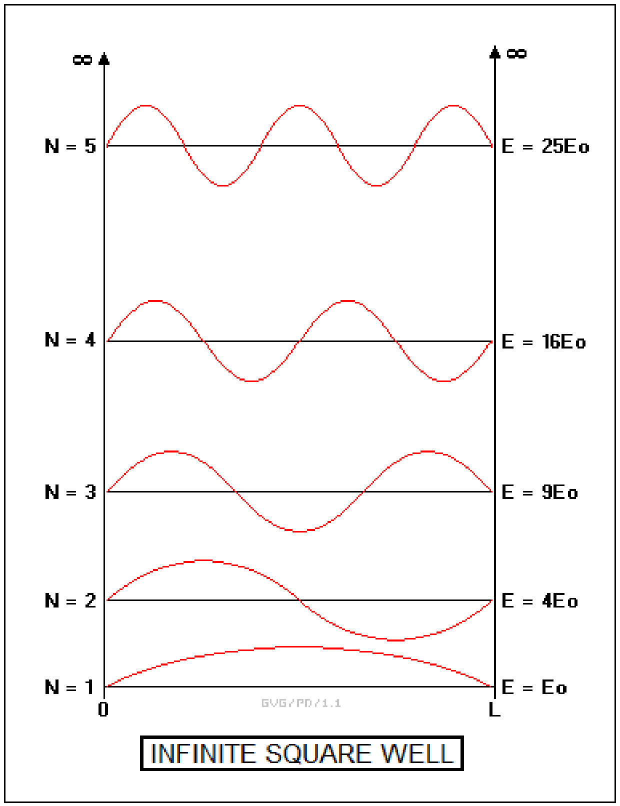


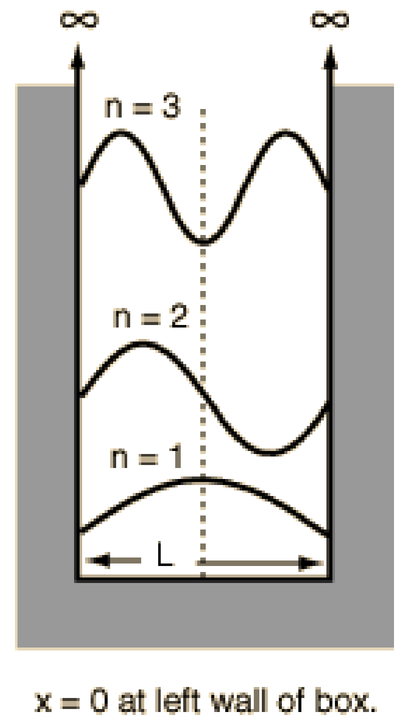
$$\Psi^{-}(x,t) = Ae^{-i(kx+\omega t)}$$

Poço infinito de potencial

Partícula em uma “caixa”:

$$\psi_n(x) = \sqrt{\frac{2}{L}} sen\, \frac{n\pi}{L} x \qquad E_n = \frac{h^2\pi^2}{2mL^2} n^2$$



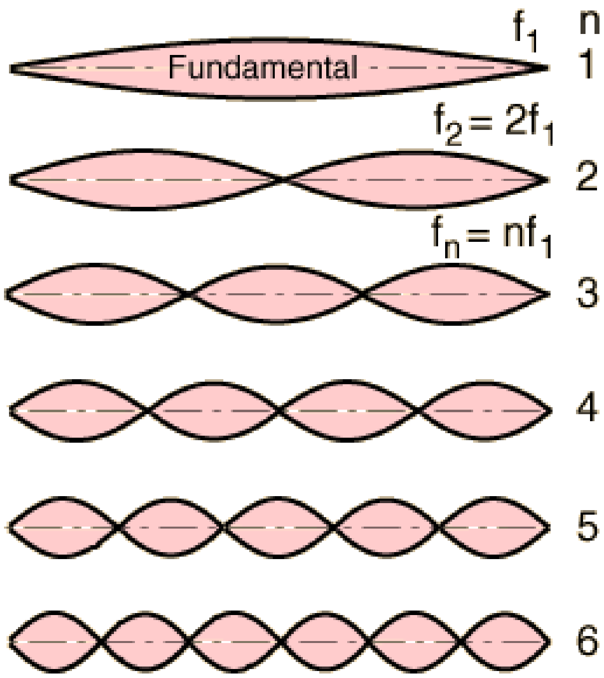


http://www.vectorsite.net/tpqm_02.html

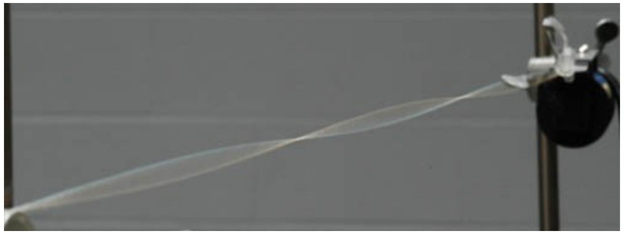
http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/pbox.html

Poço infinito de potencial

Analogia com ondas estacionárias em uma corda – modos normais e harmônicos:



$$f_1 = \frac{v}{2L}$$

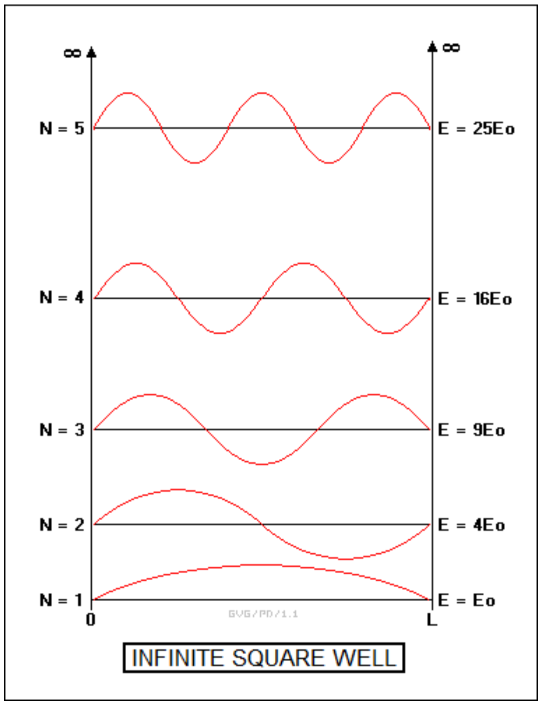


http://hyperphysics.phy-astr.gsu.edu/hbase/waves/string.html

Poço infinito de potencial

Partícula em uma “caixa”:

$$\psi_n(x) = \sqrt{\frac{2}{L}}\, sen\, \frac{n\pi}{L} x \qquad E_n = \frac{h^2\pi^2}{2mL^2} n^2$$



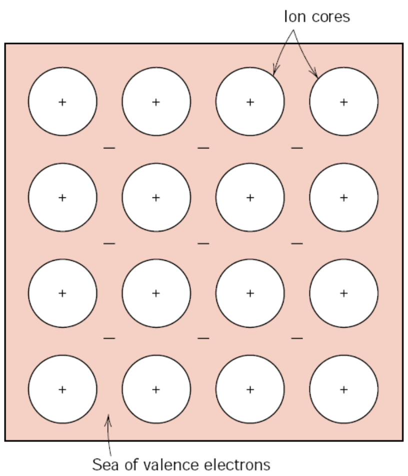
http://www.vectorsite.net/tpqm_02.html

Resultados:

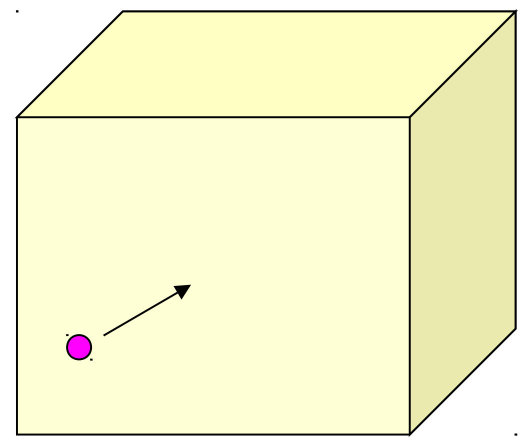
- Função de onda confinada a uma região do espaço.
- Quantização da energia da partícula (n = número quântico).
- Estado de menor energia: estado fundamental.
- Mínima energia não nula: energia de ponto zero.

Poço infinito de potencial

Aplicação do modelo de partícula em uma "caixa" - elétrons livres em metais:



Fundamentals of Materials Science and Engineering , Callister.



$$\psi_{n_x n_y n_z}(\vec{r}) = \sqrt{\frac{8}{V}}\,\mathrm{sen}\left(\frac{n_x \pi}{L_x}x\right)\mathrm{sen}\left(\frac{n_y \pi}{L_y}y\right)\mathrm{sen}\left(\frac{n_z \pi}{L_z}z\right)$$

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_x^{\,2}}{L_x^{\,2}} + \frac{n_y^{\,2}}{L_y^{\,2}} + \frac{n_z^{\,2}}{L_z^{\,2}}\right)$$

Potencial degrau

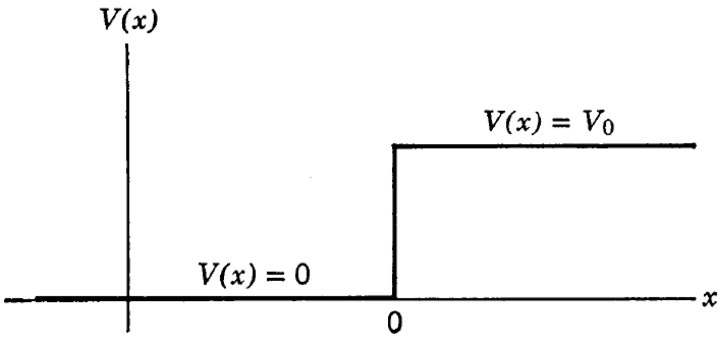


Figure 6-3 A step potential.

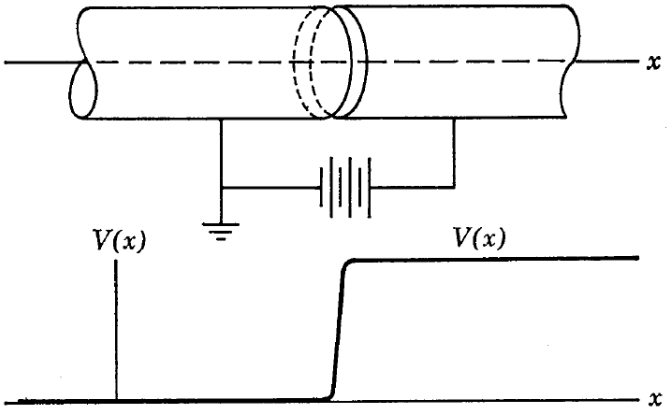
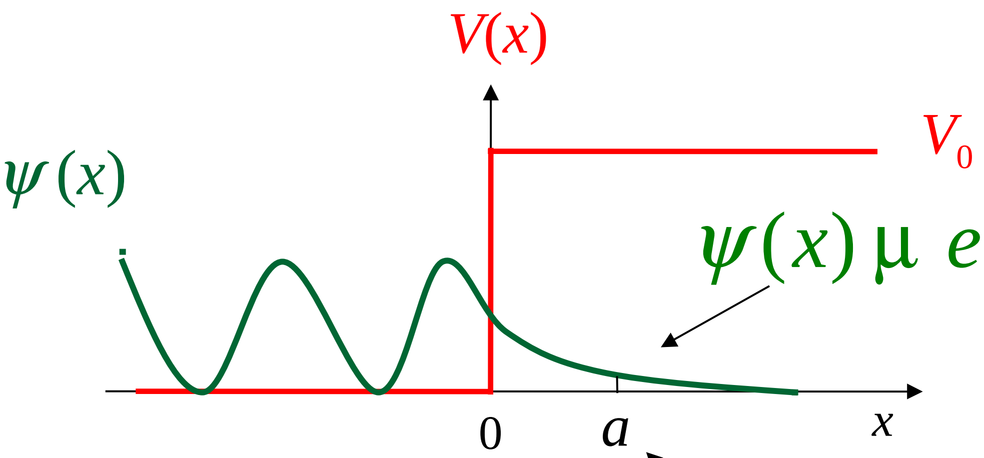


Figure 6-4 Illustrating a physical system with a potential energy function that can be approximated by a step potential. A charged particle moves along the axis of two cylindrical electrodes held at different voltages. Its potential energy is constant when it is inside either electrode, but it changes very rapidly when passing from one to the other.

Quantum Physics, Eisberg & Resnick.

Potencial degrau

Transmissão na “região classicamente proibida”:



$$\psi(x) \propto e^{-\gamma x}$$

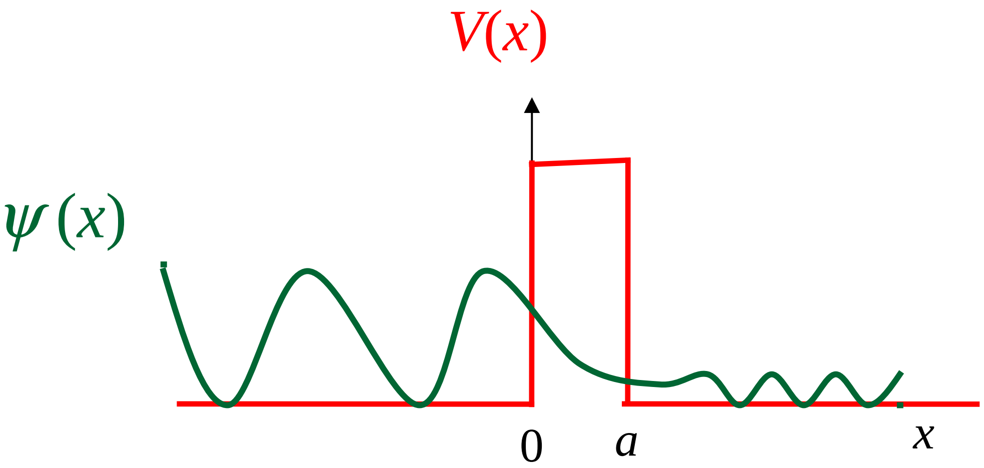
$$\gamma = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

$$|\psi(a)|^2 \propto e^{-2\gamma a}$$

http://nanotech.ica.ele.puc-rio.br/pos_notas/2010-1/Aula%202.ppt

Barreira de potencial - tunelamento

Transmissão na “região classicamente proibida”:

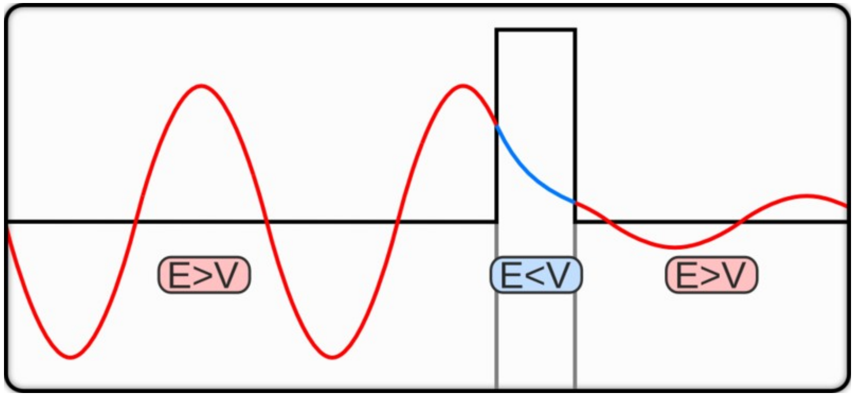


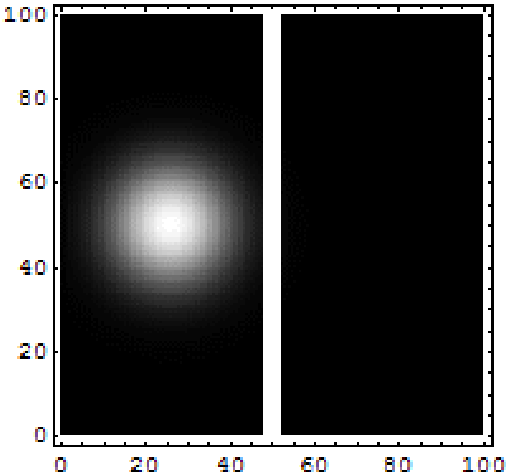
$$\text{Probabilidade de tranmissão} \simeq |\psi(a)|^2 \; \mu \; e^{-2\gamma a}$$

http://nanotech.ica.ele.puc-rio.br/pos_notas/2010-1/Aula%202.ppt

Barreira de potencial - tunelamento

Efeito túnel:

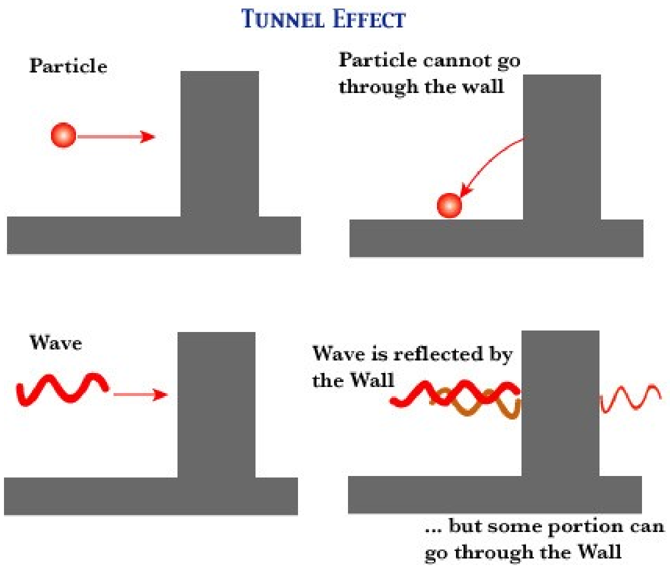


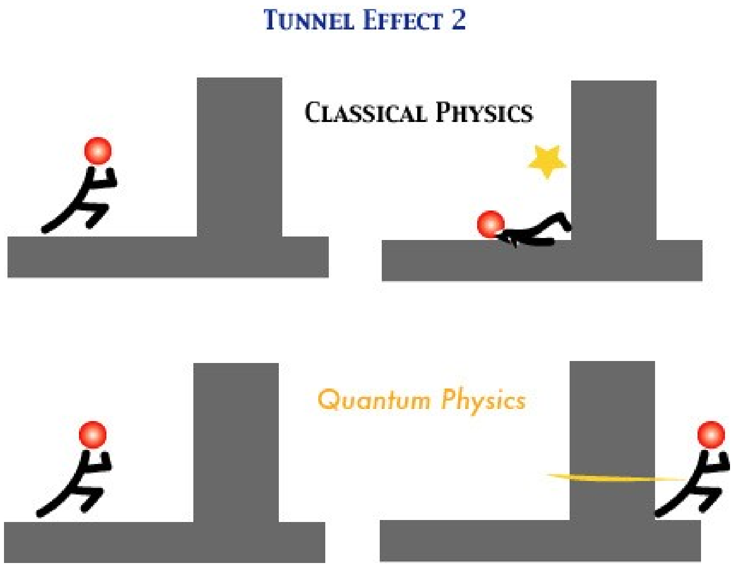


http://en.wikipedia.org/wiki/Quantum_tunneling

Barreira de potencial - tunelamento

Efeito túnel:

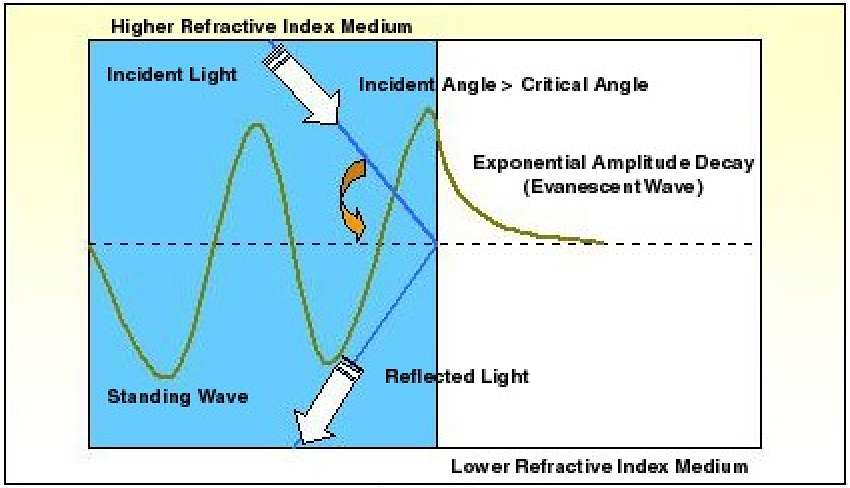




http://www.bun.kyoto-u.ac.jp/~suchii/Bohr/tunnel.html

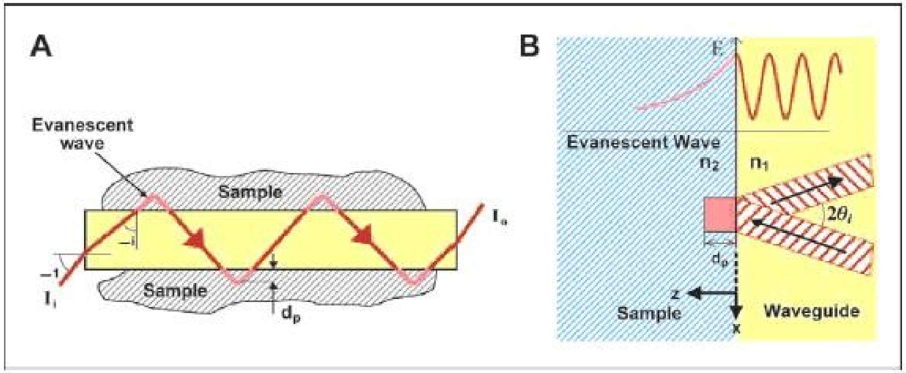
Barreira de potencial - tunelamento

Penetração na barreira - ondas evanescentes:



Evanescent Wave Generation

http://www.photonics.cusat.edu/Research_Fiber%20Sensors_EW.html

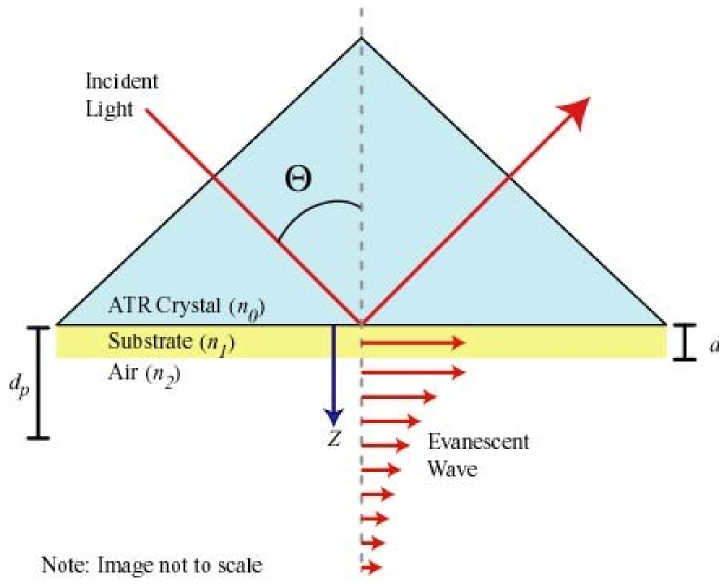


(A) *Evanescent wave in a waveguide, in contact with a sample.* (B) *Evanescent wave at the interface between two media, under total internal reflection.*

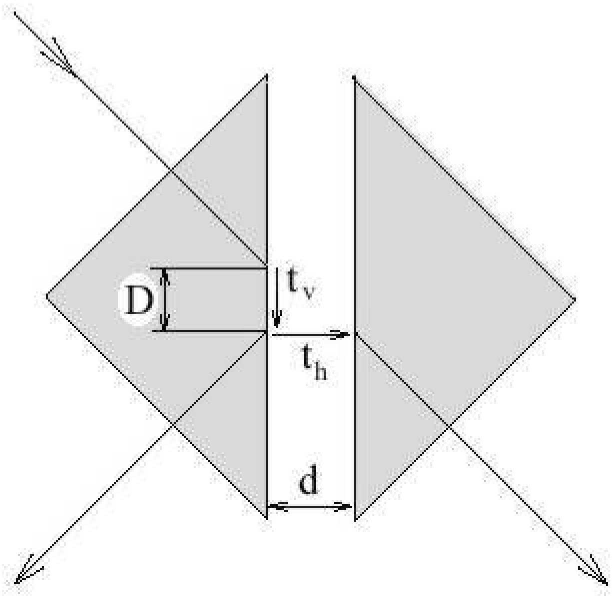
http://www.tau.ac.il/~applphys/research_fews.htm

Barreira de potencial - tunelamento

Efeito túnel em ótica – reflexão interna total frustrada:



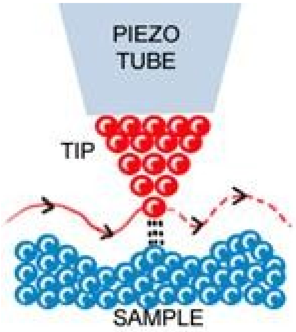
http://www.nano.psu.edu/~aad/current_projects.htm

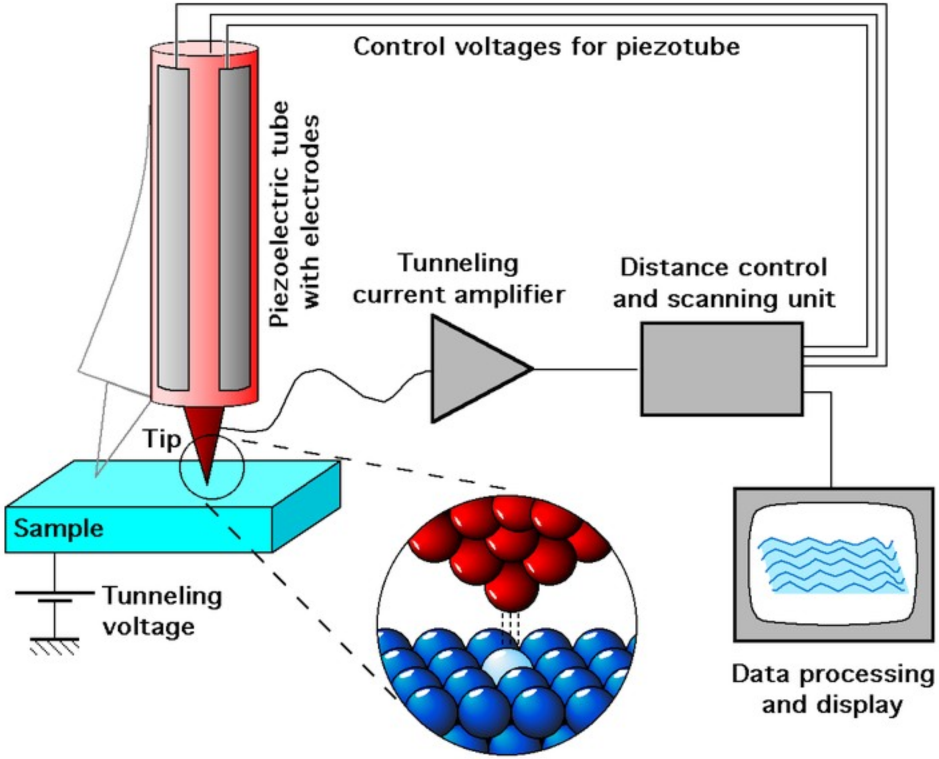


http://www.popularscience.co.uk/features/feat11.htm

Aplicações do efeito túnel

Exemplos: decaimento alfa, emissão eletrônica, junção túnel, diodo Josephson, microscópio de tunelamento (STM – “scanning tunneling microscope”), ...



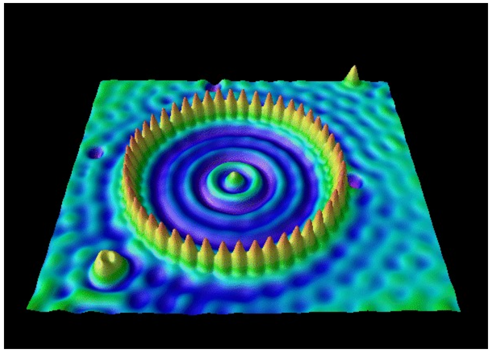


http://en.wikipedia.org/wiki/Scanning_tunnelling_microscope

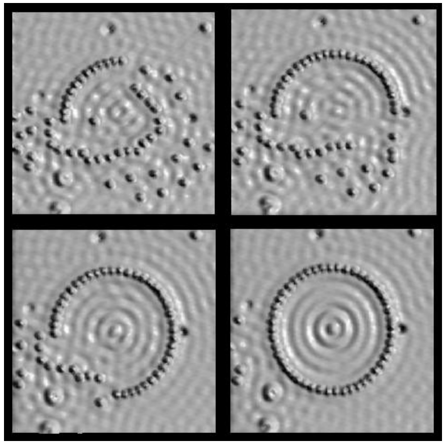
Microscopia eletrônica de tunelamento

Algumas imagens de STM - nanomateriais:

Superfície de Cu/Fe:

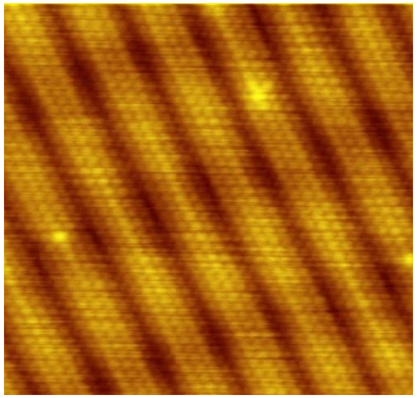


Superfície de Cu/Fe:

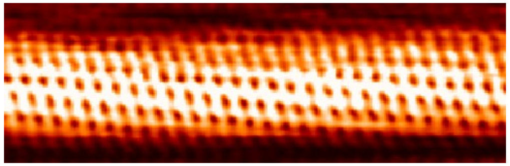


http://www.almaden.ibm.com/vis/stm/

Superfície de ouro:



Nanotubo de carbono:



http://en.wikipedia.org/wiki/Scanning_tunnelling_microscope

Átomo de hidrogênio

Equação de Schrödinger em 3D:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})+V(\vec{r})\psi(\vec{r})=E\psi(\vec{r})$$

$$\psi(\vec{r})=R(r)Y(\theta,\phi)$$

$$V(\vec{r})=V(r)$$

Separação de variáveis:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}[V(r)-E]=l(l+1)$$

$$\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\}=-l(l+1)$$

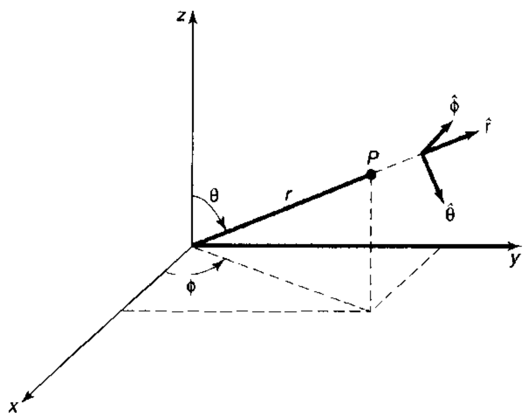


Figure 4.1: Spherical coordinates: radius r, polar angle θ, and azimuthal angle ϕ.

Introduction to Quantum Mechanics, Griffiths, 1995.

Átomo de hidrogênio

Equação de Schrödinger em 3D:

$$V(\vec{r}) = V(r) = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

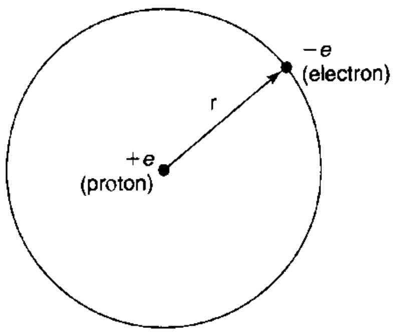


Figure 4.3: The hydrogen atom.

Introduction to Quantum Mechanics, Griffiths, 1995.

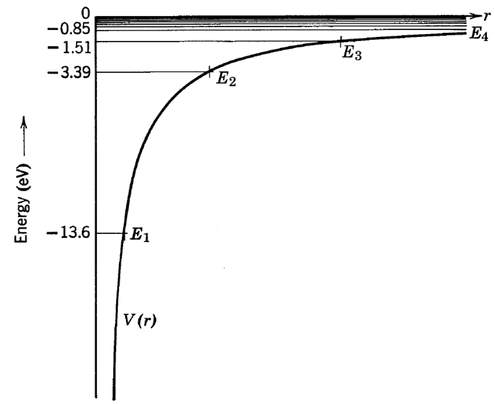


Figure 7-3 The Coulomb potential $V(r)$ and its eigenvalues E_n. For large values of n the eigenvalues become very closely spaced in energy since E_n approaches zero as n approaches infinity. Note that the intersection of $V(r)$ and E_n, which defines the location of one end of the classically allowed region, moves out as n increases. Not shown in this figure is the continuum of eigenvalues at positive energies corresponding to unbound states.

Quantum Physics, Eisberg & Resnick.

Átomo de hidrogênio

Harmônicos esféricos:

$$\psi(\vec{r}) = R(r)Y_l^m(\theta,\phi)$$

Table 4.2: The first few spherical harmonics, $Y_l^m(\theta,\phi)$.

$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$	$Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm 2i\phi}$
$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$	$Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta)$
$Y_1^{\pm 1} = \mp\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\phi}$	$Y_3^{\pm 1} = \mp\left(\frac{21}{64\pi}\right)^{1/2} \sin\theta(5\cos^2\theta - 1)e^{\pm i\phi}$
$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$	$Y_3^{\pm 2} = \left(\frac{105}{32\pi}\right)^{1/2} \sin^2\theta\cos\theta e^{\pm 2i\phi}$
$Y_2^{\pm 1} = \mp\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta e^{\pm i\phi}$	$Y_3^{\pm 3} = \mp\left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta e^{\pm 3i\phi}$

Introduction to Quantum Mechanics, Griffiths, 1995.

Átomo de hidrogênio

Harmônicos esféricos:

$$\psi(\vec{r}) = R(r)Y_l^m(\theta,\phi)$$

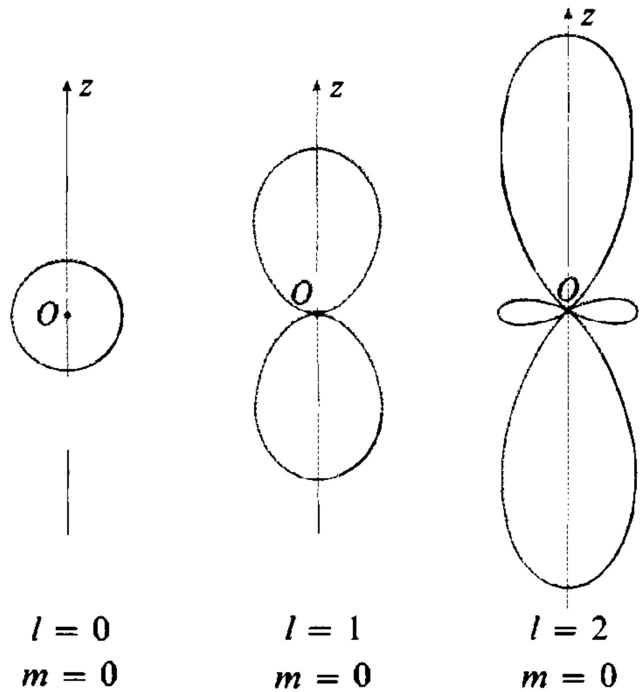


FIGURE 5

Angular dependence, $Y_l^m(\theta, \varphi)$, of some stationary wave functions of the hydrogen atom, corresponding to well-defined values of l and m. For each direction of polar angles θ, φ, the value of $|Y_l^m(\theta, \varphi)|^2$ is recorded; a surface of revolution about the Oz axis is thus obtained. When $l = 0$, this surface is a sphere centered at O; it becomes more complicated for higher values of l.

Quantum Mechanics, Cohen-Tannoudji et al., 1977.

Átomo de hidrogênio

Soluções da Equação de Schrödinger:

$$\psi(\vec{r}) = R(r)Y_l^m(\theta,\phi)$$

$$\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}}\, e^{-r/na}\left(\frac{2r}{na}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right) Y_l^m(\theta,\phi)$$

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}[V(r)-E] = l(l+1)$$

Condição de normalização:

$$\int \psi_{nlm}^* \, \psi_{n'l'm'}\, r^2 \sin\theta \, dr\, d\theta\, d\phi = \delta_{nn'}\delta_{ll'}\delta_{mm'}$$

Números quânticos:

$n \longrightarrow$ número quântico principal

$l \longrightarrow$ número quântico azimutal

$m \longrightarrow$ número quântico magnético

Table 4.4: The first few Laguerre polynomials, $L_q(x)$.

$L_0 = 1$
$L_1 = -x + 1$
$L_2 = x^2 - 4x + 2$
$L_3 = -x^3 + 9x^2 - 18x + 6$
$L_4 = x^4 - 16x^3 + 72x^2 - 96x + 24$
$L_5 = -x^5 + 25x^4 - 200x^3 + 600x^2 - 600x + 120$
$L_6 = x^6 - 36x^5 + 450x^4 - 2400x^3 + 5400x^2 - 4320x + 720$

Introduction to Quantum Mechanics, Griffiths, 1995.

Átomo de hidrogênio

Níveis de energia:

$$\psi(\vec{r}) = R(r)Y_l^m(\theta,\phi)$$

$$E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n^2}, \quad n = 1, 2, 3, \ldots.$$

Estado fundamental (*n* = 1):

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}$$

Raio de Bohr:

$$a \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}\text{ m}$$

$$E_1 = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right] = -13.6\text{ eV}$$

$\Rightarrow$ *Energia de ionização* = 13,6 eV

Introduction to Quantum Mechanics, Griffiths, 1995.

Átomo de hidrogênio

Números quânticos e observáveis:

$n \rightarrow$ número quântico principal	n = 1, 2, 3, 4, ...	Níveis: K, L, M, N, ...
$l \rightarrow$ número quântico azimutal	l = 0, 1, 2, ..., $n-1$	Orbitais: s, p, d, f
$m \rightarrow$ número quântico magnético	$m = -l, -l+1, ..., l-1, l$	$2l+1$ estados
$m_s \rightarrow$ número quântico de spin	$m_s = -1/2, 1/2$	2 estados

Energia:

$$E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2}$$

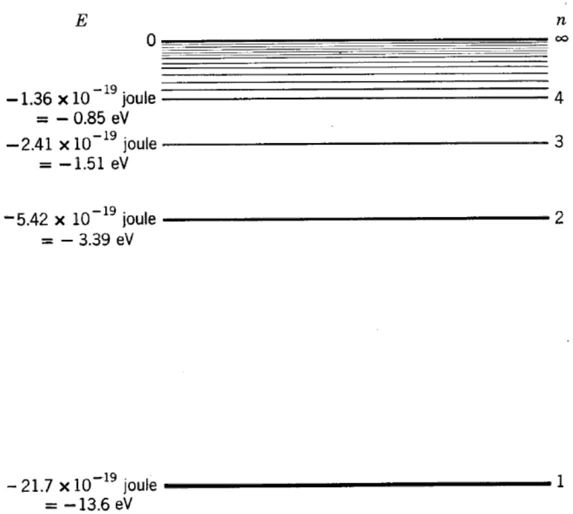


Figure 4-11 An energy-level diagram for the hydrogen atom.

Quantum Physics, Eisberg & Resnick.

Átomo de hidrogênio

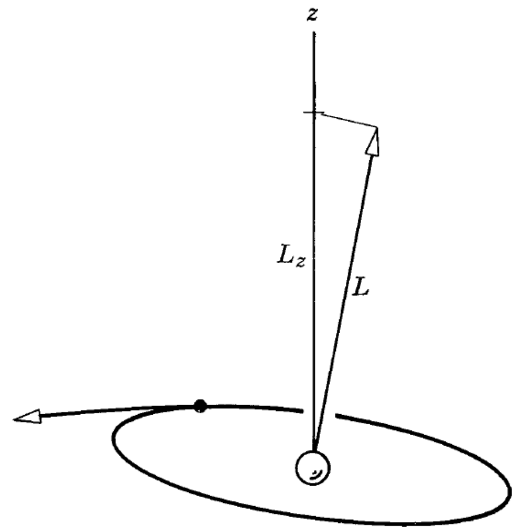
Números quânticos e observáveis:

$n \rightarrow$ número quântico principal	$n = 1, 2, 3, 4, \ldots$	Níveis: K, L, M, N, ...
$l \rightarrow$ número quântico azimutal	$l = 0, 1, 2, \ldots, n-1$	Orbitais: s, p, d, f
$m \rightarrow$ número quântico magnético	$m = -l, -l+1, \ldots, l-1, l$	$2l+1$ estados
$m_s \rightarrow$ número quântico de spin	$m_s = -1/2, 1/2$	2 estados

Momento angular orbital:

$$L^2 = l(l+1)\hbar^2$$

$$L_z = m\hbar$$



Quantum Physics, Eisberg & Resnick.

Átomo de hidrogênio

Números quânticos e observáveis:

$n \rightarrow$ número quântico principal	n = 1, 2, 3, 4, ...	Níveis: K, L, M, N, ...
$l \rightarrow$ número quântico azimutal	l = 0, 1, 2, ..., $n-1$	Orbitais: s, p, d, f
$m \rightarrow$ número quântico magnético	$m = -l, -l+1, ..., l-1, l$	$2l+1$ estados
$m_s \rightarrow$ número quântico de spin	$m_s = -1/2, 1/2$	2 estados

Momento angular de spin:

$$S^2 = s(s+1)\hbar^2 = \frac{3}{4}\hbar^2$$

$$S_z = m_s\hbar = \pm\frac{1}{2}\hbar$$

Elétrons: $s = 1/2$

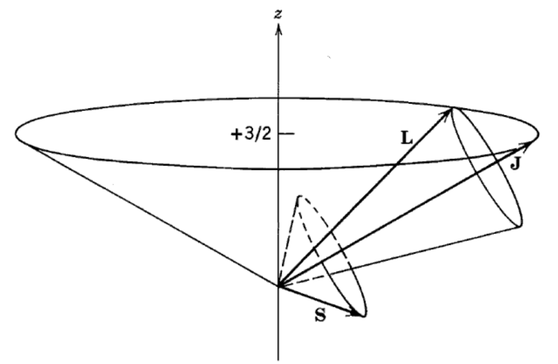


Figure 8-8 The angular momentum vectors **L**, **S**, and **J** for a typical case of a state with $l = 2$, $j = 5/2$, $m_j = 3/2$. The vectors **L** and **S** precess uniformly about their sum **J**, and **J** can be found anywhere on the cone symmetrical about the z axis.

Quantum Physics, Eisberg & Resnick.

Átomo de hidrogênio

Níveis de energia:

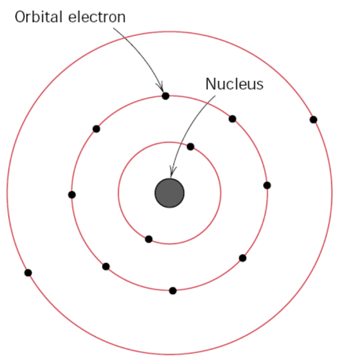
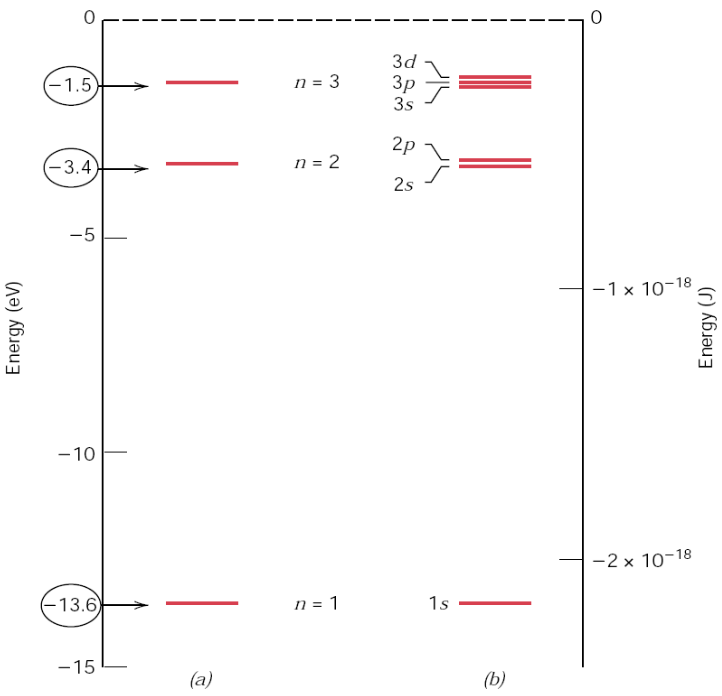


FIGURE 2.1 Schematic representation of the Bohr atom.

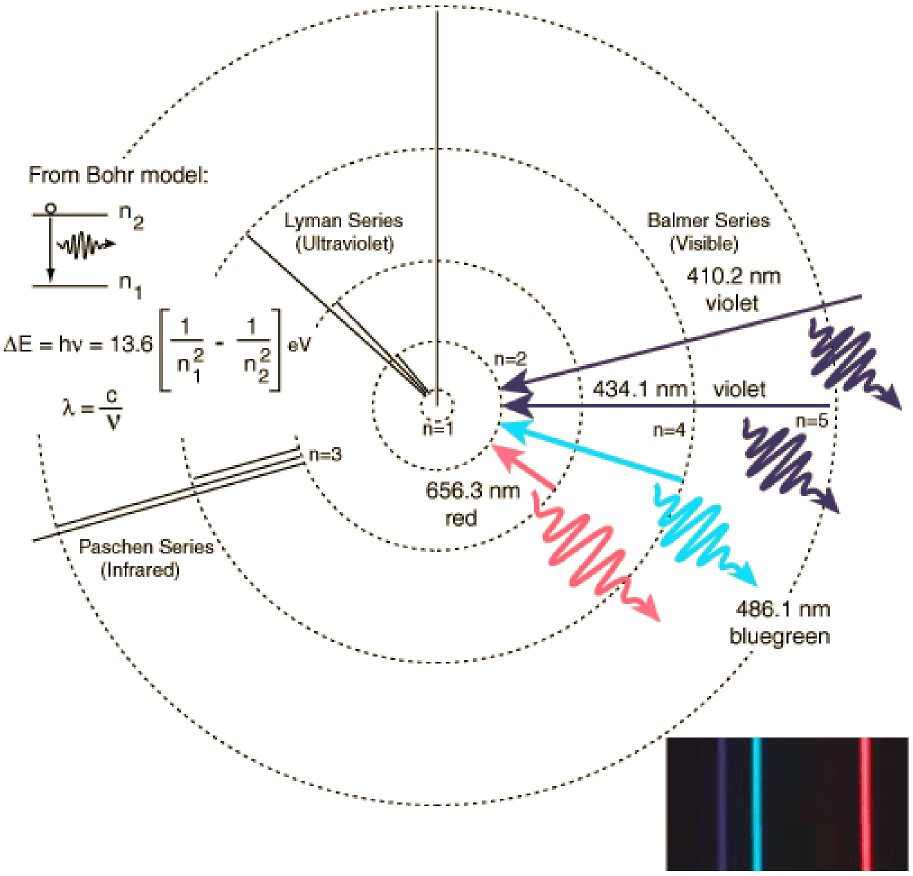
FIGURE 2.2 (*a*) The first three electron energy states for the Bohr hydrogen atom. (*b*) Electron energy states for the first three shells of the wave-mechanical hydrogen atom. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 10. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)



Fundamentals of Materials Science and Engineering , Callister.

Átomo de hidrogênio

Espectro de emissão do hidrogênio:



http://hyperphysics.phy-astr.gsu.edu/hbase/hyde.html#c4

Átomo de hidrogênio

Espectro de emissão do hidrogênio:

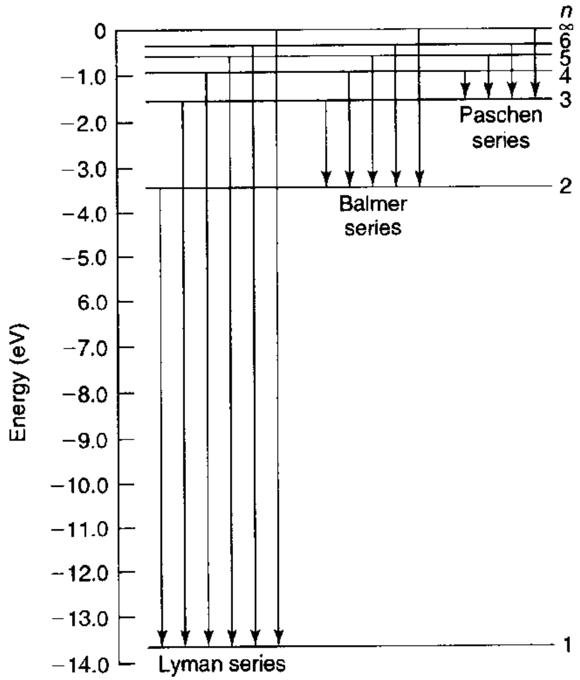


Figure 4.5: Energy levels and transitions in the spectrum of hydrogen.

$$E_n = -\frac{13{,}6\ \mathrm{eV}}{n^2}$$

http://en.wikipedia.org/wiki/Emission_spectrum

Introduction to Quantum Mechanics, Griffiths, 1995.

Átomo de hidrogênio

Funções radiais:

$$\psi(\vec{r}) = R(r)Y_l^m(\theta,\phi)$$

Table 4.6: The first few radial wave functions for hydrogen, $R_{nl}(r)$

$$R_{10} = 2a^{-3/2}\exp(-r/a)$$

$$R_{20} = \frac{1}{\sqrt{2}}a^{-3/2}\left(1-\frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$$

$$R_{21} = \frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a}\exp(-r/2a)$$

$$R_{30} = \frac{2}{\sqrt{27}}a^{-3/2}\left(1-\frac{2}{3}\frac{r}{a}+\frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$$

$$R_{31} = \frac{8}{27\sqrt{6}}a^{-3/2}\left(1-\frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$$

$$R_{32} = \frac{4}{81\sqrt{30}}a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$$

$$R_{40} = \frac{1}{4}a^{-3/2}\left(1-\frac{3}{4}\frac{r}{a}+\frac{1}{8}\left(\frac{r}{a}\right)^2-\frac{1}{192}\left(\frac{r}{a}\right)^3\right)\exp(-r/4a)$$

$$R_{41} = \frac{\sqrt{5}}{16\sqrt{3}}a^{-3/2}\left(1-\frac{1}{4}\frac{r}{a}+\frac{1}{80}\left(\frac{r}{a}\right)^2\right)\frac{r}{a}\exp(-r/4a)$$

$$R_{42} = \frac{1}{64\sqrt{5}}a^{-3/2}\left(1-\frac{1}{12}\frac{r}{a}\right)\left(\frac{r}{a}\right)^2\exp(-r/4a)$$

$$R_{43} = \frac{1}{768\sqrt{35}}a^{-3/2}\left(\frac{r}{a}\right)^3\exp(-r/4a)$$

Introduction to Quantum Mechanics, Griffiths, 1995.

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$$\psi(\vec{r}) = R(r)Y_l^m(\theta,\phi)$$

Funções radiais:

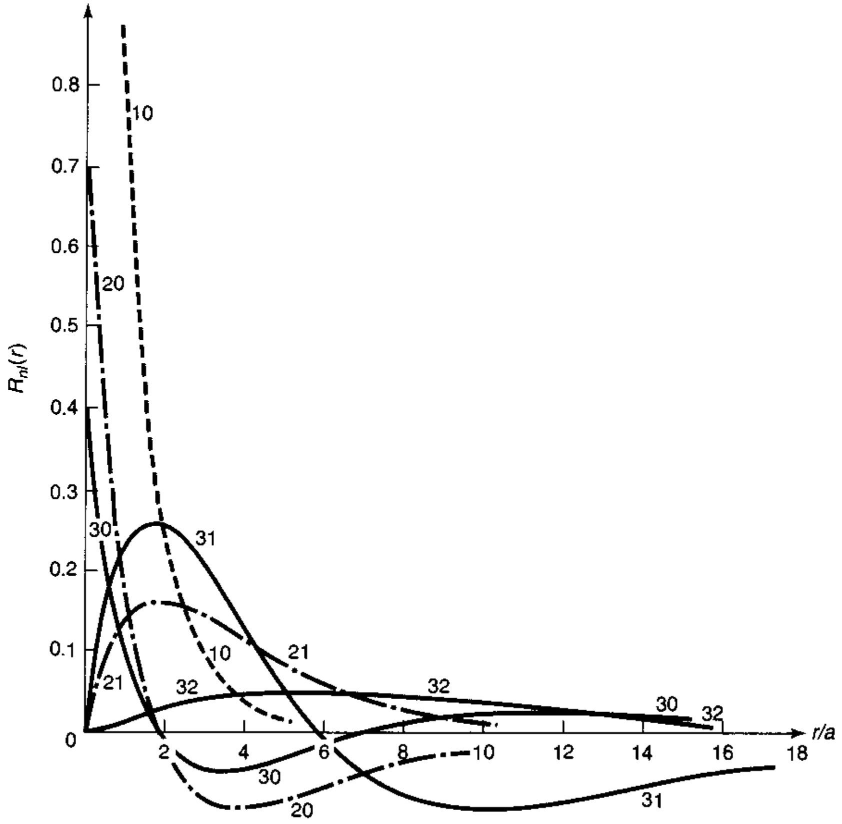

Figure 4.4: Graphs of the first few hydrogen radial wave functions, $R_{nl}(r)$.

Introduction to Quantum Mechanics, Griffiths, 1995.

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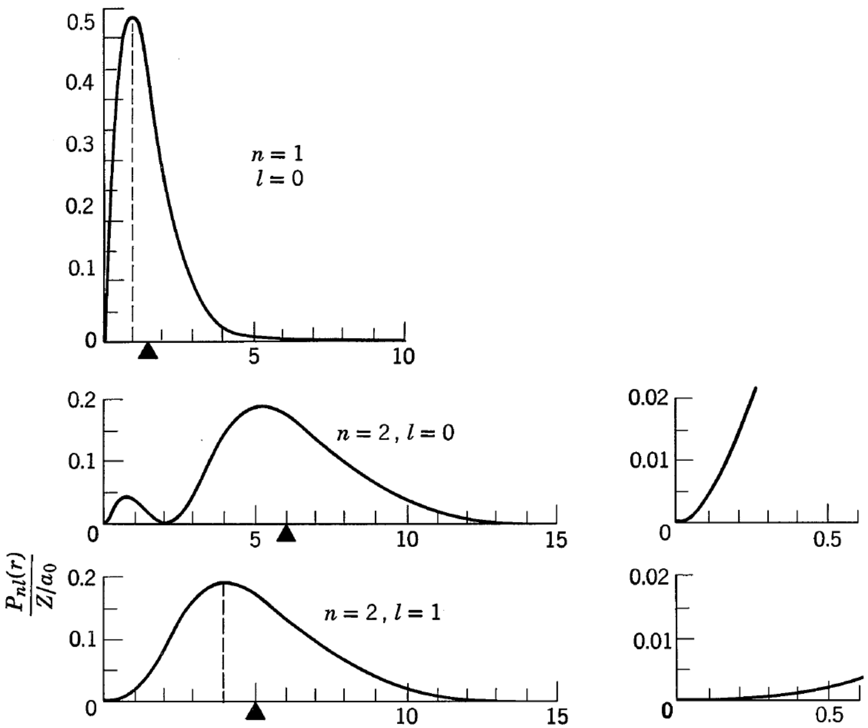
Distribuições radiais de densidade de probabilidade (densidade de carga):

$$\psi(\vec{r}) = R(r)Y_l^m(\theta,\phi)$$

$$P_{nl}(r)dr = R_{nl}^*(r)R_{nl}(r)4\pi r^2 dr$$



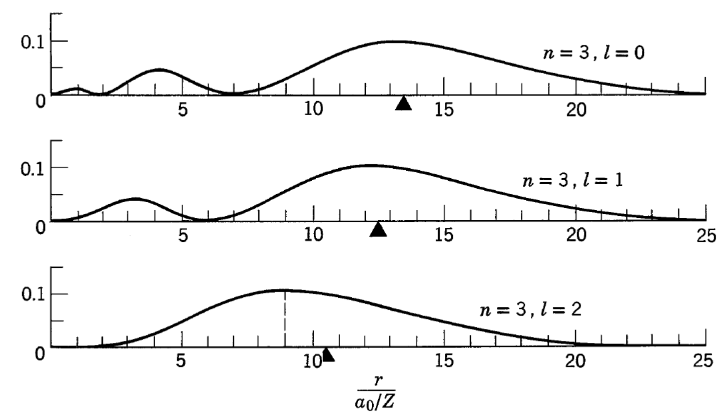


Figure 7-5 The radial probability density for the electron in a one-electron atom for $n = 1, 2, 3$ and the values of l shown. The triangle on each abscissa indicates the value of $\overline{r_{nl}}$ as given by (7-29). For $n = 2$ the plots are redrawn with abscissa and ordinate scales expanded by a factor of 10 to show the behavior of $P_{nl}(r)$ near the origin. Note that in the three cases for which $l = l_{max} = n - 1$ the maximum of $P_{nl}(r)$ occurs at $r_{Bohr} = n^2 a_0/Z$, which is indicated by the location of the dashed line.

Introduction to Quantum Mechanics, Griffiths, 1995.

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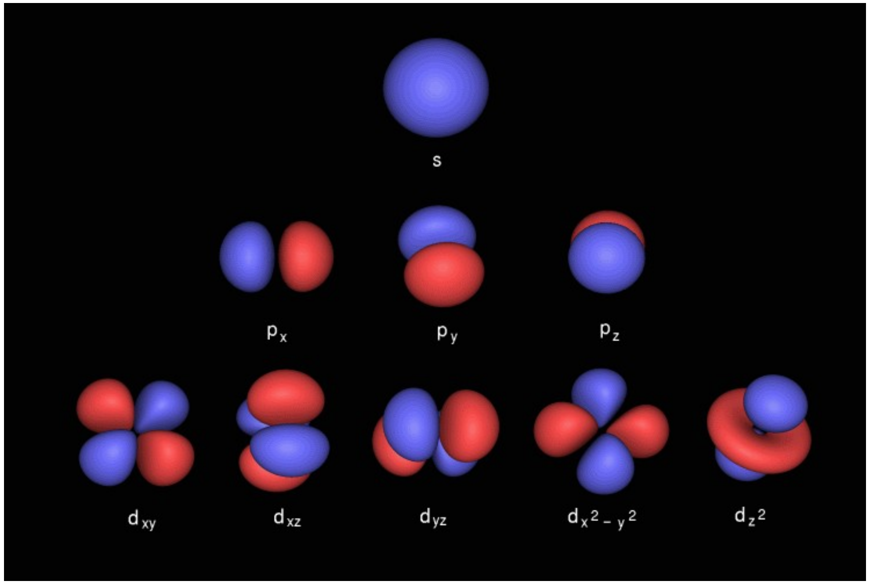
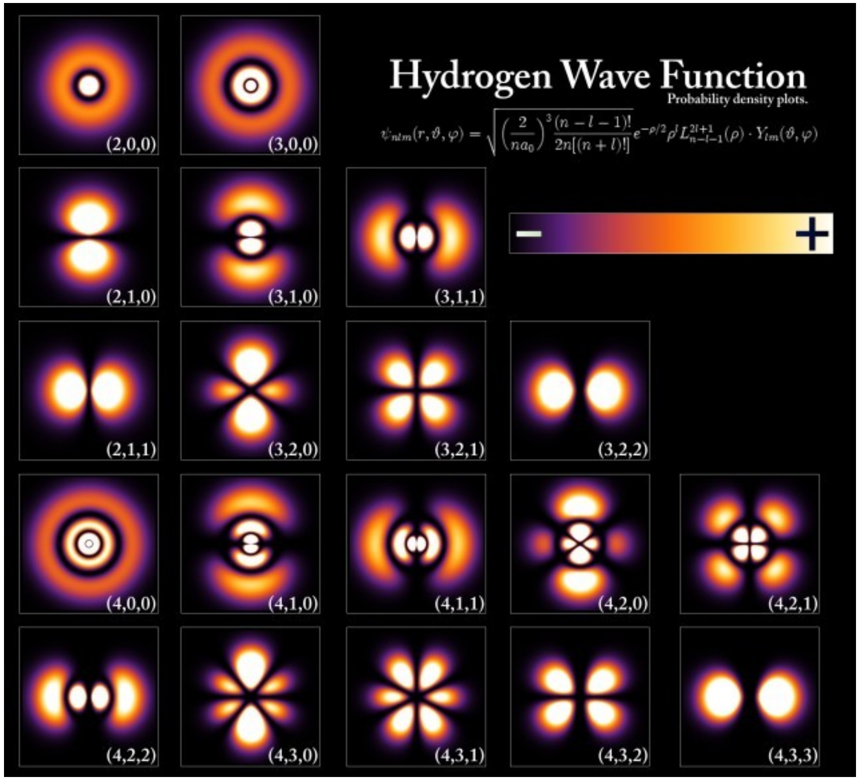
Orbitais atômicos:



http://www.chemcomp.com/journal/molorbs.htm



http://www.physicsoftheuniverse.com/topics_quantum_probability.html

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