**PHY 741 Quantum Mechanics**
**12-12:50 PM MWF Olin 103**

**Plan for Lecture 10:**
**Review Chapters #5 & 7 in Shankar;**
**Eigenstates of the one-dimensional Schrödinger equation**

1. **Charged particle in an electrostatic field**
2. **Brief introduction to numerical methods in the context of the one-dimensional Schrödinger equation.**



## Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

| | Date | F&W Reading | Topic | Assignment | Due |
|---|---|---|---|---|---|
| 1 | Mon, 8/28/2017 | Chap. 1 | Review of basic principles | #1 | 9/6/2017 |
| 2 | Wed, 8/30/2017 | Chap. 1 | Linear vector spaces | #2 | 9/6/2017 |
| 3 | Fri, 9/01/2017 | Chap. 1 | Linear vector spaces | #3 | 9/6/2017 |
| 4 | Mon, 9/04/2017 | Chap. 4 | Principles of Quantum Mechanics | #4 | 9/8/2017 |
| 5 | Wed, 9/06/2017 | Chap. 5 | Examples in 1 dimension | | |
| 6 | Fri, 9/08/2017 | Chap. 5 | Schrödinger equation in one-dimension | #5 | 9/13/201 |
| 7 | Mon, 9/11/2017 | Chap. 5 | Schrödinger equation in one-dimension | | |
| 8 | Wed, 9/13/2017 | Chap. 7 | Schrödinger equation in one-dimension | #6 | 9/15/201 |
| 9 | Fri, 9/15/2017 | Chap. 7 | Schrödinger equation in one-dimension | #7 | 9/20/201 |
| 10 | Mon, 9/18/2017 | Chap. 5 and 7 | Schrödinger equation in one-dimension | | |
| 11 | Wed, 9/20/2017 | | | | |
| 12 | Fri, 9/22/2017 | | | | |
| 13 | Mon, 9/25/2017 | | | | |
| 14 | Wed, 9/27/2017 | | | | |
| 15 | Fri, 9/29/2017 | | | | |
| | Mon, 10/02/2017 | | *Take-home exam -- No class* | | |
| | Wed, 10/04/2017 | | *Take-home exam -- No class* | | |

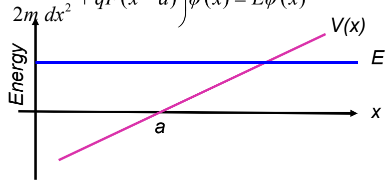


Energy eigenstates of the Schrödinger equation for one-dimensional systems

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

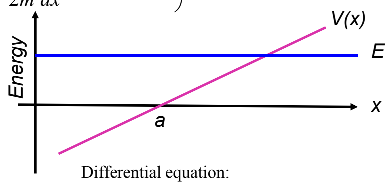
Suppose that the potential is due to an electrostatic field $F$ and the particle has charge $q$ such that $V(x)=qF(x-a)$:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+qF(x-a)\right)\psi(x)=E\psi(x)$$



One dimensional Schrödinger equation for charged particle in an electrostatic field – continued:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + qF(x-a)\right)\psi(x) = E\psi(x)$$




Differential equation:

$$\left(\frac{d^2}{dx^2} - \frac{2mqF}{\hbar^2}(x-b)\right)\psi(x) = 0 \quad \text{where } b \equiv a + \frac{E}{qF}$$

$$\left(\frac{d^2}{du^2} - \alpha u\right)\psi(u) = 0 \quad \text{where } u \equiv x - b \quad \alpha \equiv \frac{2mqF}{\hbar^2}$$

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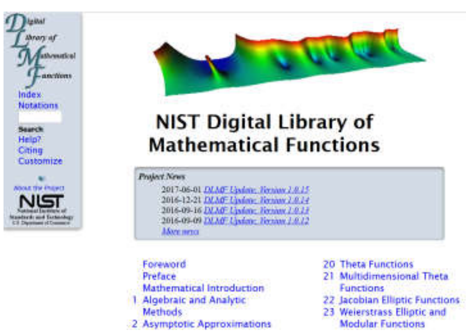
Digression – library of solutions to differential equations
http://dlmf.nist.gov/

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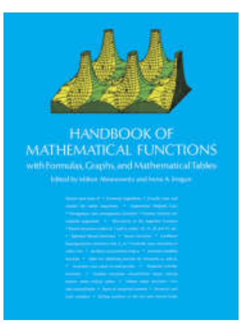


http://store.doverpublications.com/0486612724.html

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## §9.2(i) Airy's Equation

9.2.1 $$\frac{d^2w}{dz^2} = zw.$$

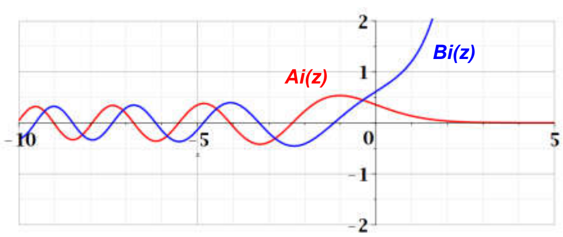
All solutions are entire functions of $z$.

Standard solutions are:

9.2.2 $$w = \mathrm{Ai}(z),\ \mathrm{Bi}(z),\ \mathrm{Ai}(z e^{\mp 2\pi i/3}).$$



$$\frac{d^2w}{dz^2} = zw$$






Differential equation:

$$\left(\frac{d^2}{dx^2} - \frac{2mqF}{\hbar^2}(x-b)\right)\psi(x) = 0 \qquad \text{where } b \equiv a + \frac{E}{qF}$$

$$\left(\frac{d^2}{du^2} - \alpha u\right)\psi(u) = 0 \qquad \text{where } u \equiv x-b \qquad \alpha \equiv \frac{2mqF}{\hbar^2}$$

Airy's equation

$$\left(\frac{d^2}{dz^2} - z\right)Ai(z) = 0$$

Note that the Schroedinger equation can be multiplied by a constant:

$$C\left(\frac{d^2}{du^2} - \alpha u\right)\psi(u) = 0$$

Changing variables: $z = C\alpha u$

$$C\frac{d^2}{du^2} = C^3\alpha^2\frac{d^2}{dz^2} \quad \Rightarrow C = \alpha^{-2/3} \quad \Rightarrow z = \alpha^{1/3}u$$

$$\Rightarrow \psi(u) = \mathcal{N}Ai(\alpha^{1/3}u)$$

normalization constant

Some properties of Airy functions –

Integral form:

$$\mathrm{Ai}(x) = \frac{1}{\pi}\int_0^\infty \cos\left(\tfrac{1}{3}t^3 + xt\right)\,dt.$$

Behavior as $z \to \infty$

$$Ai(z) \approx \frac{1}{2\sqrt{\pi}z^{1/4}} e^{-\frac{2}{3}z^{3/2}}$$

Behavior as $-z \to \infty$

$$Ai(-z) \approx \frac{1}{\sqrt{\pi}z^{1/4}} \sin\left(\frac{2}{3}z^{3/2} + \frac{\pi}{4}\right)$$

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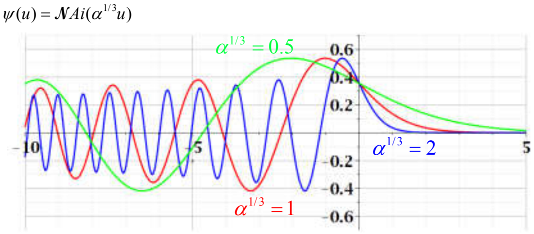
Summary of results

Differential equation:

$$\left(\frac{d^2}{dx^2} - \frac{2mqF}{\hbar^2}(x-b)\right)\psi(x) = 0 \qquad \text{where } b \equiv a + \frac{E}{qF}$$

$$\left(\frac{d^2}{du^2} - \alpha u\right)\psi(u) = 0 \qquad \text{where } u \equiv x - b \qquad \alpha \equiv \frac{2mqF}{\hbar^2}$$

$$\psi(u) = \mathcal{N} Ai(\alpha^{1/3}u)$$

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Introduction to numerical methods of solving the one-dimensional Schrödinger equation

Consider the following one-dimensional Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi_n(x) = E_n\psi_n(x), \qquad (1)$$

where $V(x)$ is a given potential function, and $E_n$ is the energy eigenvalue associated with the eigenfunction $\psi_n(x)$. This can either represent a bound state or a continuum state. One basic approach to developing accurate numerical approximations to the solution of these equations is to use a Taylor's series expansion to relate the behavior of $\frac{d^2\psi_n(x)}{dx^2}$ to $\psi_n(x')$ for points $x'$ in the neighborhood of $x$. Note that for any small distance $s$,

$$\psi_n(x \pm s) = \psi_n(x) \pm s\frac{d\psi_n(x)}{dx} + \frac{s^2}{2!}\frac{d^2\psi_n(x)}{dx^2} \pm \frac{s^3}{3!}\frac{d^3\psi_n(x)}{dx^3} + \frac{s^4}{4!}\frac{d^4\psi_n(x)}{dx^4}\ldots \qquad (2)$$

This means that if $s$ is small, we can approximate the second derivative according to

$$\frac{d^2\psi_n(x)}{dx^2} \approx \frac{\psi_n(x+s) + \psi_n(x-s) - 2\psi_n(x)}{s^2} + O(s^4). \qquad (3)$$

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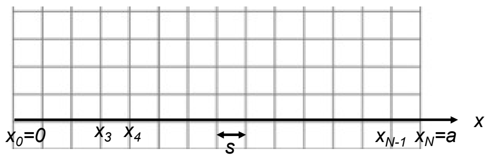
Introduction to numerical methods of solving the one-dimensional Schrödinger equation -- continued

$$\left(\frac{d^2}{dx^2}-\frac{2m}{\hbar^2}V(x)\right)\psi_n(x)=-\frac{2m}{\hbar^2}E_n\psi_n(x)$$

Simplified example: $V(x)=0$

$$\psi_n(x=0)=\psi_n(x=a)=0$$




Discretize $x$ into $N$ segments $s$, with $s=a/N$.



Introduction to numerical methods of solving the one-dimensional Schrödinger equation -- continued

$$\frac{d^2\psi_n(x)}{dx^2}\approx\frac{\psi_n(x+s)+\psi_n(x-s)-2\psi_n(x)}{s^2}+O(s^4).$$

For $x$ values on the grid points $x_i$, this means that

$$\frac{d^2\psi_n(x_i)}{dx^2}\approx\frac{1}{s^2}\left(\psi_n(x_{i+1})+\psi_n(x_{i-1})-2\psi_n(x_i)\right)\quad\text{for } i=1,2,...N-1$$

From the Schroedinger equation, we also know that

$$\frac{d^2\psi_n(x_i)}{dx^2}=\frac{2m}{\hbar^2}\left(V(x_i)-E_n\right)\psi_n(x_i)$$

For the simplified example,

we thus have a set of $N-1$ linear equations of the form:

$$\psi_n(x_{i+1})+\psi_n(x_{i-1})-2\psi_n(x_i)=-\lambda_n\psi_n(x_i)\qquad\text{where } \lambda_n=\frac{2ms^2E_n}{\hbar^2}$$



In this way, our numerical solution is cast in terms of an eigenvalue problem where the *N-1* unknown eigenvector components are $\psi_n(x_i)$

$$\begin{pmatrix}2 & -1 & 0 & \cdots & 0\\ -1 & 2 & -1 & \cdots & 0\\ 0 & -1 & 2 & \cdots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & \cdots & 2\end{pmatrix}\begin{pmatrix}\psi_n(x_1)\\ \psi_n(x_2)\\ \psi_n(x_3)\\ \vdots\\ \psi_n(x_{N-1})\end{pmatrix}=\lambda_n\begin{pmatrix}\psi_n(x_1)\\ \psi_n(x_2)\\ \psi_n(x_3)\\ \vdots\\ \psi_n(x_{N-1})\end{pmatrix}$$

Exact solution for this example:

$$\psi_n(x)=C\sin\left(\frac{n\pi x}{a}\right)\qquad E_n=\frac{\hbar^2}{2ma^2}n^2\pi^2$$

Note that for $N$ grid spacings, $\lambda_n=\frac{n^2\pi^2}{N^2}$

Example for *N=7:*

| n | λ | λ/s² | $E_v$ |
|---|---|---|---|
| 1 | 0.1980622645 | 9.7050509605 | 9.869604401 |
| 2 | 0.7530203960 | 36.897999404 | 39.47841760 |
| 3 | 1.554958132 | 76.192948468 | 88.82643960 |
| 4 | 2.445041868 | 119.80705153 | 157.9136704 |
| 5 | 3.246979605 | 159.10200064 | 246.7401100 |
| 6 | 3.801937736 | 186.29494906 | 355.3057584 |



Convergence of results with respect to *N*

Numerical results from second-order approximation:

| | N=4 | N=8 | Exact |
|---|---|---|---|
| n=1 | 9.54915028 | 9.7697954 | 9.869604404 |
| n=2 | 34.54915031 | 37.9008002 | 39.47841762 |

Numerical results from Numerov approximation:

| | N=4 | Exact |
|---|---|---|
| n=1 | 9.863097625 | 9.869604404 |
| n=2 | 39.04581620 | 39.47841762 |



More accurate algorithm – Numerov scheme

Recall the Taylor's expansion

$$\psi_n(x \pm s) = \psi_n(x) \pm s\frac{d\psi_n(x)}{dx} + \frac{s^2}{2!}\frac{d^2\psi_n(x)}{dx^2} \pm \frac{s^3}{3!}\frac{d^3\psi_n(x)}{dx^3} + \frac{s^4}{4!}\frac{d^4\psi_n(x)}{dx^4} \ldots$$

Recall that: $\frac{d^2\psi_n(x)}{dx^2} \approx \frac{\psi_n(x+s) + \psi_n(x-s) - 2\psi_n(x)}{s^2} + O(s^4).$

The Numerov scheme approximates the 4th derivative:

$$\frac{d^4\psi_n(x)}{dx^4} = \frac{d^2\psi''_n(x)}{dx^2} \approx \frac{\psi''_n(x+s) + \psi''_n(x-s) - 2\psi''_n(x)}{s^2} + O(s^6).$$

We also know that each second derivative is constrained by the Schroedinger equation:

$$\frac{d^2\psi_n(x_i)}{dx^2} = \frac{2m}{\hbar^2}\left(V(x_i) - E_n\right)\psi_n(x_i)$$