Quantum Bound States

Eigenvalues From ODEs

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Based on *A Survey of Computational Physics* by Landau, Páez, & Bordeianu

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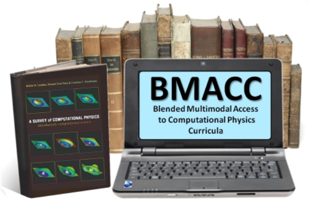
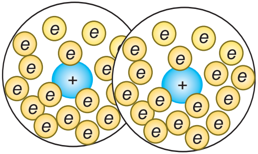
Course: **Computational Physics II**



Does QM Apply in a Nucleus?



Problem: QM Binding in Nucleus

- Know: neutron, proton $mc^2 \simeq 940\,\text{MeV}$
- Know: MeV nuclear energies
- Know: n, p bound within nucleus $R \simeq 2\,fm = 2 \times 10^{-15}$ m
- Compatible with QM bound state?
- Can electron ($mc^2 \simeq 0.5\,\text{MeV}$) be inside too?

Theory: The Quantum Eigenvalue Problem

Physics Assumptions and Semantics

- Assume stationary state $\psi(x,t) = \psi(x)e^{-iEt/\hbar}$
- $\Rightarrow$ t-independent Schrödinger equation
- Bound-State $\Rightarrow$ confined
- $\Rightarrow \psi \to 0 \Rightarrow$ eigenvalue problem
- Not just solve ODE
- Boundary conditions $\Rightarrow$ Eigen-energies, -values
- Don't sweat physics
- Elsewhere: p-space bound = matrix problem
- Elsewhere: QM wave packet; t-dependent PDE

Theory: The Quantum Eigenvalue Problem

Mathematics Formulation

- Probability in dx around x: $|\psi(x)|^2\,dx$
- 1-D time-independent Schrödinger equation

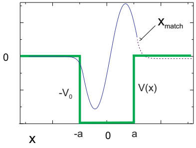
$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{1}$$

- Solve wave vector κ ($\equiv E$)

$$\kappa^2 = -\frac{2m}{\hbar^2}E = \frac{2m}{\hbar^2}|E| \tag{2}$$

$$\Rightarrow \quad \frac{d^2\psi(x)}{dx^2} - \frac{2m}{\hbar^2}V(x)\psi(x) = \kappa^2\psi(x) \tag{3}$$

Model: Nucleon in a Box



- Numerical methods any $V(x)$
- Simplicity: finite square well

$$V(x) = \begin{cases} -V_0 = -83\,\text{MeV}, & \text{for } |x| \leq a = 2\,\text{fm}, \\ 0, & \text{for } |x| > a = 2\,\text{fm} \end{cases} \tag{1}$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + \left(\frac{2m}{\hbar^2} V_0 - \kappa^2\right)\psi(x) = 0, \quad \text{for } |x| \leq a, \tag{2}$$

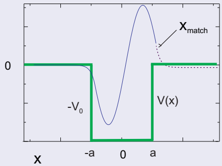
$$\frac{d^2\psi(x)}{dx^2} - \kappa^2\psi(x) = 0, \quad \text{for } |x| > a \tag{3}$$

Constants

$$\frac{2m}{\hbar^2} = \frac{2mc^2}{(\hbar c)^2} \simeq \frac{2 \times 940\,\text{MeV}}{(197.32\,\text{MeV fm})^2} = 0.0483\,\text{MeV}^{-1}\,\text{fm}^{-2} \tag{4}$$

Algorithm: ODE Solver + Search

Build in Boundary Conditions + ODE Solver (rk4, Numerov)



1. Start far left $x = -X_{\max} \ll -a \simeq -\infty$
2. Assume $\psi(x)$ satisfies Boundary Condition there:

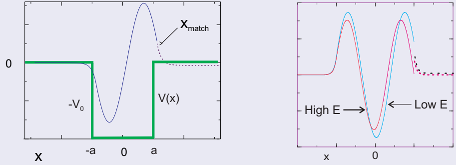
$$\psi_L(x = -X_{\max}) \simeq e^{+\kappa x} = e^{-\kappa |X_{\max}|} \quad (1)$$

3. Use ODE solver, step $\psi_L(x)$ to right
4. Continue to matching radius x_{match}
5. Start far right step left, through $V(x)$

$$\psi_R = e^{-\kappa x} = e^{-\kappa X_{\max}} \quad (2)$$

Algorithm: ODE Solver + Search

Trial-&-Error Search for E_i (Bisection, Newton-Raphson)



1. Recall $\psi_L(x = -X_{\max}) \simeq e^{+\kappa x}, \quad \psi_R = e^{-\kappa x}$
2. Require continuous probability, current at x_{match}
3. $\Rightarrow$ Continuous $\psi(x)$, $\psi'(x)$
4. $\Rightarrow \psi'(x)/\psi(x) =$ log derivative continuous (no norm)
5. Use mismatch amount to improve next guess:

$$\Delta(E, x) = \left. \frac{\psi_L'(x)/\psi_L(x) - \psi_R'(x)/\psi_R(x)}{\psi_L'(x)/\psi_L(x) + \psi_R'(x)/\psi_R(x)} \right|_{x = x_{\text{match}}} \tag{1}$$

6. Continue till L & R ψ'/ψ match within tolerance

Implementation: Eigenvalues via an ODE Solver Plus Bisection Algorithm

CODE QuantumEigen.py

1. Combine bisection algorithm search with ODE solver
2. Start with a step size $h = 0.04$
3. Write subroutine calculate matching function $\Delta(E, x)$
4. Search till change 4th decimal place $\Rightarrow \Delta(E, x = 2) = 0$
5. Print out energy for each iteration
6. Limit number iterations
7. Plot ψ, $V(x)$
8. Count nodes to label excited states
9. Search for excited states
10. Check ψ for continuity, nodes
11. Verify problem solved; MeV spacing