ECE 595, Section 10
Numerical Simulations
Lecture 10: Solving Quantum Wavefunctions

Prof. Peter Bermel

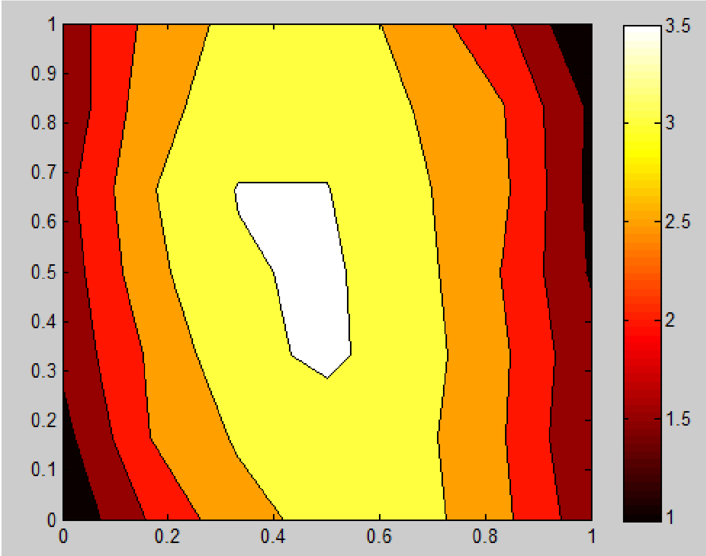
January 30, 2013

Outline

- Recap from Monday
- Schrodinger's equation
- Infinite & Finite Quantum Wells
- Kronig-Penney model
- Numerical solutions:
  - Real space
  - Fourier space

Recap from Monday

- Application Examples
  - Electrostatic potential (Poisson's equation)
    - 1D array of charge
    - 2D grid of charge
  - Arrays of interacting spins
    - 1D interaction along a chain
    - 2D nearest-neighbor coupling



Electrostatic potential in 2D (7x7 grid)

Schrodinger's Equation

- Wavefunction Ψ describes extent of particle
- Also eigenfunction of Schrodinger's equation:

$$\mathcal{H}\Psi = E\Psi$$

- Hamiltonian consists of kinetic and potential terms: $\mathcal{H} = T + V$
- Classically, $T = \frac{p^2}{2m}$; if $p = -i\hbar\nabla$, $T = -\frac{\hbar^2}{2m}\nabla^2$
- Probability of finding at *x* given by $|\Psi(x)|^2$

Free Particle

- A free particle has zero potential everywhere
- Schrodinger's equation becomes:

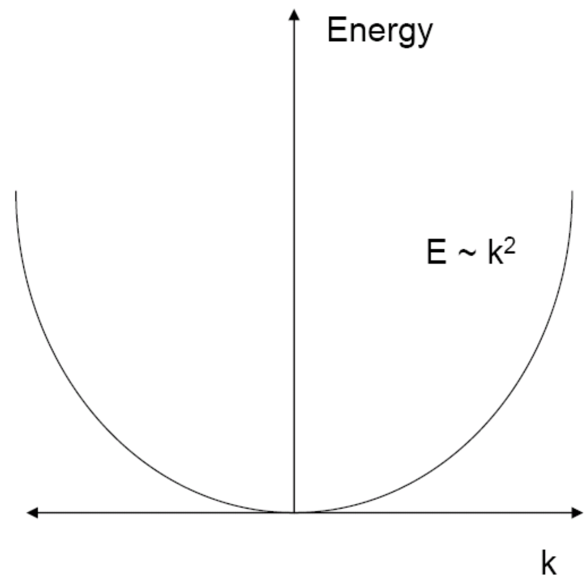
$$-\frac{\hbar^2}{2m}\nabla^2\Psi = E\Psi$$

- Eigenfunction can be obtained analytically:

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

- Energy eigenvalue thus given by:

$$E = \frac{\hbar^2 k^2}{2m}$$

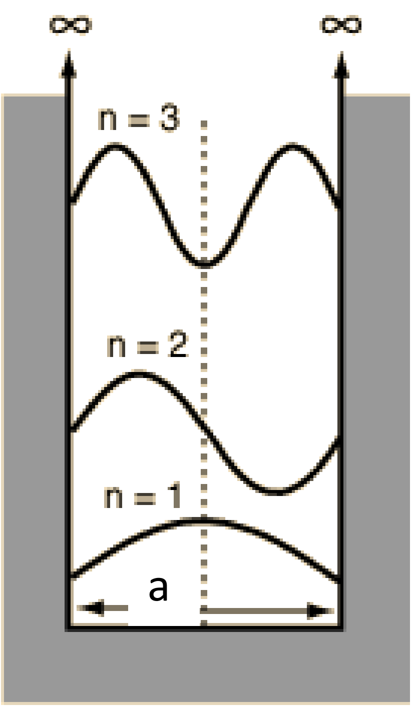


Infinite Quantum Well

- Example: proton in iron nucleus
- Potential $V(x) = \begin{cases} 0, & |x| < a/2 \\ \infty, & |x| \geq a/2 \end{cases}$
- Boundary condition:

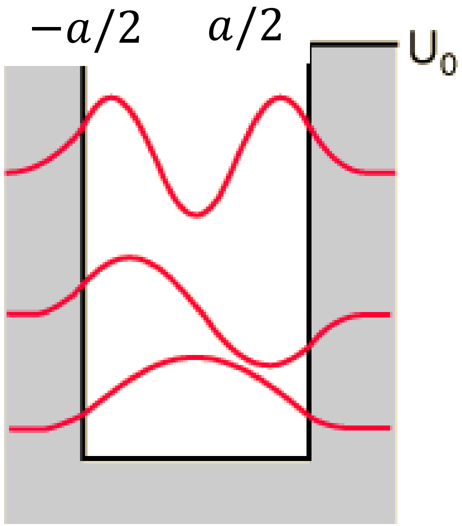
$$\Psi(\pm a/2) = 0$$

- Eigenfunctions are standing waves:
$$\Psi(x) = A\left[e^{ikx} + e^{-ikx}\right]$$
- By BC's, $k = \frac{n\pi}{a}$; $E = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$



Finite Quantum Well

- Example: α-particle in U-235 nucleus
- Potential $V(x) = \begin{cases} 0, & |x| < a/2 \\ U, & |x| \geq a/2 \end{cases}$
- Boundary conditions:
  $$\Psi[\pm(a+\epsilon)/2] = \Psi[\pm(a-\epsilon)/2]$$
  $$\Psi'[\pm(a+\epsilon)/2] = \Psi'[\pm(a-\epsilon)/2]$$
- Eigenfunctions inside box like before; outside region decays exponentially



Kronig-Penney Potential

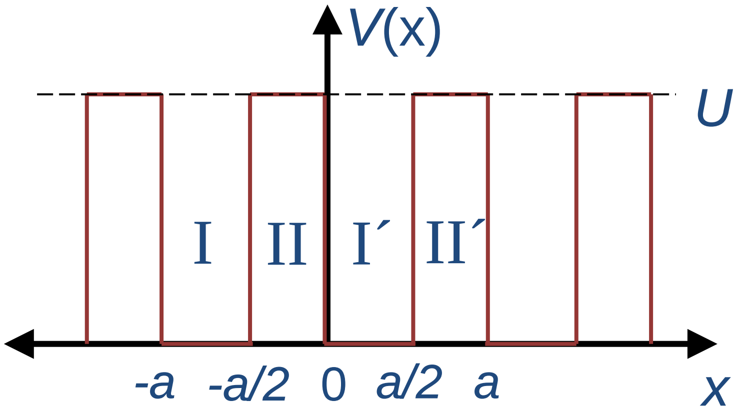
- Example: 1D atomic crystal
- Potential

$$V(x) = \begin{cases} 0, & 0 < x < a/2 \\ U, & a/2 < x < a \end{cases}$$

- And, $V(x + a) = V(x)$
- Boundary conditions:

$$\Psi(x + a) = \Psi(x)?$$

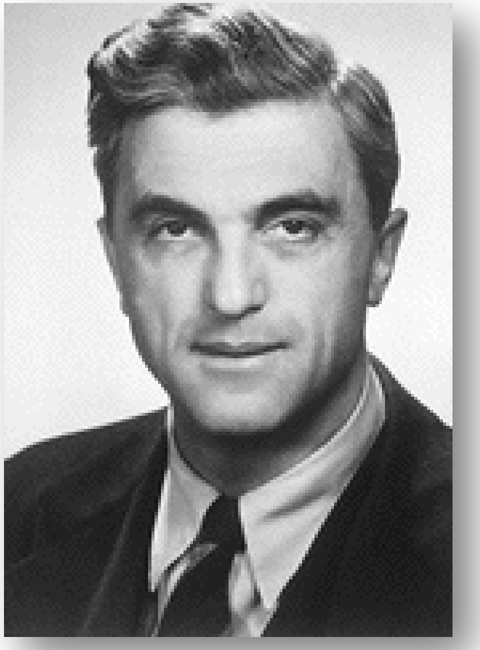
- Will each electron be stuck in its own little well?



Bloch Theorem

"When I started to think about it, I felt that the main problem was to explain how the electrons could sneak by all the ions in a metal …. By straight Fourier analysis, I found to my delight that the wave differed from the plane wave of free electron only by a periodic modulation."

--Felix Bloch, *Physics Today* (1976)



Bloch Theorem

- Asserts that solution in periodic potential is always a product of two terms:
  - a periodic function (with the same period)
  - a plane wave
- Mathematically, we can write:

$$\Psi(x) = Ae^{ikx}u(x)$$

where $u(x+a) = u(x)$

Bloch Theorem: Numerical Solution

- Use Bloch's theorem to solve the eigenproblem numerically

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\left[e^{ikx}u(x)\ \right] = E(k)e^{ikx}u(x)$$

- What basis to use for periodic function?

Bloch Theorem: Real-Space Basis

- Real space is most obvious, with uniform grid
- Pull out plane wave from eigenvector to reduce complexity:

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

- Immediate problem: not positive definite

Bloch Theorem: Real-Space Basis

```
>> N=10;A=-2*diag(ones(N,1))+diag(ones(N-1,1),1)+diag(ones(N-1,1),-1)+diag([zeros(N/2,1);ones(N/2,1)])

A =

    -2     1     0     0     0     0     0     0     0     0
     1    -2     1     0     0     0     0     0     0     0
     0     1    -2     1     0     0     0     0     0     0
     0     0     1    -2     1     0     0     0     0     0
     0     0     0     1    -2     1     0     0     0     0
     0     0     0     0     1    -1     1     0     0     0
     0     0     0     0     0     1    -1     1     0     0
     0     0     0     0     0     0     1    -1     1     0
     0     0     0     0     0     0     0     1    -1     1
     0     0     0     0     0     0     0     0     1    -1

>> [V,D]=eig(full(A)); V

V =

   -0.2494   -0.4205   -0.2483    0.4572    0.3603    0.4437    0.2943    0.2753    0.0345   -0.0043
    0.4440    0.5019    0.1766   -0.1349    0.0757    0.3504    0.3811    0.4711    0.0758   -0.0120
   -0.5410   -0.1785    0.1227   -0.4175   -0.3444   -0.1669    0.1992    0.5309    0.1317   -0.0291
    0.5189   -0.2888   -0.2639    0.2580   -0.1481   -0.4822   -0.1231    0.4374    0.2130   -0.0689
   -0.3828    0.5232    0.0650    0.3414    0.3132   -0.2140   -0.3587    0.2176    0.3356   -0.1625
    0.1625   -0.3356    0.2176   -0.3587    0.2140    0.3132   -0.3414   -0.0650    0.5232   -0.3828
   -0.0689    0.2130   -0.4374    0.1231   -0.4822    0.1481    0.2580   -0.2639    0.2888   -0.5189
    0.0291   -0.1317    0.5309    0.1992    0.1669   -0.3444    0.4175   -0.1227   -0.1785   -0.5410
   -0.0120    0.0758   -0.4711   -0.3811    0.3504   -0.0757   -0.1349    0.1766   -0.5019   -0.4440
    0.0043   -0.0345    0.2753    0.2943   -0.4437    0.3603   -0.4572    0.2483   -0.4205   -0.2494

>> diag(D)'

ans =

   -3.7801   -3.1935   -2.7113   -2.2950   -1.7898   -1.2102   -0.7050   -0.2887    0.1935    0.7801
```

Bloch Theorem: Fourier Space Basis

- If we write periodic function as Fourier series:

$$u(r) = \sum_G c_G e^{iGr}$$

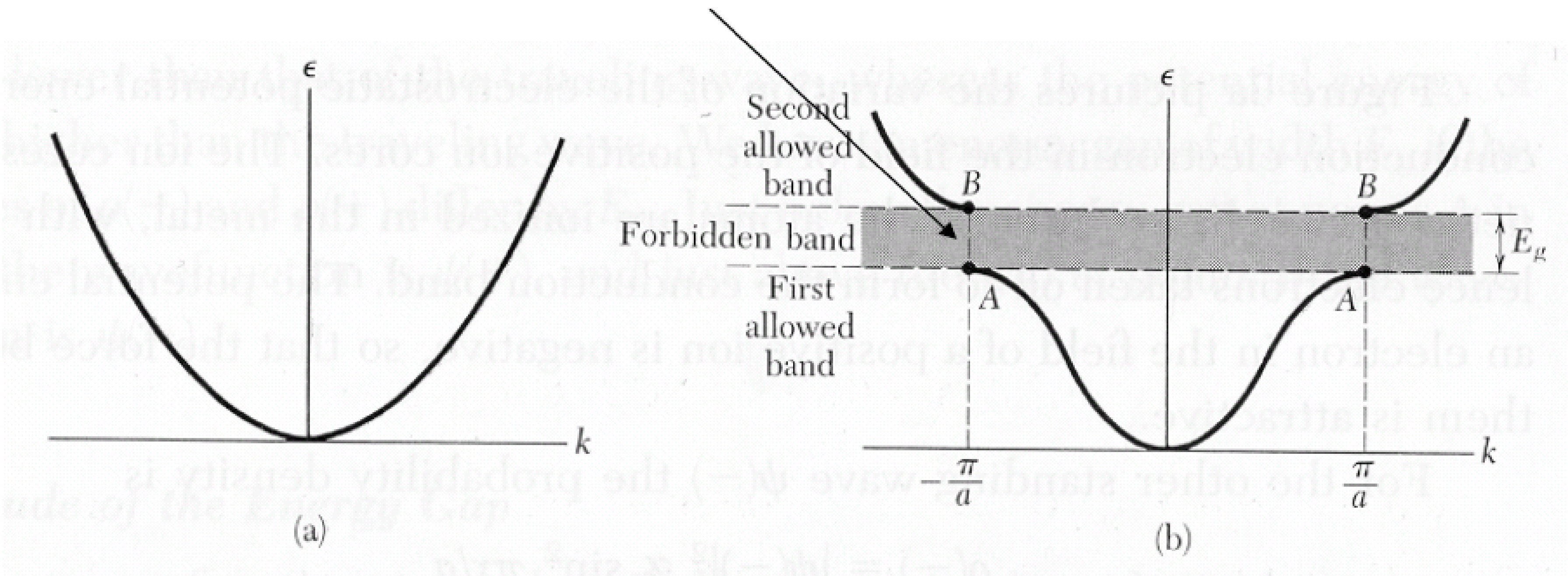
- We obtain the nice recursion relation:

$$V_{G'} c_{G-G'} = \left[E(k) - \frac{\hbar^2}{2m}(k+G)^2 \right] c_G$$

Bloch Theorem: Fourier Space Basis

```
>> N=11;k=0;G=2*pi*[-(N-1)/2:(N-1)/2];T=diag((k+G).^2)/100;ftV=fft([zeros((N-1)/2,1); 0.5; ones((N-1)/2,1)]);
>> V=diag(ones(N,1))*ftV(1)+diag(ones(N-1,1),1)*ftV(2)+diag(ones(N-2,1),2)*ftV(3)+diag(ones(N-3,1),3)*ftV(4);
>> V=V+diag(ones(N-1,1),-1)*ftV(N)+diag(ones(N-2,1),-2)*ftV(N-1)+diag(ones(N-3,1),-3)*ftV(N-2);
>> [psi,D]=eig(full(T+V)); psi(:,1:7)

ans =

  -0.0273 - 0.0066i   0.0337 - 0.0043i   0.0005 + 0.0134i  -0.1315 + 0.0147i  -0.2569 + 0.0670i   0.3022 - 0.1357i   0.0766 - 0.1116i
  -0.0278 - 0.0658i  -0.0077 - 0.0080i  -0.0830 + 0.1624i  -0.1667 - 0.3577i  -0.2441 - 0.3999i   0.2262 + 0.2727i   0.0824 - 0.0007i
   0.0144 - 0.0770i   0.1573 - 0.1405i  -0.4499 - 0.0550i   0.3569 - 0.3149i   0.1515 - 0.1548i   0.0388 - 0.0746i  -0.0507 + 0.0180i
  -0.0371 - 0.1784i   0.3876 + 0.2765i  -0.0883 - 0.4725i   0.0551 + 0.0557i  -0.2629 - 0.1100i   0.3074 + 0.0864i   0.2659 + 0.0144i
   0.2838 - 0.3985i  -0.2133 + 0.4133i   0.0711 - 0.0290i   0.0599 - 0.3008i   0.0188 - 0.0742i  -0.0203 - 0.3921i  -0.1258 - 0.4737i
   0.6517 + 0.0781i  -0.0096 - 0.1500i  -0.1585 - 0.1526i   0.0000 + 0.0007i  -0.3868 + 0.0496i   0.0115 + 0.0538i  -0.5020 + 0.2643i
   0.1817 + 0.4543i   0.2643 + 0.3827i  -0.0262 + 0.0722i  -0.0930 - 0.2923i   0.0369 + 0.0671i  -0.1421 - 0.3660i   0.3193 + 0.3718i
  -0.0781 + 0.1646i  -0.3491 + 0.3237i  -0.4755 - 0.0701i  -0.0485 + 0.0615i  -0.2267 + 0.1727i  -0.2450 + 0.2047i   0.1386 - 0.2273i
  -0.0041 + 0.0782i  -0.1739 - 0.1192i  -0.0722 - 0.4474i  -0.3897 - 0.2732i   0.1856 + 0.1116i  -0.0660 - 0.0521i  -0.0435 + 0.0316i
  -0.0426 + 0.0573i   0.0066 - 0.0089i   0.1591 - 0.0892i   0.1259 - 0.3741i  -0.1353 + 0.4485i  -0.0947 + 0.3414i   0.0473 - 0.0675i
  -0.0281            -0.0340             0.0134             0.1323            -0.2655            -0.3313             0.1354

>> mydiag=diag(D)'; mydiag(1:7)

ans =

    0.1996    1.1497    3.4376    5.6172    8.0651   10.5996   11.3658
```

Physical Observation



Free electron model

Nearly free electron model

From C. Kittel, *Introduction to Solid State Physics*

Next Class

- Is on Friday, Feb. 1
- Will discuss numerical tools for Fast Fourier Transforms
- Recommended reading: Numerical Recipes, Chapter 12