Schrödinger equation for the nuclear potential

Introduction to Nuclear Science

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Outline

1. One-dimensional Schrödinger equation
   - The wave function
   - Constant potential
   - Potential step
   - Potential barrier
   - Potential well
   - Infinitely deep potential well
   - Harmonic oscillator

Outline

Description of a quantum-mechanical system

- Evolution of a non-relativistic quantum-mechanical system is described by the Shrödinger equation.

- In its most general form the Shrödinger equation is the second-order differential equation in space coordinates and the first-order differential equation in the time coordinate.

- For interactions constant in time, which are defined by the potential energy V, the Schödinger equation represents conservation of energy:

$$E = K + V = \frac{p^2}{2m} + V \tag{1}$$

- The difference from the classical description is a consequence of the fact that p^2 in quantum mechanics is a differential operator

$$p^2 = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \tag{2}$$

Wave function for a single particle

- Let us consider a single particle in one dimension.

- Let the interactions be defined by the potential energy $V(x)$

- The probability for a particle to be located at position x is defined by $\mid \psi(x) \mid^2$ with $\psi(x)$ being a solution of the Shrödinger equation

$$E\psi(x) = (K + V)\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) \quad (3)$$

- Energy E is a constant, the equation can be re-written as

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}\left(E - V(x)\right)\psi(x) \quad (4)$$

- The last equation has a simple solution for a constant potential

$$V(x) = \text{const.} \quad (5)$$

Constant potential: $E > V$

- Let us consider a constant potential $V(x) = V$. In this case the Shrödinger equation can be written as

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

- For the case of $E > V$ one can define

$$k^2 = \frac{2m}{\hbar^2}(E - V), \quad \hbar k = \sqrt{2m(E - V)}$$

- The equation reads

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$$

- The solution, called a plane wave solution, is

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

Constant potential: normalization

- A constrain for constants A and B in the plane wave solution is imposed by the wave function normalization condition

$$\mid \psi(x) \mid^2 = 1$$

- Let us consider the special case of $B = 0$. The normalization condition for A reads

$$1 = \mid \psi(x) \mid^2 = \int_{=\infty}^{\infty} A^2 \sin^2(kx) dx = A^2 \int_{-\infty}^{\infty} \sin^2(kx) dx$$

- But the integral $\int_{-\infty}^{\infty} \sin^2(kx) dx$ diverges, thus a plane wave solution can not be normalized in the full space.

- However, plane wave solution can be normalized if the spacial dimensions are restricted, yielding finite limits for the integration. Such restriction leads to a "particle in a well" model discussed later.

Constant potential: $E < V$

- For the case of $E < V$ one can define

$$\kappa^2 = \frac{2m}{\hbar^2}(V - E), \quad \hbar\kappa = \sqrt{2m(V - E)}$$

- The equation reads

$$\frac{d^2\psi(x)}{dx^2} = \kappa^2 \psi(x)$$

- The solution is

$$\psi(x) = C\exp(-\kappa x) + D\exp(\kappa x)$$

- Note that this solution diverges very rapidly with increasing x if $D \neq 0$ or for decreasing x if $C \neq 0$.

Potential step

- Let us consider a potential step

$$V = \left\{ \begin{array}{cc} 0 & x < 0 \\ -V_0 & x \geq 0 \end{array} \right.$$

- The strategy for solving the Shrödinger equation is to
  - obtain two solutions, $\psi_<(x)$ for $x < 0$, and $\psi_>(x)$ for $x \geq 0$
  - match the solution on the step, at $x = 0$ in such a way that the wave function and its derivative is continues on the step

$$\begin{array}{rcl} \psi_<(0) & = & \psi_>(0) \\ \dfrac{d\psi_<}{dx}(0) & = & \dfrac{d\psi_>}{dx}(0) \end{array}$$

Potential step, $E > 0$

- For $E > 0$ the solutions are

$$\psi_<(x) = A_< \sin(k_< x) + B_< \cos(k_< x) \qquad \hbar k_< = \sqrt{2mE}$$
$$\psi_>(x) = A_> \sin(k_> x) + B_> \cos(k_> x) \qquad \hbar k_> = \sqrt{2m(E + V)}$$

  note that the wavelength is shorter for $x > 0$ reflecting larger momentum in this region $\hbar k_> > \hbar k_<$.

- The continuity conditions require that

$$\psi_<(0) = \psi_>(0) \quad \implies \quad B_< = B_>$$
$$\frac{d\psi_<}{dx}(0) = \frac{d\psi_>}{dx}(0) \quad \implies \quad k_< A_< = k_> A_>$$

- For numerical solution see this link.

Potential step, $-V_0 < E < 0$

- For $-V_0 < E < 0$ the solutions are

$$\psi_<(x) = D\exp(\kappa x) \qquad \hbar\kappa = \sqrt{-2mE}$$
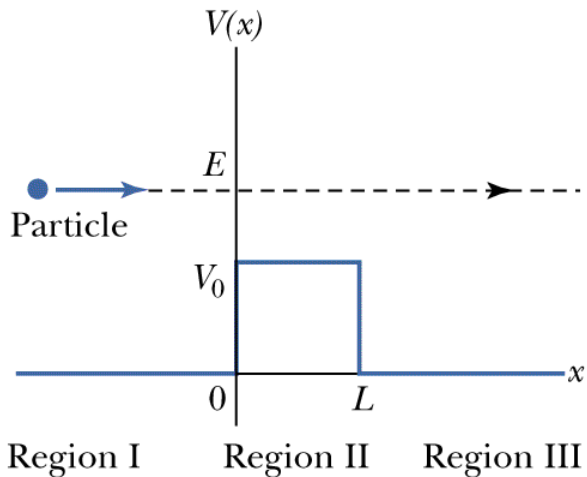$$\psi_>(x) = A\sin(kx) + B\cos(kx) \qquad \hbar k = \sqrt{2m(E - V_0)}$$

note that $C\exp(-\kappa x)$ should not be included as it diverges with $x \to -\infty$.

- The continuity conditions require that

$$\psi_<(0) = \psi_>(0) \quad \Longrightarrow \quad B = D$$
$$\frac{d\psi_<}{dx}(0) = \frac{d\psi_>}{dx}(0) \quad \Longrightarrow \quad kA = \kappa D$$

- For numerical solution see this link. Note the wave function penetrating into the step.
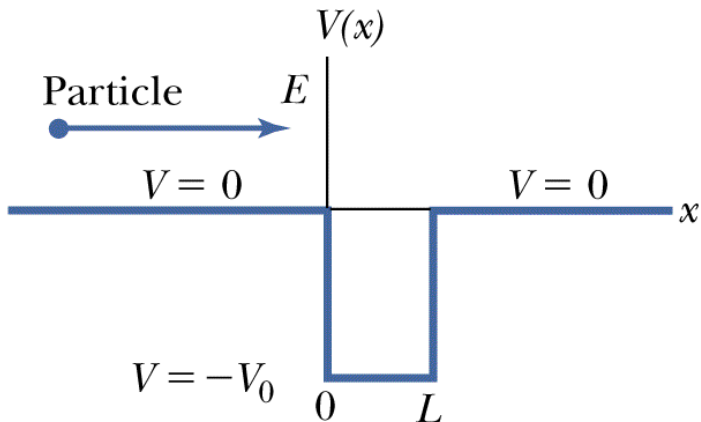
Potential barrier

For numerical solution see this link.

Potential well

- In the case of the potential well one seeks solutions in three regions.

- Continuity equations of the wave function and its first derivative have to be applied on the boundaries between regions I and II and regions II and III.
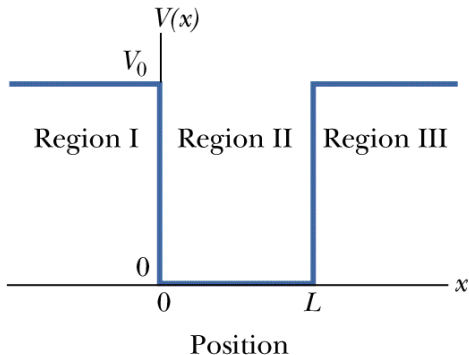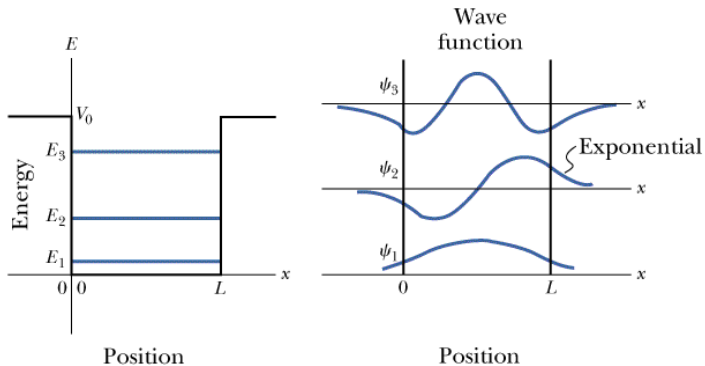
Potential well: unbound states

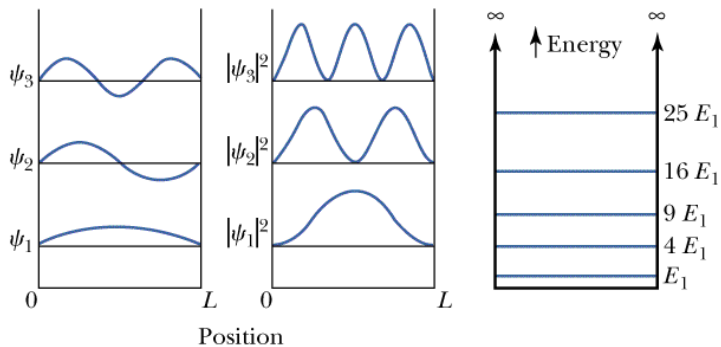For numerical solution see this link.

Potential well: bound states

Continuity conditions for bound states lead to quantization of states.

For numerical solution see this link.

Infinitely deep potential well

If the well is infinitely deep the continuity equations require that the wave function vanishes on the boundaries.

Position

Infinitely deep potential well

- For the well on the graph

$$\psi(0) = 0 \quad \psi(L) = 0 \quad \implies \quad \psi(x) = A\sin(\frac{n\pi}{L}x)$$

- But at the same time
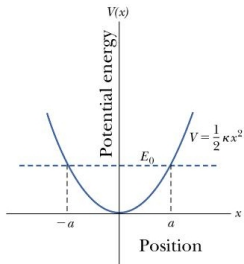
$$\psi(x) = A\sin(kx) \qquad \hbar k = \sqrt{2mE}$$

- This leads to

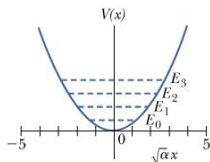$$k = \frac{1}{\hbar}\sqrt{2mE} = \frac{n\pi}{L} \quad \text{or}$$

$$E = n^2\frac{\pi^2\hbar^2}{2mL^2} = n^2 E_1 \quad E_1 = \frac{h^2}{8mL^2}$$

- Note that the wave function for the ground state is symmetric with respect to the middle of the well (has positive parity), for the next state the wave function is asymmetric (has negative parity) etc.

Harmonic oscillator

$$E = \hbar\omega(n + \tfrac{1}{2}) = h\nu(n + \tfrac{1}{2}) = E_0(n + \tfrac{1}{2})$$

Wave functions

$$\psi_3(x) = \left(\tfrac{\alpha}{\pi}\right)^{1/4} \tfrac{1}{\sqrt{3}} \left(\sqrt{\alpha}x\right)(2\alpha x^2 - 3)\, e^{-\alpha x^2/2}$$
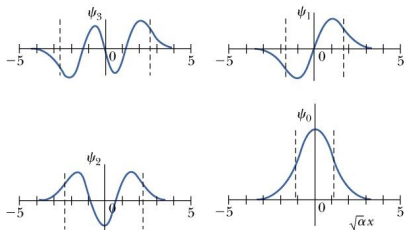
$$\psi_2(x) = \left(\tfrac{\alpha}{\pi}\right)^{1/4} \tfrac{1}{\sqrt{2}} (2\alpha x^2 - 1)\, e^{-\alpha x^2/2}$$

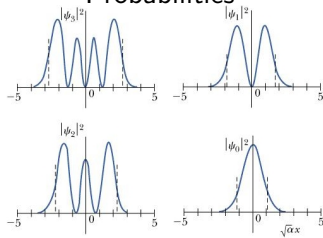$$\psi_1(x) = \left(\tfrac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha}\; x e^{-\alpha x^2/2}$$

$$\psi_0(x) = \left(\tfrac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$
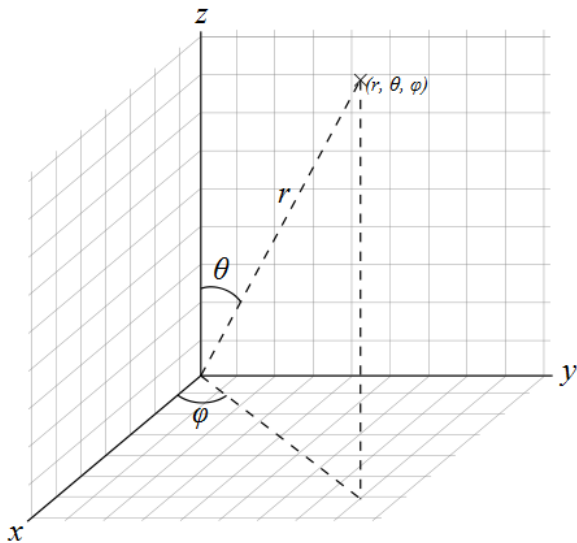
Harmonic oscillator

A step to three dimensions

- In one dimension the Schrödinger equation is a differential equation of a single variable: the single position coordinate of a particle.

- In three dimensions there are three coordinates defining position of a particle.

- Thus the Schrödinger equation relevant to nuclear and atomic sciences (thus also to Chemistry) is a partial second-order differential equation of (at least) three variables: the three position coordinates of a particle.

- Note that for particles with spin, the Schrödinger equation may depend on spin orientation. We are not going to consider such cases today, but we will come back to an example later.

Separation of variables

- In general, it is easier to solve three separate differential equations of a single variable, than a single differential equation of three variables.

- The complication in the latter case comes from the correlations between variables. It is easier to handle uncorrelated variables which do not impact each other rather than correlated variables which are coupled together.

- This observation leads to a strategy in solving differential equations named separation of variables. This strategy attempts to find a set of variables which describe the case of interest (position of a particle) but lead to separation of the equation of interest (the Schrödinger equation) into a set of decoupled equations of a single variable.

- For atoms and nuclei (potential dependent on the distance $V(r)$) this is achieved using a set of spherical rather than Cartesian coordinates.

The spherical coordinates

$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\cos\theta = \frac{z}{\sqrt{x^2 + y^2}}$$

$$\tan\phi = \frac{y}{x}$$

$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

$$z = r\cos\theta \qquad (6)$$

The Schrödinger equation is spherical coordinates

- Nuclear and atomic potential depends on a distance

$$V = V(r) = V(\sqrt{x^2 + y^2 + z^2}) \qquad (7)$$

- Three-dimensional Schrödinger equation in Cartesian coordinates is:

$$
\begin{aligned}
E\psi(x, y, z) = & - \frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] \psi(x, y, z) \\
& + V(x, y, z)\psi(x, y, z) \qquad (8)
\end{aligned}
$$

- Three-dimensional Schrödinger equation in spherical coordinates is:

$$
\begin{aligned}
& E\psi(r, \theta, \phi) = \\
& -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right] \psi(r, \theta, \phi) \\
& + V(r)\psi(r, \theta, \phi) \qquad (9)
\end{aligned}
$$

The azimuthal equation

- The first step in solving Eq. 9 is to separate the azimuthal equation which depends only on the azimuthal coordinate ϕ.

- As a consequence of this separation, the wave function $\psi(r, \theta, \phi$ separates into a product of the azimuthal wave function $\Phi_m(\phi)$ and a wave function which depends on r and θ.

- The equation for the azimuthal wave function reads
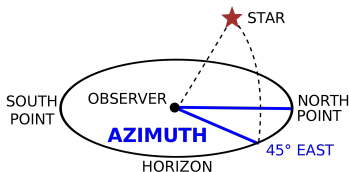
$$\frac{d^2\Phi_m(\phi)}{d\phi^2} = -m^2\Phi_m(\phi) \qquad (10)$$

- The solutions are

$$\Phi_m(\phi) = \exp(-im\phi) = \cos(m\phi) - i\sin(m\phi) \qquad (11)$$

with m called the azimuthal quantum number is an integer.

The azimuthal quantum number

- The fact that the azimuthal quantum number is an integer follows from the condition that the rotation over the full angle brings the system into the same orientation.

$$
\begin{aligned}
\Phi_m(\phi + 2\pi) &= \cos(m(\phi + 2\pi)) - i\sin(m(\phi + 2\pi)) = \\
&= \cos(m\phi) - i\sin(m\phi) = \Phi_m(\phi) \quad (12)
\end{aligned}
$$

if m is an integer.

The orbital equation

- The next step in solving Eq. 9 is to separate the orbital equation which depends only on the variable θ and the value of the azimuthal quantum number m. For the solution function $P_{l,m}(\theta)$:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP_{l,m}(\theta)}{d\theta}\right) - \frac{m^2}{\sin^2\theta}P_{l,m}(\theta) = l(l+1)P_{l,m}(\theta) \quad (13)$$

- Note that the orbital equation does not depend on the azimuthal coordinate ϕ, however, it does depend on the azimuthal quantum number m.

- As a consequence, there is a different solution of the orbital equation for different value of m.

- The integer number $l \leq |m|$ is called the orbital quantum number.

Spherical harmonics

- The functions

$$Y_{l,m}(\theta, \phi) = P_{l,m}(\theta, \phi)\Phi_m(\phi) \qquad (14)$$

  are called spherical harmonics.

- These are functions of the polar (θ) and azimuthal (ϕ) angles in spherical coordinates which correspond to the solution of the orbital and azimuthal part of the Schrödinger equation.

- A spherical harmonic $Y_{l,m}(\theta, \phi)$ corresponds to an orbital motion with squared angular momentum $L^2 = l(l+1)\hbar^2$ and the projection of the angular momentum on the quantization axis of $L_z = m\hbar$.

- In a hydrogen atom as well as in a nucleus spherical harmonics define angular shapes of the orbitals for single particle motion with quantum numbers corresponding to their order.

Spherical harmonics

Single Harmonics

$$\cos(m\phi)\ P_\ell^m(\cos\theta)$$

$\ell = 0$

$\ell = 1$

$\ell = 2$

$\ell = 3$

$\ell = 10$
$m = 5$
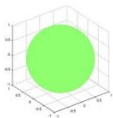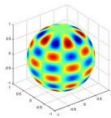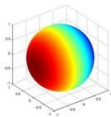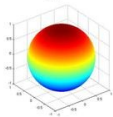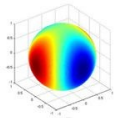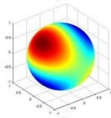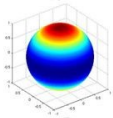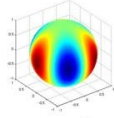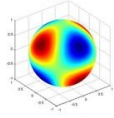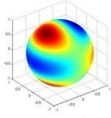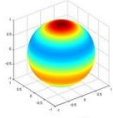
$m = 0$ $m = 1$ $m = 2$ $m = 3$

The radial equation

- The last step in solving Eq. 9 is to separate the radial equation which depends only on the variable r and the value of the orbital angular momentum quantum number l. For the solution function $R_{n,l}(r)$

$$\frac{d}{dr}\left(r^2\frac{dR_{n,l}(r)}{dr}\right) + \frac{2mr^2}{\hbar^2}(E - V(r))R_{n,l}(r) = l(l+1)R_{n,l}(r) \quad (15)$$

- Note, that the radial equation depends on the energy E and on the potential $V(r)$ which is not the case for the orbital and azimuthal equations.

- Note also that the radial equation depends only on the variable r but not on θ and ϕ. However, it does depend on the angular momentum quantum number l. This means that there are different solutions for different value of l.

- Also note that the radial equation does not depend on the azimuthal quantum number m.

The role of the potential

- The radial equation depends on the potential $V(r)$.

- In particular, if the Coulomb potential for and interaction between a proton and an electron is used

$$V(r) = -\frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r} \tag{16}$$

  the solutions describe the hydrogen atom and define the atomic shell model.

- If the nuclear potential is used the solutions describe nuclei and define the nuclear shell model.

- Note that in both cases the orbital part which depends on angles θ and ϕ is the same, given by spherical harmonics $Y_{l,m}(\theta, \phi)$.
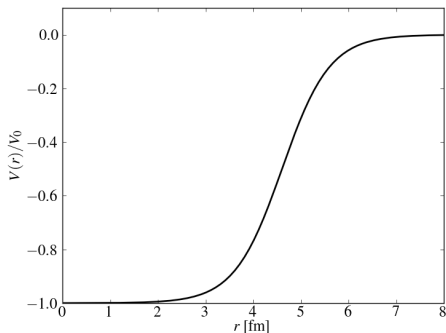
The nuclear potential

- So far everything is fine, except for the fact that we did not discuss what the nuclear potential is and where does it come from.

- This is an important point since the nuclear case is different than the atomic one.

- We are going to address this point at the start of the next lecture. For now let us assume a potential which is attractive and proportional to nuclear density distribution.

- Often used is potential proportional to the Fermi function called the Wood-Saxon potential.

- Another frequent choice is a harmonic oscillator potential (note, however, that harmonic oscillator describes an infinitely deep potential which is not the case for nuclei.)

The Wood-Saxon potential

$$V(r) = -V_0 \frac{1}{1+\exp\left(\frac{r-R}{a}\right)}$$

$$V_0 \approx 50 \text{ [MeV]} \quad R = 1.1 \times A^{\frac{1}{3}} \text{ [fm]} \quad a = 0.5 \text{ [fm]} \tag{17}$$

Solutions for the nuclear potential

- Bound ($E < 0$) solutions of the Schrödinger equation with the nuclear potential are quantized.

- The energies are defined by the principle quantum number n and the orbital quantum number l.

- The energies do not depend on the azimuthal quantum number m.

- The energies are bunched into shells: the regions of high number of states (shells) are separated by regions withouth states (shell gaps).

- The wavefunctions are given by the product of the radial wave function and a spherical harmonics

$$\psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r) Y_{l,m}(\theta, \phi) \tag{18}$$