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

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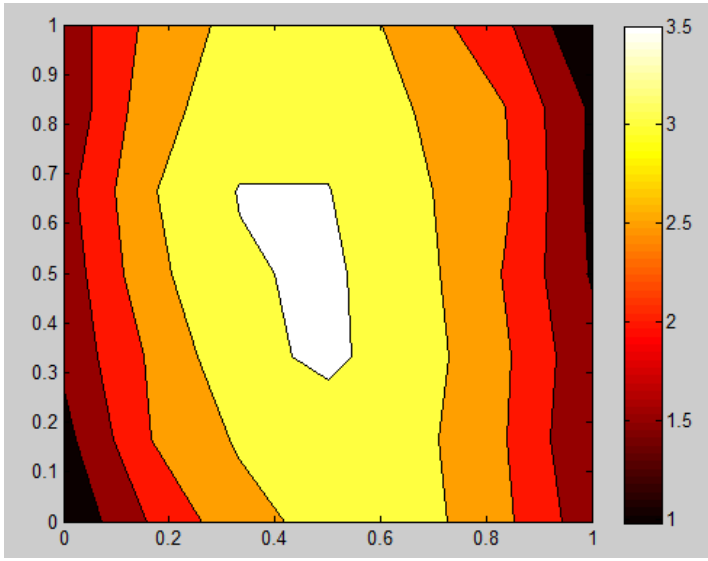
Outline

- 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:

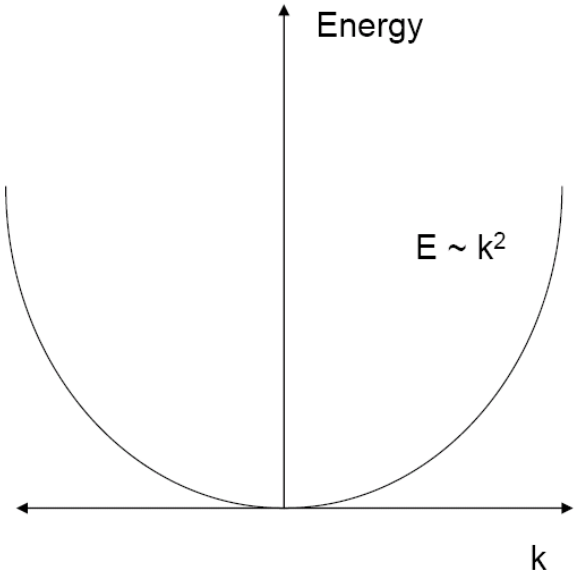
$$-\frac{\hbar^2}{2m}\nabla^2\Psi = E\Psi$$

- Eigenfunction can be obtained analytically:

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

- Energy eigenvalue thus given by:

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

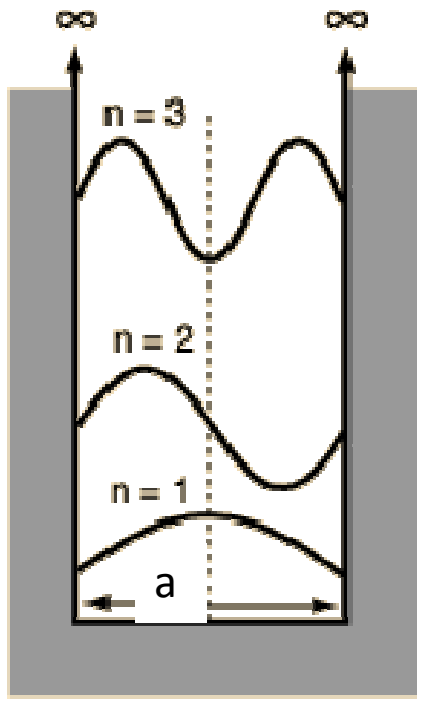


Infinite Quantum Well

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

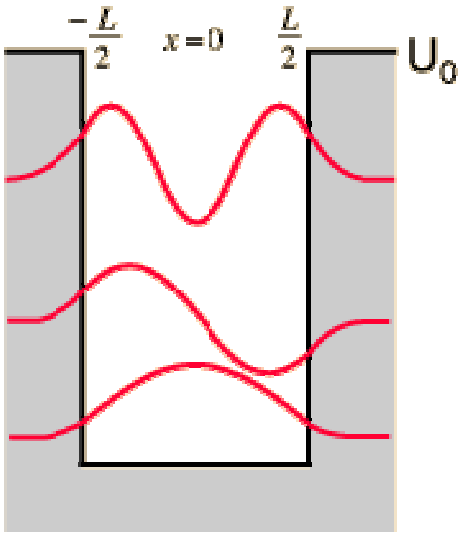


Finite Quantum Well

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

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

- Eigenfunctions inside box like before; outside region decays exponentially



Kronig-Penney Potential

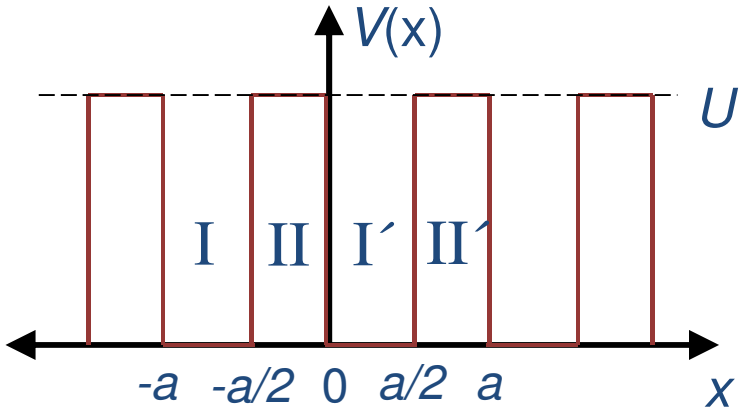
- Example: 1D atomic crystal
- Potential

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

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

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

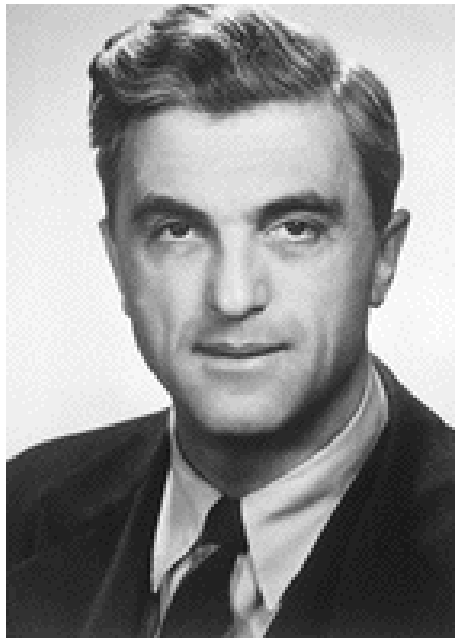
- Will each electron be stuck in its own little well?



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:

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

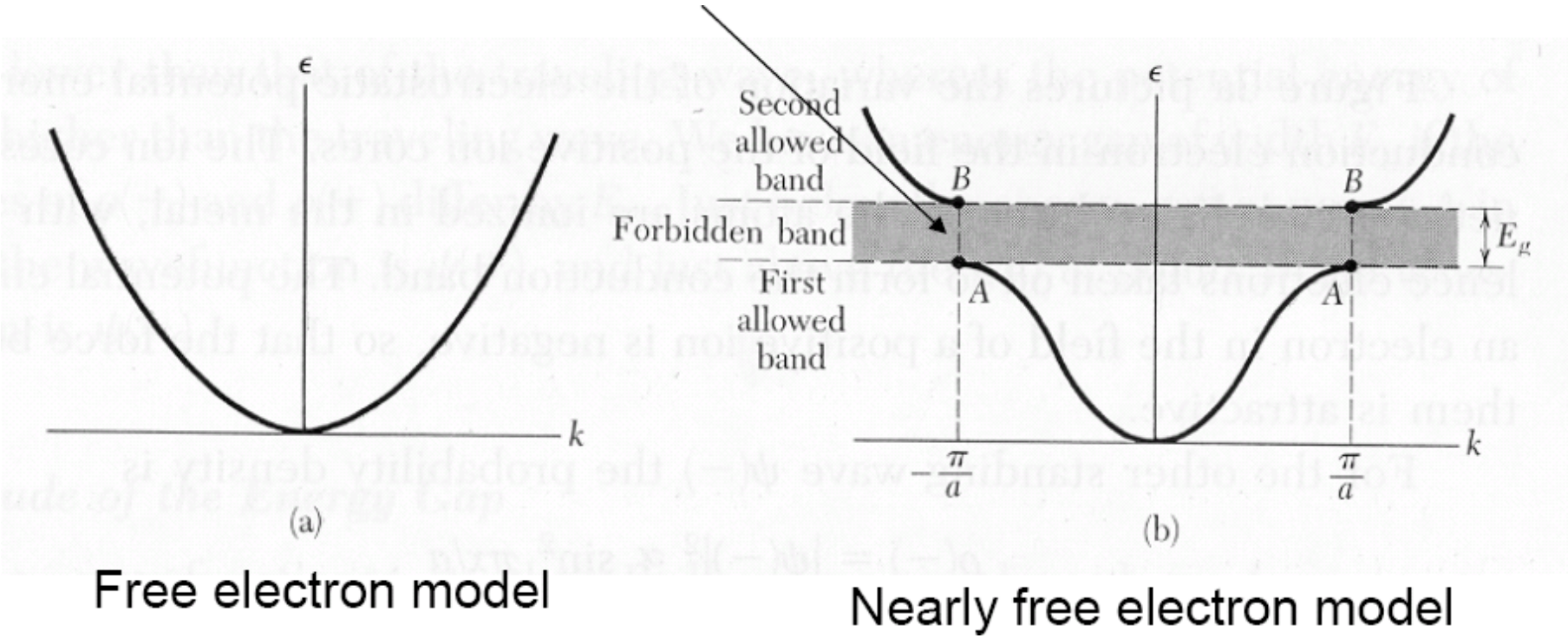
- We obtain the nice recursion relation:

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

Bloch Theorem: Fourier Space Basis

```
>> N=11;k=0;G=2*pi*[-(N-1)/2:(N-1)/2];T=diag((k+G).^2);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-1,1),-1)*ftV(N);
>> [V,D]=eig(full(T+V)); V=abs(V)

V =

    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0001    0.0098    0.0000    1.0000
    0.0000    0.0000    0.0000    0.0001    0.0001    0.0089    0.0089    0.0152    0.9998    0.0000    0.0098
    0.0000    0.0002    0.0002    0.0125    0.0125    0.7070    0.7069    0.0002    0.0126    0.0000    0.0001
    0.0019    0.0207    0.0207    0.7067    0.7067    0.0125    0.0125    0.0000    0.0001    0.0000    0.0000
    0.0863    0.7068    0.7015    0.0207    0.0208    0.0001    0.0001    0.0000    0.0000    0.0000    0.0000
    0.9925    0.0000    0.1220    0.0000    0.0009    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000
    0.0863    0.7068    0.7015    0.0207    0.0208    0.0001    0.0001    0.0000    0.0000    0.0000    0.0000
    0.0019    0.0207    0.0207    0.7067    0.7067    0.0125    0.0125    0.0001    0.0000    0.0000    0.0000
    0.0000    0.0002    0.0002    0.0125    0.0125    0.7069    0.7070    0.0126    0.0002    0.0001    0.0000
    0.0000    0.0000    0.0000    0.0001    0.0001    0.0089    0.0089    0.9998    0.0152    0.0098    0.0000
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0098    0.0001    1.0000    0.0000

>> abs(diag(D))'

ans =

    4.8954   44.8764   45.4808  163.4545  163.4546  360.8233  360.8233  637.1644  637.1644  992.4945  992.4945
```

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