PHY 742 Quantum Mechanics II
1-1:50 AM MWF Olin 103

Plan for Lecture 9

Single particle states of molecules and solids

1. **Part of this material is mentioned in Chapters 2 and 6 of Professor Carlson's textbook**
   a. **Comparison of the eigenstate analysis of a single well potential, a double well, and of a periodic array of wells.**
   b. **Comparison of the eigenstate analysis of a H atom and an H_2^+ molecular ion – next time**

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Topics for Quantum Mechanics II

Single particle analysis
- Single particle interacting with electromagnetic fields – EC Chap. 9
- Scattering of a particle from a spherical potential – EC Chap. 14
- More time independent perturbation methods – EC Chap. 12, 13
- Single electron states of a multi-well potential ➔ molecules and solids – EC Chap. 2,6
- Time dependent perturbation methods – EC Chap. 15
- Path integral formalism (Feynman) – EC Chap. 11.C
- Relativistic effects and the Dirac Equation – EC Chap. 16

Multiple particle analysis
- Quantization of the electromagnetic fields – EC Chap. 17
- Photons and atoms – EC Chap. 18
- Multi particle systems; Bose and Fermi particles – EC Chap. 10
- Multi electron atoms and materials
  - Hartree-Fock approximation
  - Density functional approximation

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Course schedule for Spring 2020

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	Reading	Topic	HW	Due date
1	Mon: 01/13/2020	Chap. 9	Quantum mechanics of electromagnetic forces	#1	01/22/2020
2	Wed: 01/15/2020	Chap. 9	Quantum mechanics of particle in electrostatic field	#2	01/24/2020
3	Fri: 01/17/2020	Chap. 9	Quantum mechanics of particle in magnetostatic field	#3	01/27/2020
	Mon: 01/20/2020	No class	Martin Luther King Holiday		
4	Wed: 01/22/2020	Chap. 14	Scattering theory	#4	01/29/2020
5	Fri: 01/24/2020	Chap. 14	Scattering theory	#5	01/31/2020
6	Mon: 01/27/2020	Chap. 14	Scattering theory	#6	02/03/2020
7	Wed: 01/29/2020	Chap. 12	Variational methods	#7	02/05/2020
8	Fri: 01/31/2020	Chap. 12	Variational and other approximation methods	#8	02/07/2020
9	Mon: 02/03/2020	Chap. 2,6	Single particle states of molecules and solids	#9	02/10/2020
10	Wed: 02/05/2020				
11	Fri: 02/07/2020				
12	Mon: 02/10/2020				
13	Wed: 02/12/2020				
14	Fri: 02/14/2020				

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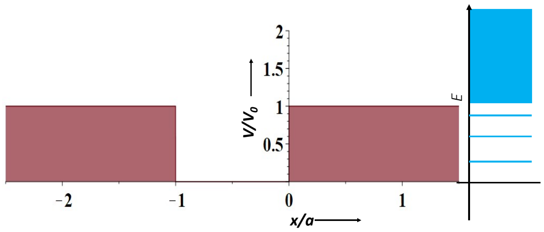
Examples of eigenstate analyses of the time independent Schrödinger equation for a single particle in a potential

Consider a single potential well

Spectrum



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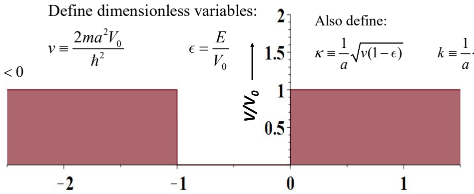
Some details

Define dimensionless variables:

$$V(x)=\begin{cases} V_0 & x<-a \\ 0 & -a<x<0 \\ V_0 & x>0 \end{cases} \qquad v \equiv \frac{2ma^2V_0}{\hbar^2} \qquad \epsilon = \frac{E}{V_0}$$

Also define:

$$\kappa \equiv \frac{1}{a}\sqrt{v(1-\epsilon)} \qquad k \equiv \frac{1}{a}\sqrt{v\epsilon}$$



For $x<-a$

$$\Psi(x) = Ae^{-\kappa(-a-x)}$$

For $-a<x<0$

$$\Psi(x) = B\begin{cases}\cos(k(x+\frac{a}{2})) \\ \sin(k(x+\frac{a}{2}))\end{cases}$$

For $x>0$

$$\Psi(x) = \pm Ae^{-\kappa x}$$

Matching equation for + (cos) solution:

$$\tan\left(\frac{ka}{2}\right)=\frac{\kappa}{k} \qquad \tan\left(\frac{1}{2}\sqrt{v\epsilon}\right)=\sqrt{\frac{1-\epsilon}{\epsilon}}$$

Matching equation for − (sin) solution:

$$\cot\left(\frac{ka}{2}\right)=-\frac{\kappa}{k} \qquad \cot\left(\frac{1}{2}\sqrt{v\epsilon}\right)=-\sqrt{\frac{1-\epsilon}{\epsilon}}$$

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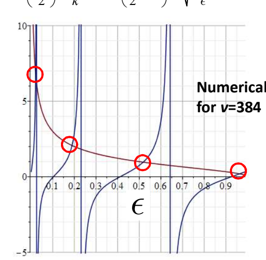
Matching equation for + (cos) solution:

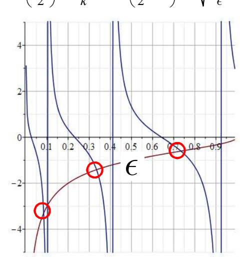
$$\tan\left(\frac{ka}{2}\right)=\frac{\kappa}{k} \qquad \tan\left(\frac{1}{2}\sqrt{v\epsilon}\right)=\sqrt{\frac{1-\epsilon}{\epsilon}}$$



Numerical results for *v*=384

Matching equation for − (sin) solution:

$$\cot\left(\frac{ka}{2}\right)=-\frac{\kappa}{k} \qquad \cot\left(\frac{1}{2}\sqrt{v\epsilon}\right)=-\sqrt{\frac{1-\epsilon}{\epsilon}}$$



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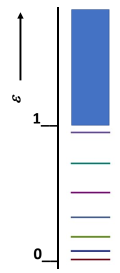
Summary of results for the case *v*=384



Maple syntax:

fsolve(tan(1/2*sqrt(384*EE)) = sqrt((1 - EE)/EE), EE = 0.95);
0.9634380037

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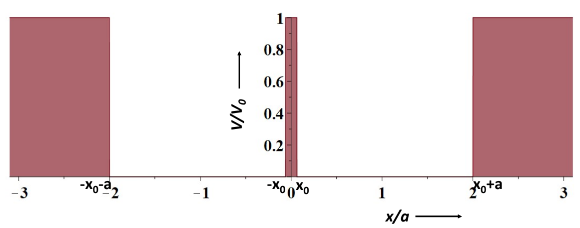
Example of a particle in a double well



even and odd solutions wrt x=0

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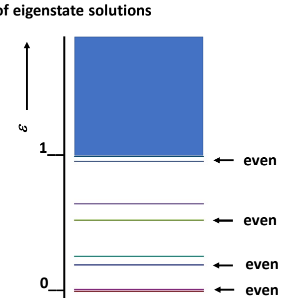
Form of eigenstate solutions



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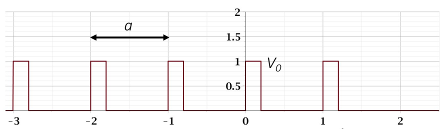
Another example of a one-dimensional system

Consider an electron moving in a one-dimensional model potential (Kronig and Penney, *Proc. Roy. Soc. (London)* **130,** 499 (1931)



Schroedinger equation for electron:

$$\left(-\frac{\hbar^2\nabla^2}{2m}+V(x)\right)\Psi(x)=E\Psi(x)$$

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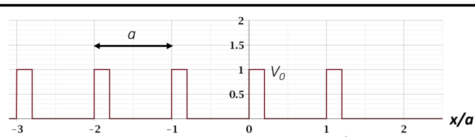

Effects of periodicity: $V(x)=V(x+na)$

$$\left(-\frac{\hbar^2\nabla^2}{2m}+V(x)\right)\Psi(x)=E\Psi(x)$$

$$\left(-\frac{\hbar^2\nabla^2}{2m}+V(x+na)\right)\Psi(x+na)=E\Psi(x+na)$$

$$\left(-\frac{\hbar^2\nabla^2}{2m}+V(x)\right)\Psi(x+na)=E\Psi(x+na)$$

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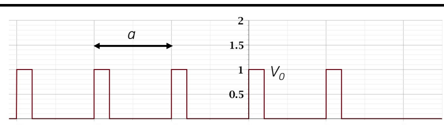

Since $\Psi(x+na)$ and $\Psi(x)$ are solutions of the same eigenvalue problem: $\Psi(x+na)=K\Psi(x)$

Assume $K=e^{i\theta}=e^{ikna}$

Bloch theorem: $\Psi_k(x+na)=e^{ikna}\Psi_k(x)$

$\Psi_k(x)=e^{ikx}u_k(x)$

where $u_k(x+na)=u_k(x)$

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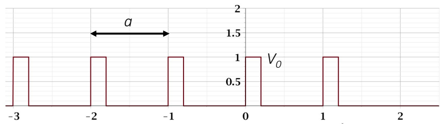
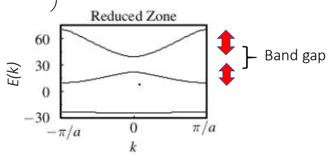


Eigenstates:

$$\left(-\frac{\hbar^2\nabla^2}{2m}+V(x)\right)\Psi_k(x)=E(k)\Psi_k(x)$$



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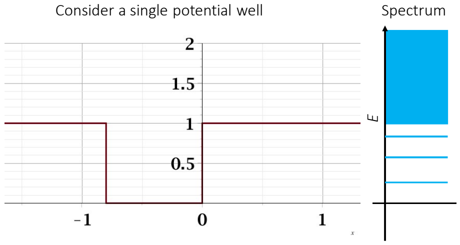
Consider a single potential well

Spectrum



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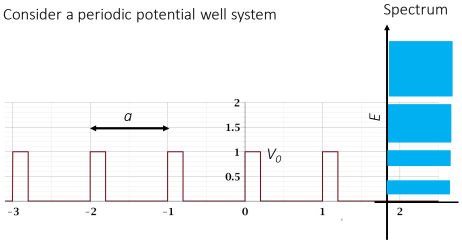
Consider a periodic potential well system

Spectrum



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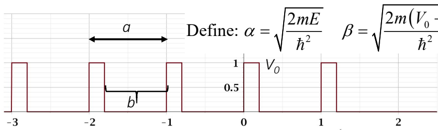

Define: $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$ $\quad \beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$

For $0 \le x \le (a-b)$ $\quad \Psi_1(x) = Ae^{\beta x} + Be^{-\beta x}$

For $(a-b) \le x \le a$ $\quad \Psi_2(x) = Ce^{i\alpha x} + De^{-i\alpha x}$

Continuity conditions: $\Psi_1(0) = \Psi_2(0)$ $\quad \frac{d\Psi_1(0)}{dx} = \frac{d\Psi_2(0)}{dx}$

$$\Psi_1(a-b) = \Psi_2(a-b) \qquad \frac{d\Psi_1(a-b)}{dx} = \frac{d\Psi_2(a-b)}{dx}$$

Also note: $\Psi(x+a) = e^{ika}\Psi(x)$

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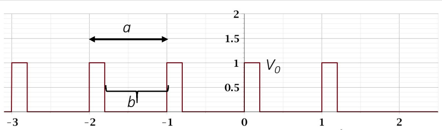

Matching conditions reduce to:

$$\cos(ka) = F(E)\cos\left(\alpha b - \Delta(E)\right)$$

$$F(E) \equiv \left(1 + \frac{V_0^2}{4E(E-V_0)}\sinh^2\left(\beta(a-b)\right)\right)^{1/2}$$

$$\tan\Delta(E) = \frac{V_0 - 2E}{2\sqrt{E(V_0 - E)}}\tanh\left(\beta(a-b)\right)$$

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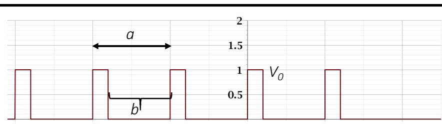

Details for $V_0 = \frac{\hbar^2}{2m}\frac{(2\pi)^2 49}{16b^2}$; $\quad b = \frac{16}{17}a$

Let $\quad f \equiv \frac{E}{V_0}$

$$\cos(ka) = \left(1 + \frac{\sinh^2\left(0.687\sqrt{1-f}\right)}{4f(1-f)}\right)^{1/2}\cos\left(11.7\sqrt{f} - \Delta(f)\right)$$

$$\tan\Delta(f) = \frac{1-2f}{2\sqrt{f(1-f)}}\tanh\left(0.687\sqrt{1-f}\right)$$

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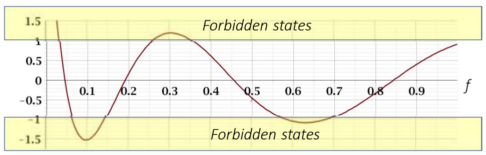
$$\cos(ka) = \left(1 + \frac{\sinh^2\left(0.687\sqrt{1-f}\right)}{4f(1-f)}\right)^{1/2} \cos\left(11.7\sqrt{f} - \Delta(f)\right) \equiv X(f)$$

$$\tan\Delta(f) = \frac{1-2f}{2\sqrt{f(1-f)}} \tanh\left(0.687\sqrt{1-f}\right)$$



$$X(f) = \left(1 + \frac{\sinh^2\left(0.687\sqrt{1-f}\right)}{4f(1-f)}\right)^{1/2} \cos\left(11.7\sqrt{f} - \Delta(f)\right)$$

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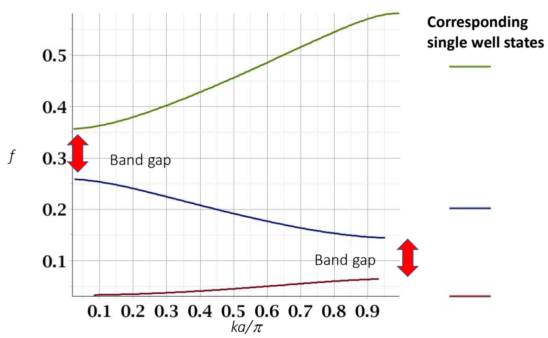

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