PY410 / 505
Computational Physics 1

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Boundary-value and eigenvalue problems

- We've completed solutions to solve "unbounded" ODE's
- Now we turn to boundary-value problems and eigenvalue problems
- These are closely related (of course, they solve the same mathematical constructs)
- Key complication : the boundary values must be met, so "marching" methods like RK4 are not always the most accurate

"1d PDEs"

Boundary-value and eigenvalue problems

- Consider a second-order ODE :

$$\frac{d^2u}{dx^2} = f(x, u, u') , \qquad u'(x) = du/dx$$

- We specify values on two boundaries (left and right)

$$x_{lb} \leq x \leq x_{rb}$$

- We can have :
  – Dirichlet : specify u(x) on the boundaries
  – Neumann : specify u'(x) on the boundaries
  – Periodic : specify u(x_lb) = u(x_rb), u'(x_lb) = u'(x_rb)
  – Mixed are also possible

Boundary-value and eigenvalue problems

- Can also consider the eigenvalue problems :

$$\frac{d^2u}{dx^2} = f(x, u, u', \lambda) \ ,$$

- We've already encountered them earlier in the semester, too

- Will build upon the matrix methods we've already established!

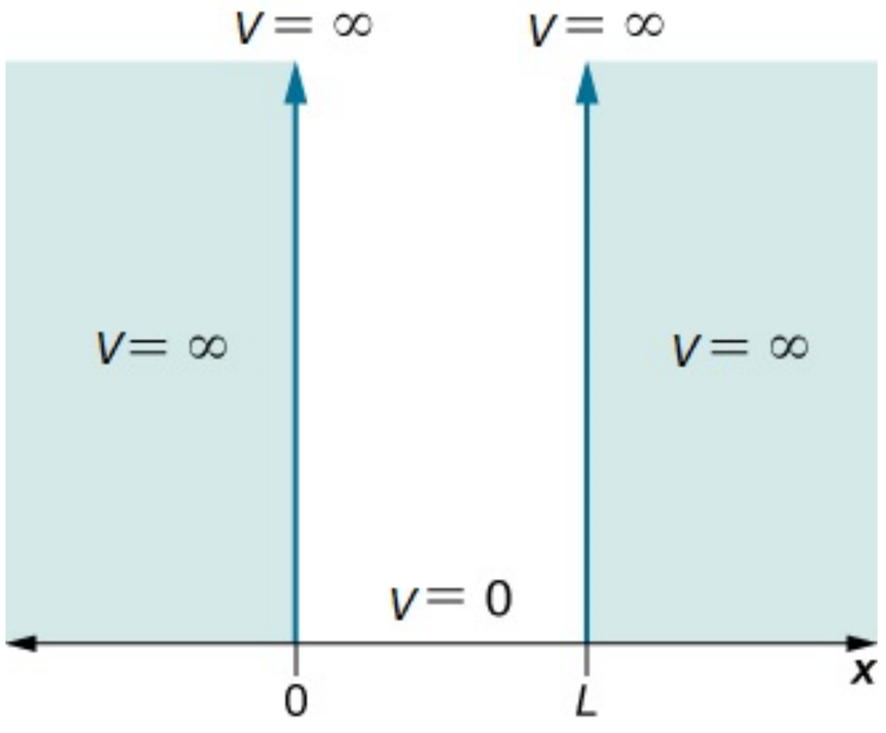
Boundary-value and eigenvalue problems

- Example : time-independent Schroedinger equation :

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

- Say V(x) is a potential well :

$$V(x) = 0 \quad |x| < L$$
$$= \infty \quad x \geq L$$



- We have Dirichlet boundary conditions : $\psi(0) = 0, \psi(L) = 0$

Boundary-value and eigenvalue problems

- Analytically, we have within the well :

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

- This is a free particle, so we guess

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

- Applying the boundary conditions we get

$$\begin{aligned}\psi(0) &= 0 = A + B \\ \psi(L) &= 0 = 2A\sin kL = 0 \\ k &= \frac{n\pi}{L}\end{aligned}$$

Boundary-value and eigenvalue problems

- Applying normalization :

$$
\begin{aligned}
1 &= \int_0^L dx \;\; 4A^2 \sin^2(\frac{n\pi}{L}x) \\
&= 4A^2 \left(\frac{x}{2} - \frac{\sin\left(\frac{n\pi}{L}x\right)}{4n\pi/L} \right)\Bigg|_0^L
\end{aligned}
$$

– So we get : $\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$

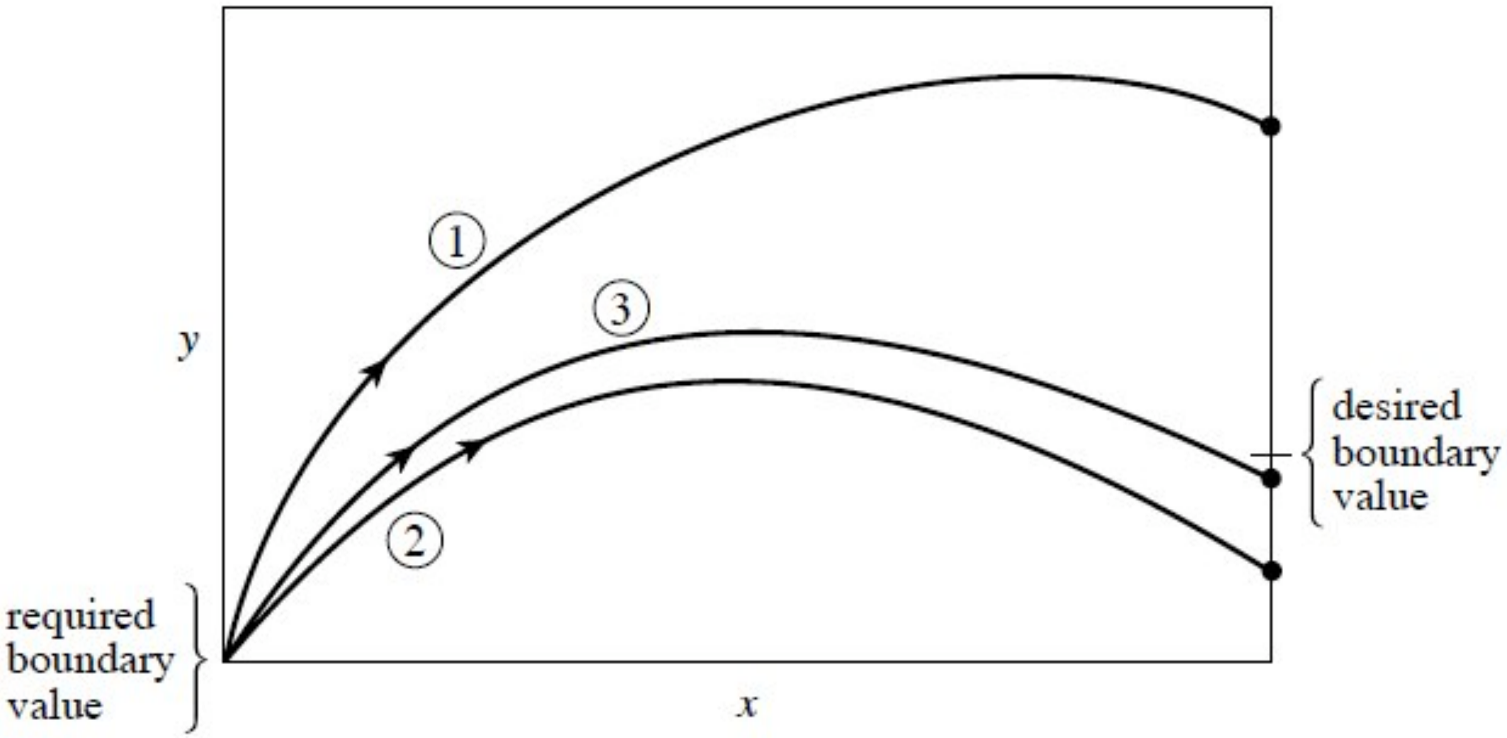
– Energy eigenvalues are $E = \hbar\omega = \dfrac{\hbar^2 k^2}{2m}$

Boundary-value and eigenvalue problems

- General strategy is to either "shoot" or "relax" :
- "Shoot" : pick values via a guess, "shoot" the ODE to the other side, and correct iteratively
- "Relax" : pick values via a guess, check points on the interior, and relax until the correction is small
- When in doubt of which to use, from NR : Be a gunslinger!
  - "Shoot first, then relax later"

Boundary-value and eigenvalue problems

- Iterative shooting procedure :
  - Guess unknown initial parameter
  - Generate trial solution with a “marching” algorithm
  - Compute difference at boundary
  - Iterate until difference i small
    - Use a root-finding metho



Boundary-value and eigenvalue problems

- Iterative shooting procedure :
  - Guess unknown initial parameter
  - Generate trial solution with a “marching” algorithm
  - Compute difference at boundary
  - Iterate until difference is small
    - Use a root-finding method!

Boundary-value and eigenvalue problems

- Iterative relaxation procedure :
  - Guess solution at all values of x AND the boundary
  - Compute the difference in the ODE

$$G(x) = \frac{d^2 u_g}{dx^2} - f\left(x, u_g, u'_g\right) \ ,$$

  - Iterate adjustments until G(x) tends to zero

Boundary-value and eigenvalue problems

- Specifically we use Jacobi's relaxation algorithm :
  - Discretize the space, compute second derivative:

$$h = \frac{1}{N}\ , \qquad x_i = ih\ , \qquad u_i \equiv u(x_i)\ , \qquad i = 1, \ldots, N-1$$

$$\left.\frac{d^2u}{dx^2}\right|_{x=x_i} = \frac{u_{i+1} + u_{i-1} - 2u_i}{h^2}\ , \qquad i = 1, \ldots, N-1$$

  - Compute difference:

$$G(x_i) \approx \frac{u_{g,i+1} + u_{g,i-1} - 2u_i}{h^2} - f\left(x_i, u_{g,i}, u'_{g,i}\right) \approx 0$$

  - Solve for the next guess :

$$u_i \approx \frac{1}{2}\left[u_{g,i+1} + u_{g,i-1} + h^2 f\left(x_i, u_{g,i}, u'_{g,i}\right)\right]$$

  - Like the Euler algorithm, Jacobi method will be the "workhorse" for many more advanced algorithms

Boundary-value and eigenvalue problems

- Specifically we use Jacobi's relaxation algorithm :
  - Discretize the space, compute second derivative:
  - Compute difference:
  - Solve for the next guess

Boundary-value and eigenvalue problems

- Examples:
  - bvpexample
  - qmbox

Boundary-value and eigenvalue problems

- For eigenvalue problems, we've already seen this once

- Recall : $$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} = -\frac{\pi^2}{4}(u+1)\ ,$$

  with u(0) = 0, u(1) = 1

- We discretized this :

$$\frac{2u_i - u_{i+1} - u_{i-1}}{h^2} = \frac{\pi^2}{4}(u_i + 1)\ , \qquad i = 1, \ldots, N-1$$

- And put this into the matrix form:

$$\mathbf{Mu} = \mathbf{b}\ ,$$

Boundary-value and eigenvalue problems

- We write M as a tridiagonal matrix :

$$\mathbf{M} = \begin{pmatrix} 2-c & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2-c & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2-c & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2-c & -1 \\ 0 & 0 & 0 & \cdots & -1 & 2-c \end{pmatrix},$$

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} u_0 + c \\ c \\ c \\ \vdots \\ c \\ u_N + c \end{pmatrix},$$

- You played with this in your homework, so we won't belabor the point, but realize that this is intricately tied!

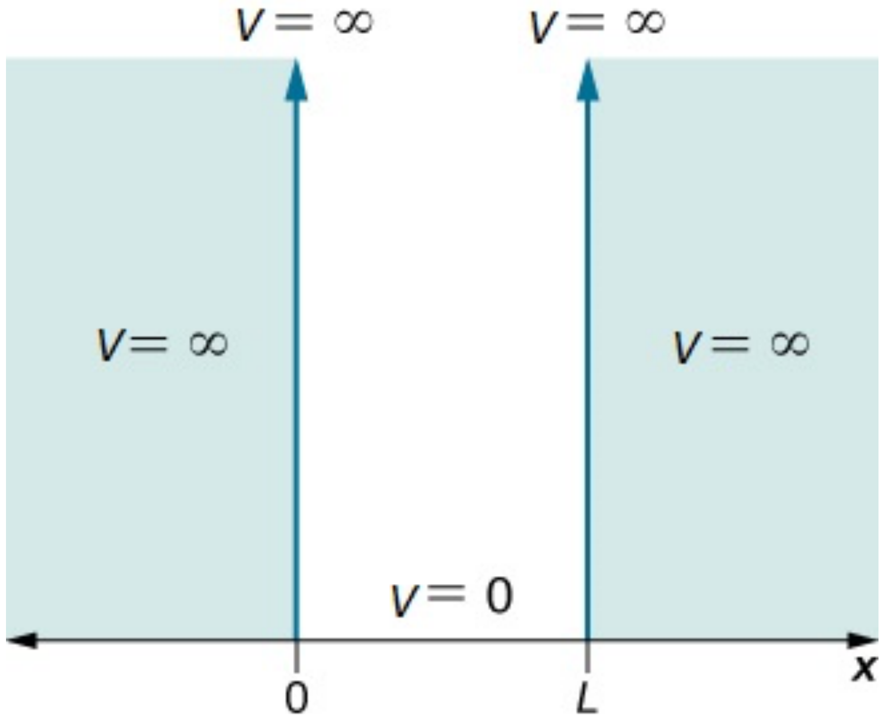
Boundary-value and eigenvalue problems

- Can also solve for eigenvalues by adjusting the parameters until the boundary conditions are met

- Example : particle in a box

- In this case we know psi(x=0) and psi(x=1) are both equal to zero

- So, adjust energy until this occurs!



Boundary-value and eigenvalue problems

- To continue our investigation of BVP and eigenvalue problems, consider

$$\frac{d^2u}{dx^2} + d(x)\frac{du}{dx} + q(x)u = s(x) \ ,$$

  - where d(x), q(x) and s(x) are given functions
- The s(x) term makes the equation inhomogeneous
- The Sturm-Liouville theory deals with linear homogeneous second order equations of the form

$$-\frac{d}{dx}\left[p(x)\frac{du}{dx}\right] + r(x)u(x) = \lambda w(x)u(x) \ ,$$

  - where p(x), r(x), w(x) are given, and lambda is a parameter, p(x) >0 and w(x) >0 in integration domain
- Need boundary conditions! Consider homogenous and linear BC's like :

$$c_1u(a) + c_2u'(a) = 0 \ , \qquad c_3u(b) + c_4u'(b) = 0 \ ,$$

Boundary-value and eigenvalue problems

- Strum and Liouville showed :
  - Non-trivial solutions exist only for eigenvalues lambda
  - If eigenvalues are arranged in increasing order, eigenfunctions have one additional node or zero per step

- Can solve these types of equations with the Numerov's Method
- If we have a second-order ODE without a first-order derivative term : $$\frac{d^2u}{dx^2} + q(x)u(x) = s(x) \ ,$$
- Then the symmetric three-point difference is :

$$\frac{u_{n+1} + u_{n-1} - 2u_n}{h^2} = u_n'' + \frac{h^2}{12}u_n'''' + \mathcal{O}(h^4) \ .$$

Boundary-value and eigenvalue problems

- With the differential equation, we can write :

$$u_n'''' = \frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(-q(x)u(x)+s(x)\right)\Big|_{x=x_n}$$
$$= -\frac{q_{n+1}u_{n+1}-2q_nu_n+q_{n-1}u_{n-1}}{h^2}+\frac{s_{n+1}-2s_n+s_{n-1}}{h^2}+\mathcal{O}(h^2)\ .$$

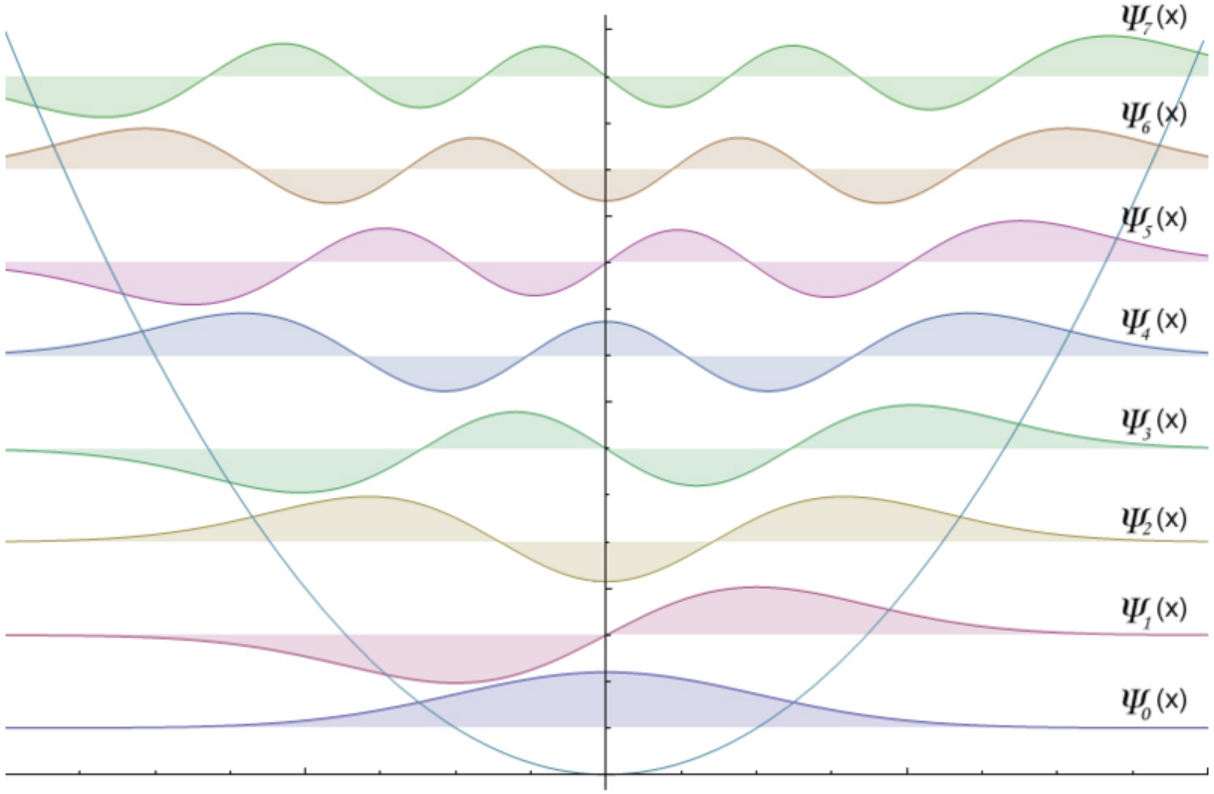
- If we plug this into the difference formula and simplify we get:

$$\left(1+\frac{h^2}{12}q_{n+1}\right)u_{n+1}-2\left(1+\frac{5h^2}{12}q_n\right)u_n+\left(1+\frac{h^2}{12}q_{n-1}\right)u_{n-1}$$
$$=\frac{h^2}{12}\left(s_{n+1}+10s_n+s_{n-1}\right)+\mathcal{O}(h^6)\ .$$

- Already better than RK4!
- But, this is a three-point formula, so needs u0 and u1 to start it

Boundary-value and eigenvalue problems

- Now we consider the Quantum harmonic oscillator



- Hamiltonian is :

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 ,$$

- Eigenfunctions are :

$$\psi_n(x) = \frac{1}{\sqrt{2^n\, n!}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot e^{-\frac{m\omega x^2}{2\hbar}} \cdot H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right), \qquad n = 0, 1, 2, \ldots.$$

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right)$$

- Energy levels are :

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

Boundary-value and eigenvalue problems

- Obviously can't compute for x in +- infinity
  - Need to get appropriate boundary conditions
  - Choose left and right boundaries that are "big enough" and then apply approximate boundary conditions :
    - Since psi(x) ~ 0 there, just set psi(x) = 0
- We can use the Numerov algorithm to solve this
- Some caveats :
  - There are unphysical solutions that march to infinity (mathematical property of QHO)
  - From symmetry, need to make sure that the solutions are appropriately symmetric or antisymmetric!

Boundary-value and eigenvalue problems

- How to deal with this?
  - March twice!
    - Once from left
    - Once from right
  - Ensure that they match at some x value
  - We can actually multiply one of the solutions by a constant (still solves the ODE) so we ensure

$$\phi_{\mathrm{left}}(x_{\mathrm{match}}) = \phi_{\mathrm{right}}(x_{\mathrm{match}}) \; .$$

  - If we have a true match, then we can test

$$\left.\frac{d\phi_{\mathrm{left}}}{dx}\right|_{x_{\mathrm{match}}} = \left.\frac{d\phi_{\mathrm{right}}}{dx}\right|_{x_{\mathrm{match}}} \; .$$

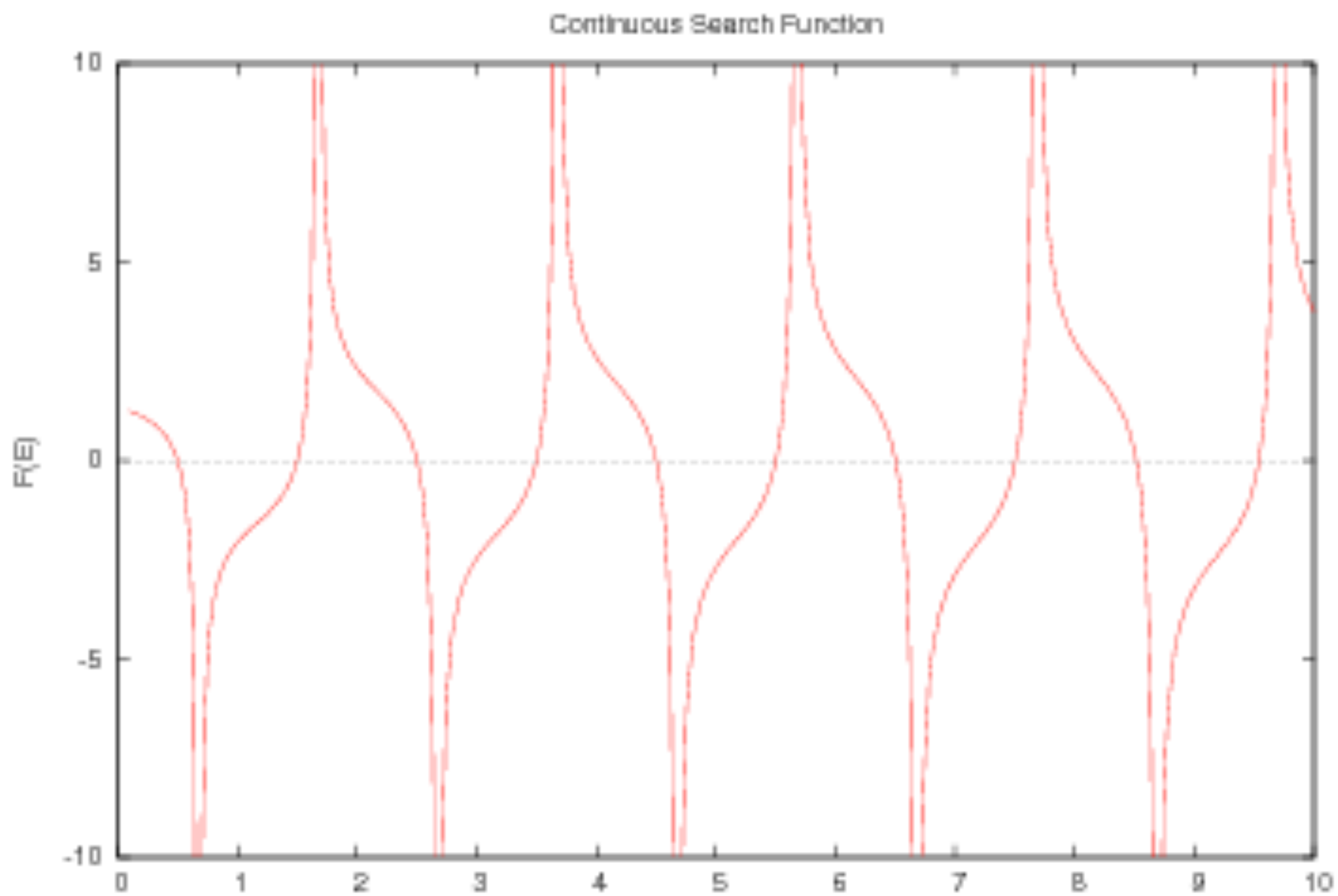
Boundary-value and eigenvalue problems

- Can pick a matching point near the classical turning point with E = V(x)

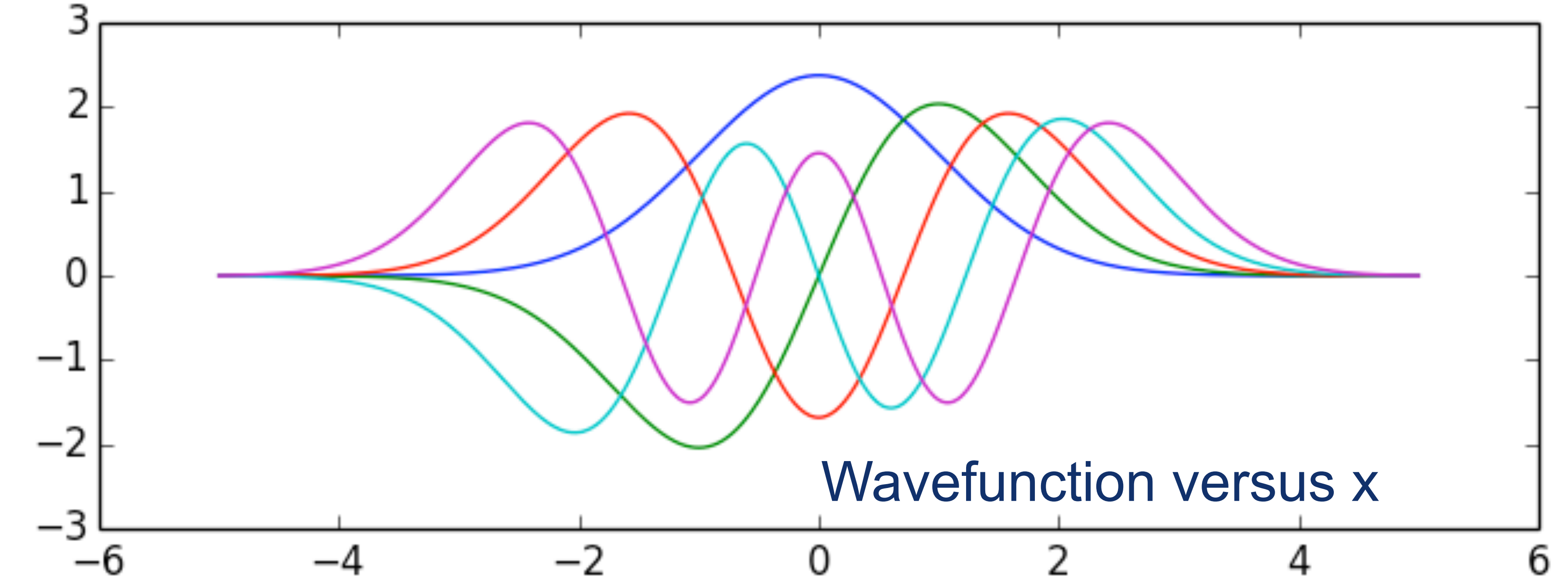
- Matching condition is :

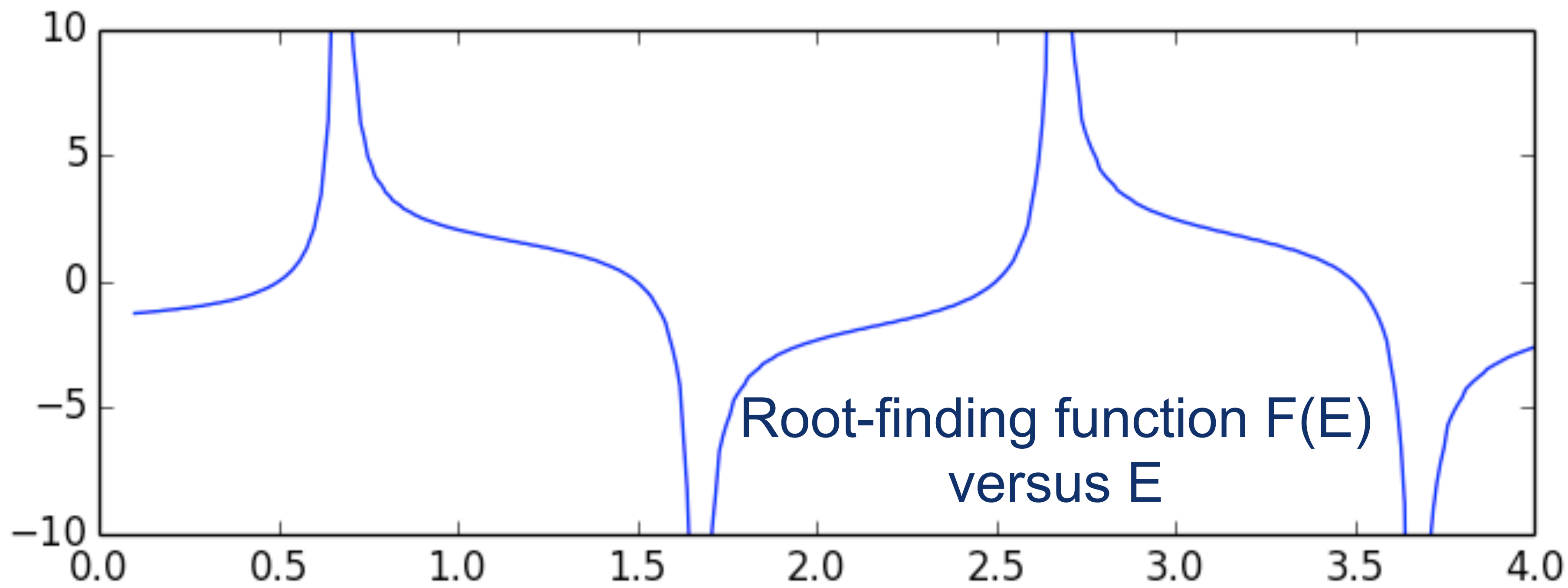
$$F(E) = \pm\left[\phi_{\text{left}}(x_{\text{match}}+h) - \phi_{\text{left}}(x_{\text{match}}-h)\right] - \left[\phi_{\text{right}}(x_{\text{match}}+h) - \phi_{\text{right}}(x_{\text{match}}-h)\right] / (2h\phi(x_{\text{match}})) = 0\,.$$

- Finally, we can find the matching functior F(E) numerically and find the roots!



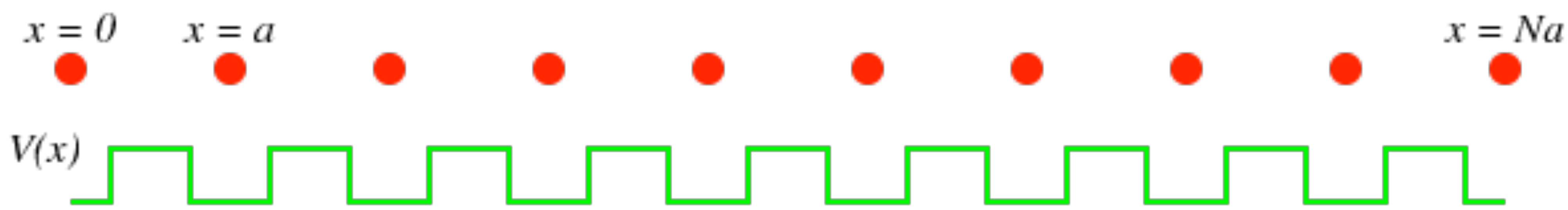
Results of Schroedinger





Boundary-value and eigenvalue problems

- Another popular problem is to investigates Particle in a periodic potential
  - Kronig-Penney model : 1-d "crystal"
  - N heavy nuclei at fixed lattice sites with spacing a



- This is easier to solve in the Fourier domain!

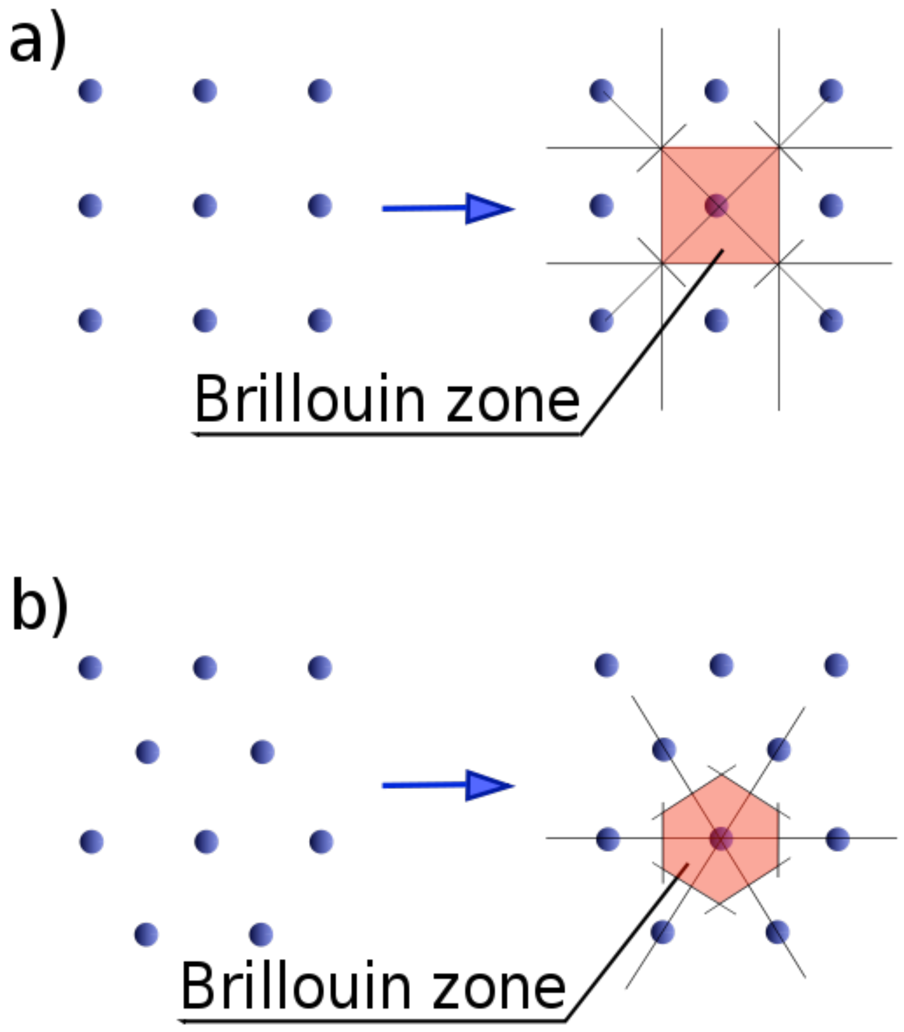
$$f(x) = \sum_k e^{ikx} f_k \ ,$$

- Then we have periodic boundary conditions :

$$e^{ik(x+Na)} = e^{ikx} \quad \Rightarrow \quad k = \frac{2\pi n}{Na} \ , \text{ where } n = 0, \pm 1, \pm 2, \ldots$$

Boundary-value and eigenvalue problems

- Define the Brillouin zone :
  - http://en.wikipedia.org/wiki/Brillouin_zone
- Space of nearest neighbors!
- Also known as the Voronoi cell
  - http://en.wikipedia.org/wiki/Voronoi_cell



Boundary-value and eigenvalue problems

- Define the lattice point by translating the objects by some basis vector a, and the “reciprocal” basis vectors b:

$$\mathbf{R} = n\mathbf{a}\ , \ \text{where } \mathbf{a} = a\hat{x}\ , \ \text{and } n = 0, \pm 1, \pm 2, \ldots ,$$

$$\mathbf{a}\cdot\mathbf{b} = 2\pi \qquad \text{that is} \qquad \mathbf{b} = (2\pi/a)\hat{x}\ .$$

$$\mathbf{K} = n\mathbf{b}\ , \ \text{where } n = 0, \pm 1, \pm 2, \ldots$$

- The first Brillouin zone is :

$$k = 0, \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, \pm\frac{6\pi}{Na}, \ldots \pm \frac{(N-1)\pi}{Na}, \frac{\pi}{a}\ .$$

- A general wave number q can be decomposed into a wave number k in the first Brillouin zone and a wave number of the reciprocal lattice $q = k + K\ .$

Boundary-value and eigenvalue problems

- Can use “Bloch’s theorem” to solve the problem
- We know: $$V(x) = \sum_K e^{iKx} V_K \ ,$$
- The eigenstates satisfy: $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x) \ .$$
- Then we expand in Fourier series:

$$\psi(x) = \sum_q e^{iqx} C_q = \sum_{K,k} e^{i(k+K)x} C_{k+K} \ ,$$

- Plugging this into Schroedinger’s equation we get:

$$\sum_{K,k} \left\{ \left[\frac{1}{2}(k+K)^2 - E \right] e^{i(k+K)x} C_{k+K} \right\} + \sum_{K'} V_{K'} \sum_{K,k} e^{i(k+K+K')x} C_{k+K} = 0 \ .$$

$$\hbar^2/m = 1$$

Boundary-value and eigenvalue problems

- k and k' are both reciprocal lattice vectors, so we just change the notation:

$$\sum_{K,k} e^{i(k+K)x} \left\{ \left[\frac{1}{2}(k+K)^2 - E \right] C_{k+K} + \sum_{K'} V_{K-K'} C_{k+K'} \right\} = 0 \,.$$

- The functions are linearly independent so :

$$\left[\frac{1}{2}(k+K)^2 - E \right] C_{k+K} + \sum_{K'} V_{K-K'} C_{k+K'} = 0 \,.$$

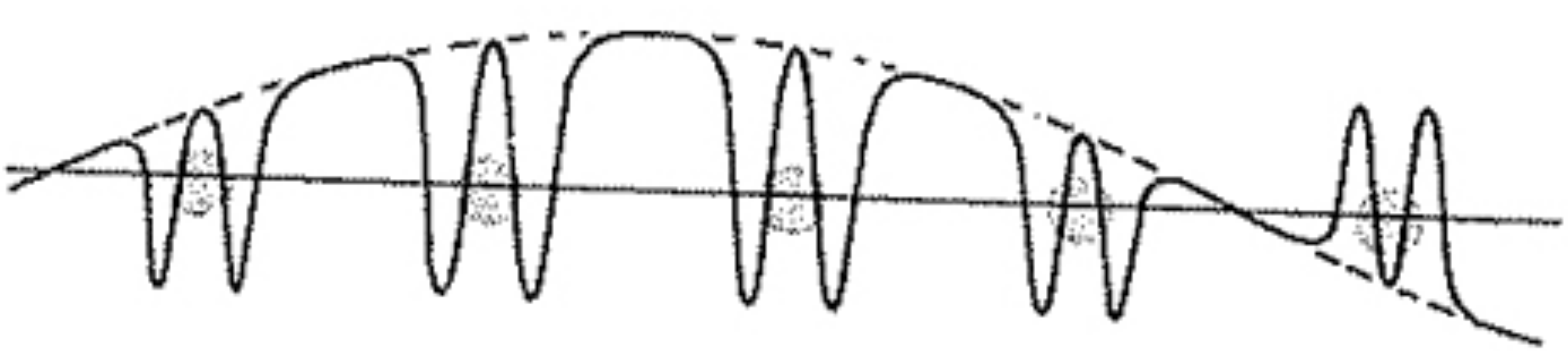
  - Modes with different wave numbers k **decouple** from one another!
- Can state this as: $\psi_k(x) = e^{ikx} \sum_{K} e^{iKx} C_{k+K} = e^{ikx} u_k(x) \,,$
  - where :

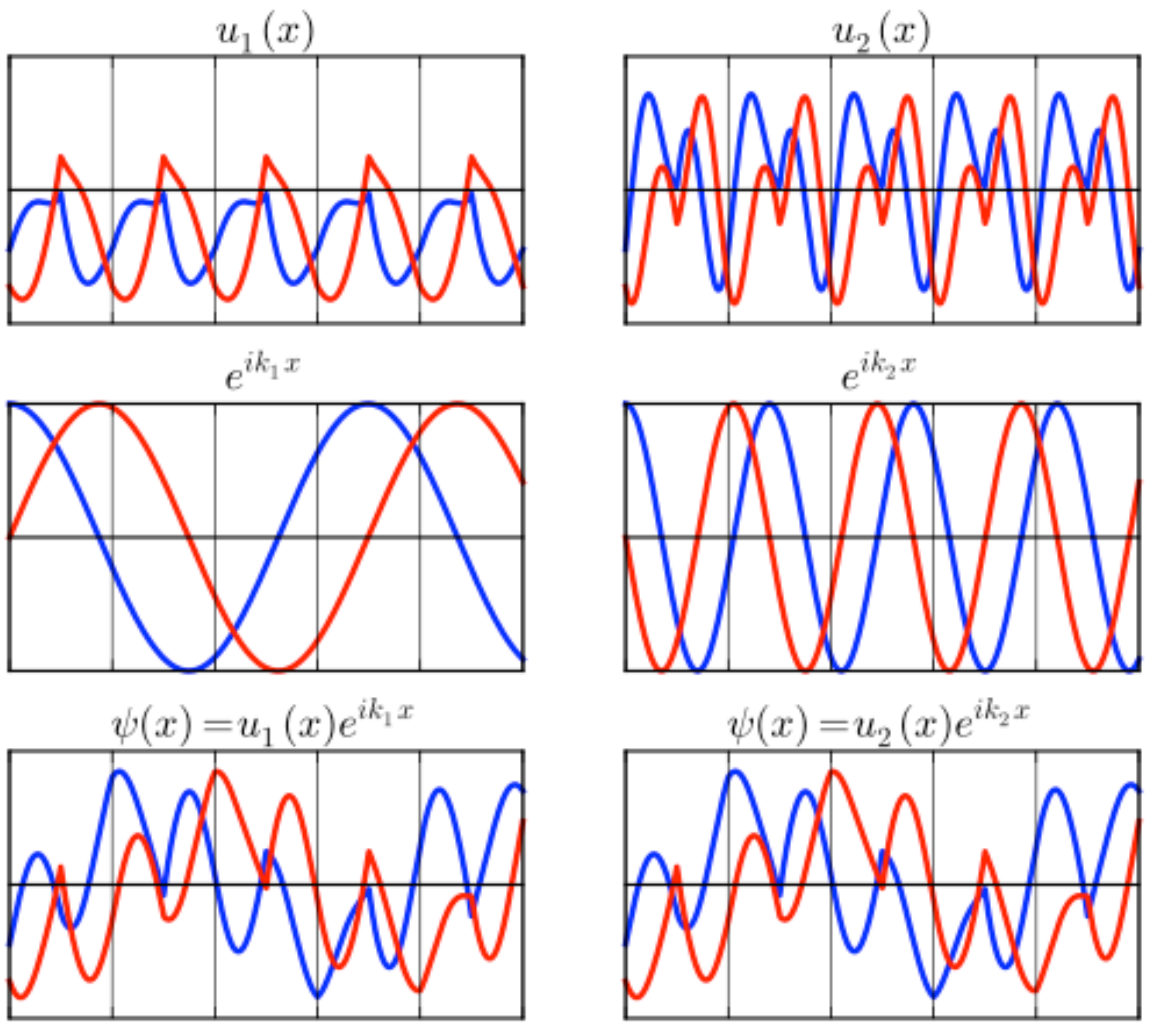
$$u_k(x+na) = u_k(x) \,,$$

- This is Bloch's theorem!

Boundary-value and eigenvalue problems

- So this "feels like" the solution to the first Brillouin zone, shifted by a simple plane wave!





Boundary-value and eigenvalue problems

- To solve for the band structure we look at the eigenvalue equation :

$$\left[\frac{1}{2}(k+K)^2 - E\right] C_{k+K} + \sum_{K'} V_{K-K'} C_{k+K'} = 0 \, .$$

- Actually infinite-dimensional, so we need to cut it off somewhere

- Looking at the spectrum of states as a function of k over the first Brillouin zone is a “band”

Boundary-value and eigenvalue problems

- Concretely, consider a single cell on the lattice :

$$V(x) = \begin{cases} 0 & \text{for } -\frac{a}{2} < x < -\frac{\Delta}{2} \\ V_0 & \text{for } -\frac{\Delta}{2} < x < \frac{\Delta}{2} \\ 0 & \text{for } \frac{\Delta}{2} < x < \frac{a}{2} \end{cases} ,$$

- Between barriers we have

$$\psi(x) = A_n e^{iq(x-na)} + B_n e^{-iq(x-na)} ,$$

- Inside the barrier we have

$$\psi(x) = C_n e^{i\kappa(x-na)} + D_n e^{-i\kappa(x-na)} ,$$

- Here : $q = \sqrt{2E} \qquad \kappa = \sqrt{2(E - V_0)}$

- Determine A,B,C,D's by matching psi and psi', then we have recursion relation to solve for n+1 given n:

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \mathbf{T}(E) \begin{pmatrix} A_n \\ B_n \end{pmatrix} ,$$

Boundary-value and eigenvalue problems

- T(E) is the "transfer matrix", with elements :

$$T_{11} = T_{22}^* = \frac{e^{iq(a-\Delta)}}{4q\kappa}\left[e^{i\kappa\Delta}(q+\kappa)^2 - e^{-i\kappa\Delta}(q-\kappa)^2\right] ,$$

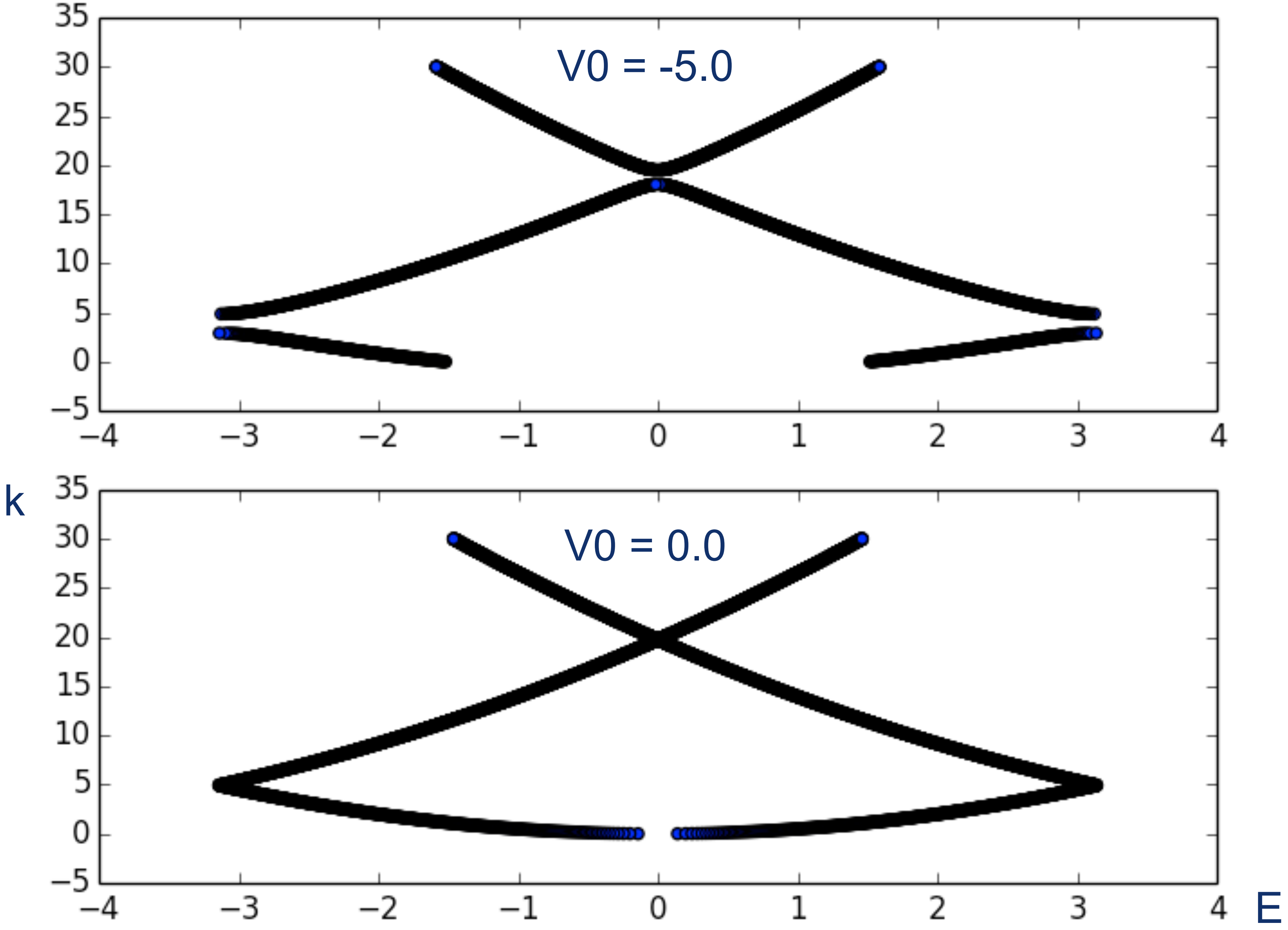
$$T_{12} = T_{21}^* = -\frac{ie^{iq(a-\Delta)}}{2q\kappa}(q^2-\kappa^2)\sin(\kappa\Delta) .$$

- From Bloch's theorem, eigenvalues are of the form exp(ika), where k is the reduced wave number in the first Brillouin zone
- T(E) is 2x2 so can easily solve the characteristic equation:

$$\det\left[\mathbf{T} - e^{ika}\mathbf{1}\right] = 0 .$$

- This yields a quadratic equation with two solutions for k(E) equal in magnitude and opposite in sign

Results of Kronig-Penney



Results of Kronig-Penney