Exploring Quantum Physics

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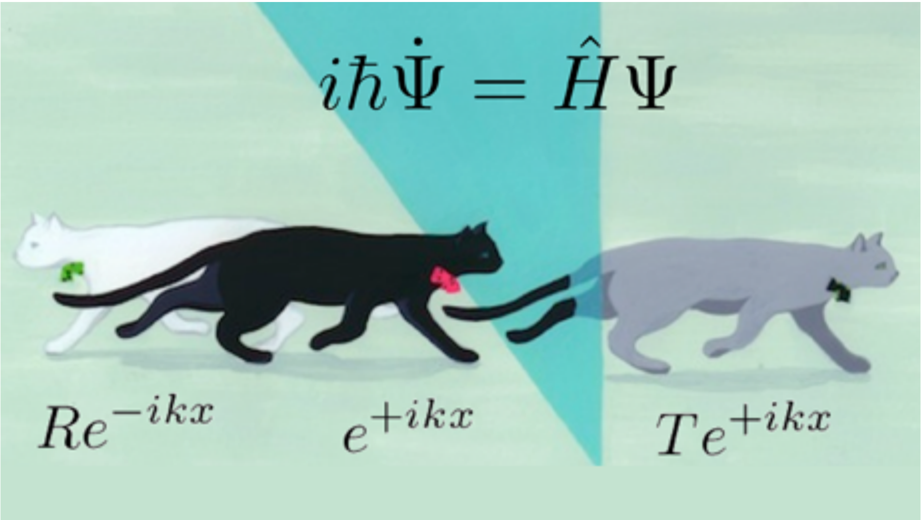
Symmetry in Quantum Physics

Part IX. Solution of Schroedinger Equations for Systems with Definite Angular Momemtum



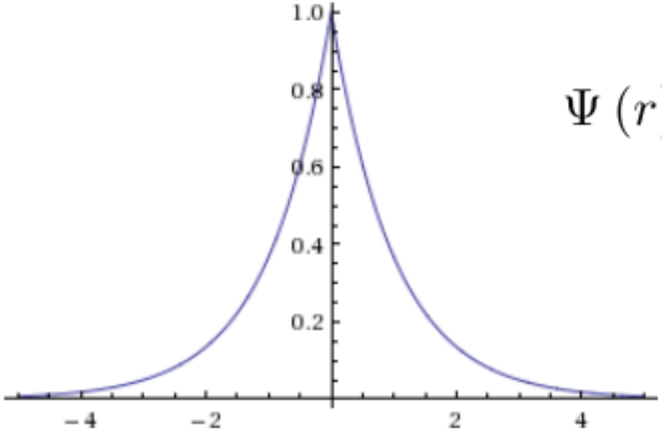
Symmetry in quantum physics

$$L_u = \frac{\hbar}{i}\epsilon_{uvw}x_v\partial_w$$

$$[L_u, L_v] = i\hbar\epsilon_{uvw}L_w$$

$$[L_u, x_v] = i\hbar\epsilon_{uvw}x_w$$

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{L^2}{\hbar^2 r^2}$$



$$\Psi(r) = \frac{\exp(-r/a_0)}{\sqrt{\pi a_0^3}}$$

a section cut along the axis x_1 – note cusp at 0

Use constructive approach to find potential : $-\frac{1}{\Psi}\left[\frac{\hbar^2}{2m_e}\nabla^2\Psi\right] = E - V(r)$

$$V(r) = -\frac{e^2}{r}$$

Coulomb potential

$$E = -\frac{\hbar^2}{2m_e a_0^2} = -R_\infty hc$$

1s ground state of hydrogen atom

$$a_0 = \frac{\hbar^2}{m_e e^2}$$

Bohr radius

Symmetry in quantum physics

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{L^2}{\hbar^2 r^2}$$

$$L^2|l,m> = \hbar^2 l(l+1)|l,m>$$

$$\Psi = \Psi(r) Y_{l,m}(\theta,\phi)$$

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + V(r)\right]\Psi = E\Psi$$

$$\left[-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right) + V(r)\right]\Psi(r) = E\Psi(r)$$

Go to dimensionless variable ρ NOW. $r = a\rho$

$$\left[\frac{1}{2}\left(\frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} - \frac{l(l+1)}{\rho^2}\right) + \epsilon - U(\rho)\right]\psi(\rho) = 0$$

$$\Psi(r) = a^{-3/2}\psi(r/a)$$

$$\frac{Ma^2}{\hbar^2}E = \epsilon \qquad U(\rho) = \frac{Ma^2}{\hbar^2}V(a\rho)$$

Invideo quiz

$E = \epsilon \frac{\hbar^2}{M a^2}$ where E is an energy, $\hbar$ is the reduced Planck constant and a is a length. What are the dimensional units of ϵ?

\vspace {8 pt}

$[M][L]^2[T]^{-2}$

\vspace {8 pt}

$[M][L]^2[T]^{-1}$

\vspace {8 pt}

$[M]^0[L][T]^{-2}$

\vspace {8 pt}

$[M]^0[L]^0[T]^0$ correct

\vspace {8 pt}

Symmetry in quantum physics

$$\Psi = \Psi(r) Y_{l,m}(\theta, \phi)$$

$$\Psi(r) = a^{-3/2} \psi(r/a)$$

$$r = a\rho \qquad \frac{Ma^2}{\hbar^2} E = \epsilon$$

$$U(\rho) = \frac{Ma^2}{\hbar^2} V(a\rho)$$

$$\left[\frac{1}{2}\left(\frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} - \frac{l(l+1)}{\rho^2}\right) + \epsilon - U(\rho)\right]\psi(\rho) = 0$$

Isolate singular points now. First near ρ = 0.

Symmetry in quantum physics

http://dlmf.nist.gov/10

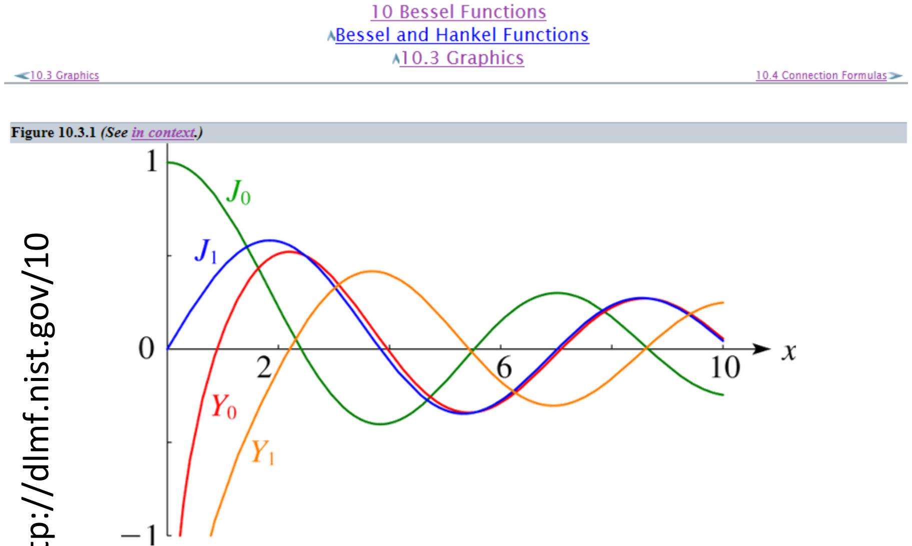


Figure 10.3.1: $J_0(x), Y_0(x), J_1(x), Y_1(x), 0 \le x \le 10$.

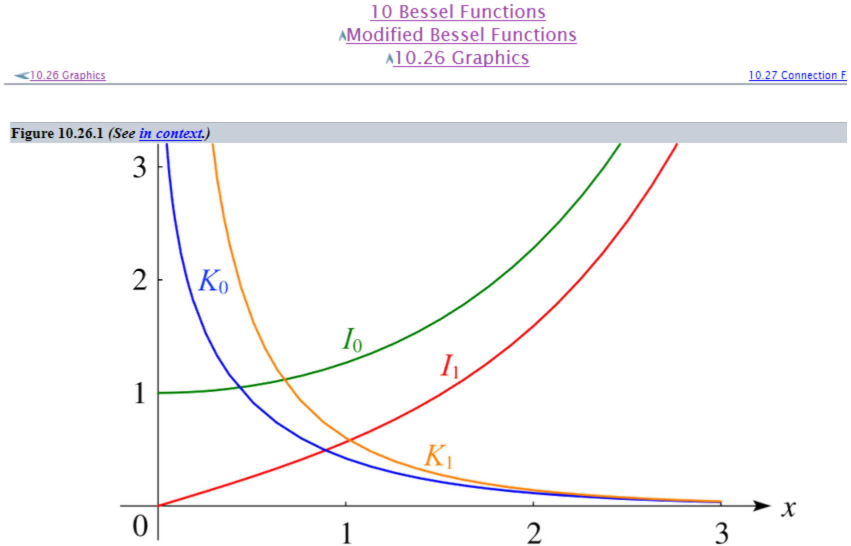


Figure 10.26.1: $I_0(x), I_1(x), K_0(x), K_1(x), 0 \le x \le 3$.

r = 0 is a singular point for the kinetic energy operator. Need regular solutions there.

Symmetry in quantum physics

$$\Psi = \Psi(r) Y_{l,m}(\theta, \phi)$$

$$\Psi(r) = a^{-3/2} \psi(r/a)$$

$$r = a\rho \qquad \frac{Ma^2}{\hbar^2} E = \epsilon$$

$$U(\rho) = \frac{Ma^2}{\hbar^2} V(a\rho)$$

$$\left[\frac{1}{2}\left(\frac{\partial^2}{\partial\rho^2} + \frac{2}{\rho}\frac{\partial}{\partial\rho} - \frac{l(l+1)}{\rho^2}\right) + \epsilon - U(\rho)\right]\psi(\rho) = 0$$

Isolate singular points now. First near ρ = 0.

$$\psi(\rho) = \phi(\rho)\rho^{\nu} \qquad \nu = l,\ -(l+1)$$

$$\left[\frac{1}{2}\frac{\partial^2}{\partial\rho^2} + \frac{l+1}{\rho}\frac{\partial}{\partial\rho} + \epsilon - U(\rho)\right]\phi(\rho) = 0$$

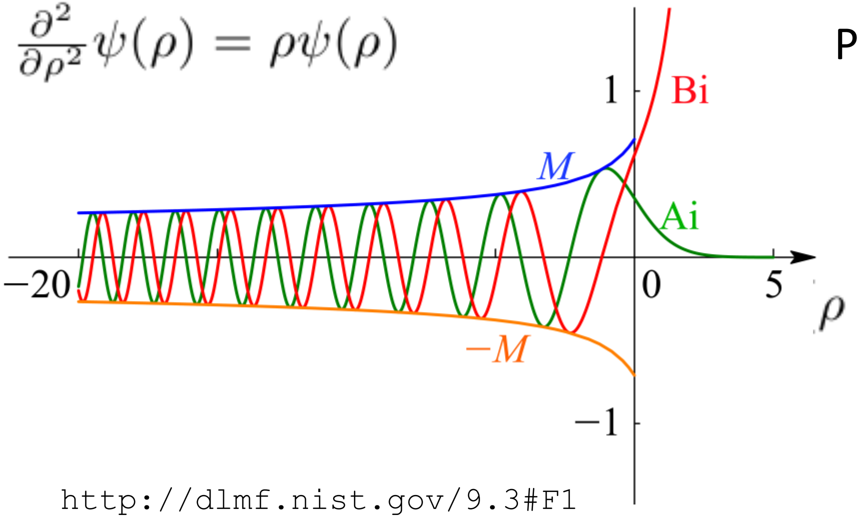
Now we face the issue of large-ρ behavior. Square-normalizable states eventually encounter a barrier region, $\epsilon < U(\rho)$, where divergence must be suppressed.

Solving the Schrödinger Equation

$$V(x) = V_0 + V_1 x$$

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V_0 + V_1 x\right]\Psi(x) = E\Psi(x) \qquad x = \frac{\alpha\rho + E - V_0}{V_1} \qquad \alpha = \left[\frac{\hbar^2 V_1^2}{2M}\right]^{1/3}$$

$$\frac{\partial^2}{\partial\rho^2}\psi(\rho) = \rho\psi(\rho)$$



http://dlmf.nist.gov/9.3#F1

Pair of universal solutions: Airy functions

$$\mathrm{Ai}(\rho),\ \mathrm{Bi}(\rho)$$

Both oscillatory for $\rho < 0$

Ai: quantum bouncing ball

Bi: scanning tunneling microscope

Symmetry in quantum physics

$$\Psi = \Psi(r) Y_{l,m}(\theta,\phi)$$

$$\Psi(r) = a^{-3/2}\psi(r/a)$$

$$r = a\rho \qquad \frac{Ma^2}{\hbar^2}E = \epsilon$$

$$U(\rho) = \frac{Ma^2}{\hbar^2}V(a\rho)$$

$$\psi(\rho) = \phi(\rho)\rho^l$$

$$M = m_e$$

$$a = a_0 = \frac{\hbar^2}{m_e e^2}$$

$$\left[\frac{1}{2}\frac{\partial^2}{\partial\rho^2} + \frac{l+1}{\rho}\frac{\partial}{\partial\rho} + \epsilon - U(\rho)\right]\phi(\rho) = 0$$

Here we get specific, and treat the hydrogen atom (with infinite nuclear mass). Hence $M = m_e$ and (in Gaussian units)

$$V(r) = -\frac{e^2}{r} \qquad\qquad U(\rho) = -\frac{1}{\rho}$$

when $a = a_0$, the Bohr radius.

$$\left[\frac{1}{2}\frac{\partial^2}{\partial\rho^2} + \frac{l+1}{\rho}\frac{\partial}{\partial\rho} + \epsilon + \frac{1}{\rho})\right]\phi(\rho) = 0$$

Symmetry in quantum physics

$$\Psi = \Psi(r) Y_{l,m}(\theta, \phi)$$

$$\Psi(r) = a^{-3/2} \psi(r/a)$$

$$r = a\rho \qquad \frac{Ma^2}{\hbar^2} E = \epsilon$$

$$U(\rho) = \frac{Ma^2}{\hbar^2} V(a\rho)$$

$$\psi(\rho) = \phi(\rho) \rho^l$$

$$M = m_e$$

$$a = a_0 = \frac{\hbar^2}{m_e e^2}$$

$$V(r) = -\frac{e^2}{r}$$

$$\left[\frac{1}{2}\frac{\partial^2}{\partial\rho^2} + \frac{l+1}{\rho}\frac{\partial}{\partial\rho} + \epsilon + \frac{1}{\rho})\right] \phi(\rho) = 0$$

Now for bound states we have $\varepsilon = -\kappa^2/2 < 0$, so we set

$$\phi(\rho) = f(\rho) \exp(-\kappa\rho)$$

$$\frac{1}{2}\frac{\partial^2 f}{\partial\rho^2} + \frac{l+1}{\rho}\frac{\partial f}{\partial\rho} - \kappa\frac{\partial f}{\partial\rho} + \frac{1-\kappa(l+1)}{\rho} f = 0$$

$$f(\rho) = \sum_{j=0}^{n} f_j \rho^j$$

Two-term recurrence relationship in *j*: **solvable**

Symmetry in quantum physics

$$\Psi = \Psi(r) Y_{l,m}(\theta, \phi)$$

$$\Psi(r) = a^{-3/2}\psi(r/a)$$

$$r = a\rho \qquad \frac{Ma^2}{\hbar^2}E = \epsilon$$

$$U(\rho) = \frac{Ma^2}{\hbar^2}V(a\rho)$$

$$\psi(\rho) = \phi(\rho)\rho^l$$

$$M = m_e$$

$$a = a_0 = \frac{\hbar^2}{m_e e^2}$$

$$V(r) = -\frac{e^2}{r}$$

$$\epsilon = -\frac{\kappa^2}{2}$$

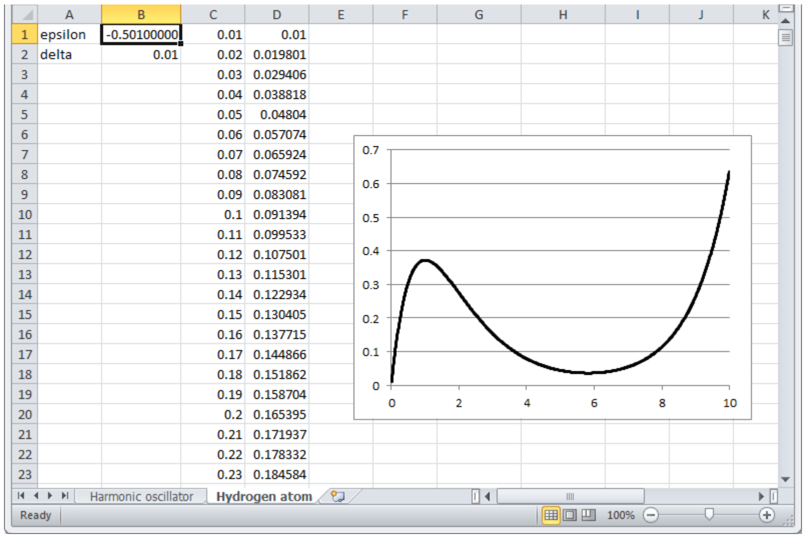
Bottom line: if *n* is highest non-vanishing term in series, then

$$E_{nl} = -\frac{\hbar^2}{2m_e a_0^2}\frac{1}{(n+l+1)^2} = -\frac{R_\infty hc}{(n+l+1)^2}$$

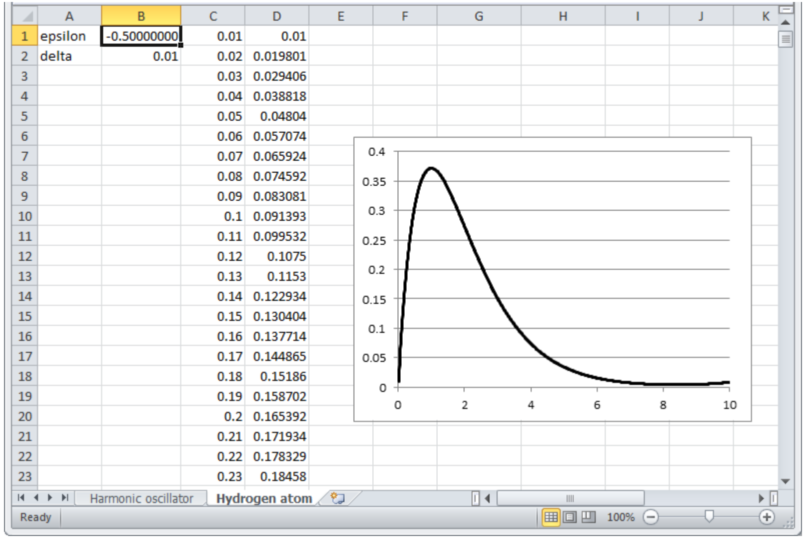
Otherwise solution diverges exponentially at large ρ.

$$\phi(\rho) = f(\rho)\exp(-\kappa\rho) \qquad f(\rho) = \sum_{j=0}^{n} f_j \rho^j$$

Solving the Schrödinger Equation



	A	B	C	D
1	epsilon	-0.50100000	0.01	0.01
2	delta	0.01	0.02	0.019801
3			0.03	0.029406
4			0.04	0.038818
5			0.05	0.04804
6			0.06	0.057074
7			0.07	0.065924
8			0.08	0.074592
9			0.09	0.083081
10			0.1	0.091394
11			0.11	0.099533
12			0.12	0.107501
13			0.13	0.115301
14			0.14	0.122934
15			0.15	0.130405
16			0.16	0.137715
17			0.17	0.144866
18			0.18	0.151862
19			0.19	0.158704
20			0.2	0.165395
21			0.21	0.171937
22			0.22	0.178332
23			0.23	0.184584



	A	B	C	D
1	epsilon	-0.50000000	0.01	0.01
2	delta	0.01	0.02	0.019801
3			0.03	0.029406
4			0.04	0.038818
5			0.05	0.04804
6			0.06	0.057074
7			0.07	0.065924
8			0.08	0.074592
9			0.09	0.083081
10			0.1	0.091393
11			0.11	0.099532
12			0.12	0.1075
13			0.13	0.1153
14			0.14	0.122934
15			0.15	0.130404
16			0.16	0.137714
17			0.17	0.144865
18			0.18	0.15186
19			0.19	0.158702
20			0.2	0.165392
21			0.21	0.171934
22			0.22	0.178329
23			0.23	0.18458

Try iterative approximate numerical solution using spreadsheet in Additional Materials