PHOT 301: Quantum Photonics

LECTURE 06

Michaël Barbier, Summer (2024-2025)

OVERVIEW

week	Topic	Reading
Week 1	Introduction & Required Mathematical Methods. Waves and Schrödinger's equation, Probability, Uncertainty and Time evolution. Infinite square well.	
Week 2	The harmonic oscillator, Creation and annihilation operators. Free particle, 1D Bound states & Scattering/Transmission, Finite well	
Week 3	Quantum mechanics formalism: Functions and operators, uncertainty. Approximation methods.	Ch. 3
Week 4	Angular momentum and the Hydrogen atom, Spin Magnetic fields, The Pauli equation, Minimal Coupling, Aharonov Bohm Perturbation: Fine Structure of Hydrogen, The Zeeman Effect	
Week 5	Identical particles, Periodic table, Molecular bonds, Periodic structures, Band structure, Bloch functions Time-dependent perturbation: Absorption, spontaneous emission, and stimulated emission	
Week 6	Final exam	

FOR NEXT WEEK

- Textbook Chapter 2: 2.31, 2.34, 2.41, 2.53
- Textbook Chapter 3: 2.31, 2.34, 2.41, 2.53
- Homework documents:
  - phot301_homework_braket.pdf
- Reading (by Thursday 7 August 2025): Chapter 4 of Griffiths

INTRODUCTION TO DIFFERENT APPROXIMATIONS

APPROXIMATIONS

	Method	Approximates?
1	Transfer matrix method	piece-wise constant $V(x)$
2	Finite basis method	limited ψ_n, E_n: Matrix-formalism
3	Finite difference method	discretizes wave function
4	Perturbation theory (stat.)	small perturbation known solutions
5	Time-dependent perturbation	small perturbation known solutions
6	Tight-binding approx.	electrons strongly bound (covalent)
7	Variational method	finding energy minima

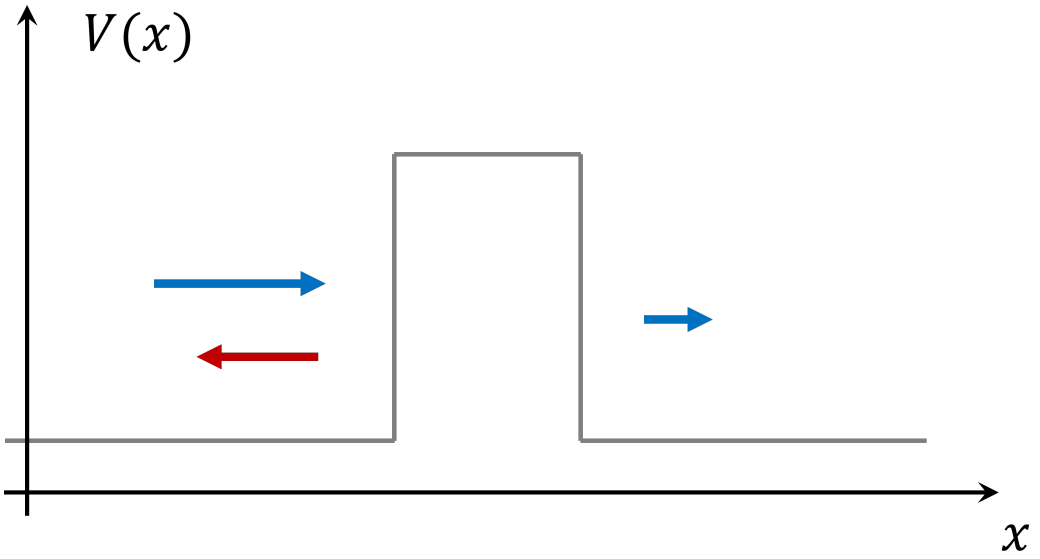
Usage of simple examples to compare over approximations

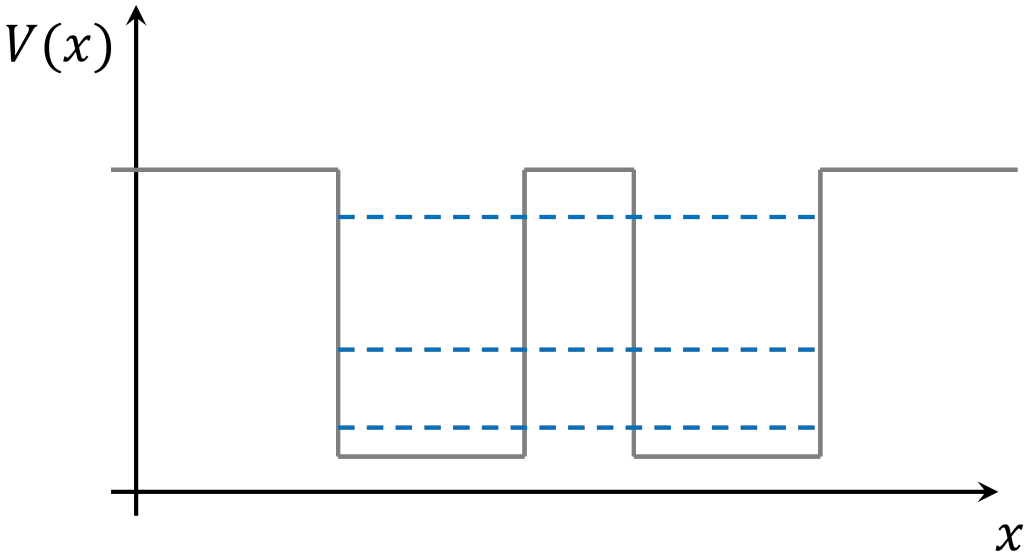
- Infinite square well with E-field (David Miller's book)
- Harmonic oscilator
- Transmission: Smoothed finite barrier

TRANSFER MATRIX METHOD IN 1D

INTRO: TRANSFER MATRIX METHOD

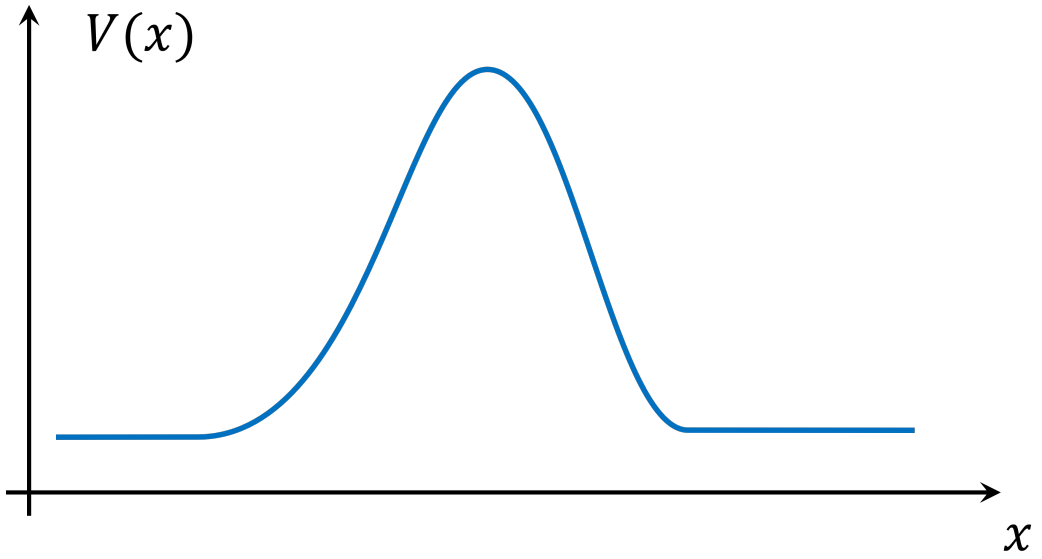
- For 1D potential energy functions $V(x)$ (here assume 1D systems)
- Approximation of potential energy $V(x)$ by piece-wise constant V_i
- Transmission or bound states

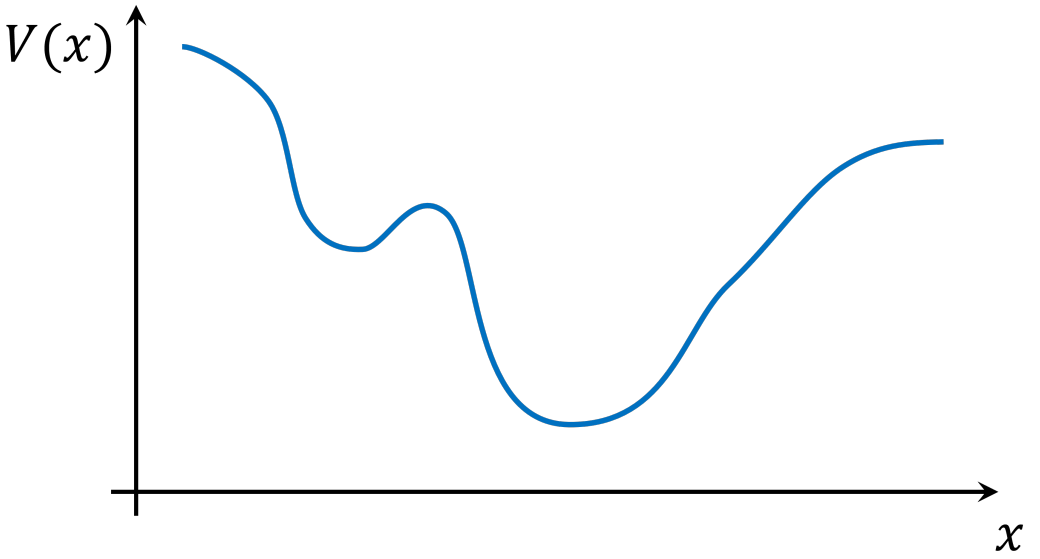




INTRO: TRANSFER MATRIX METHOD

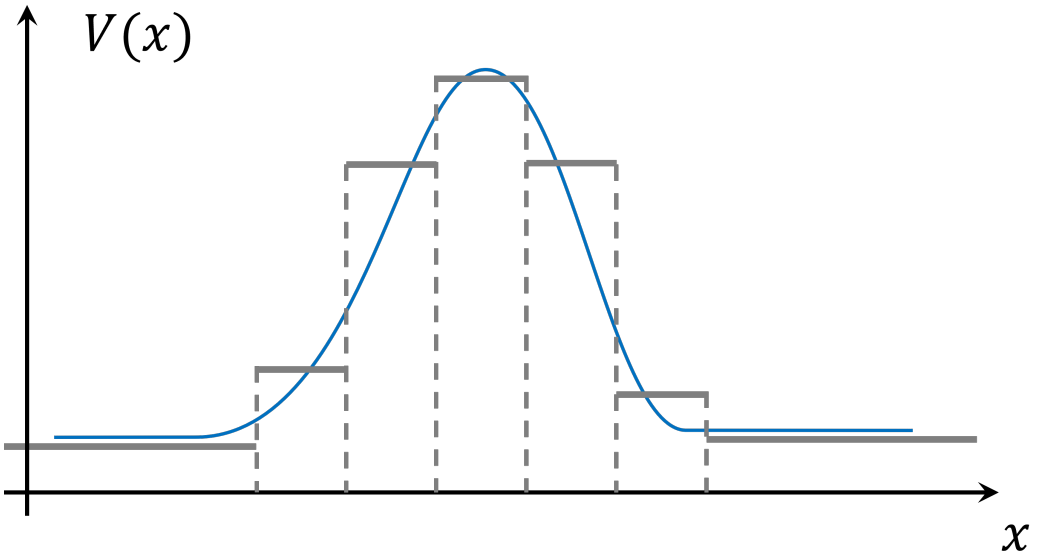
- For 1D potential energy functions $V(x)$ (here assume 1D systems)
- Approximation of potential energy $V(x)$ by piece-wise constant V_i
- Transmission or bound states

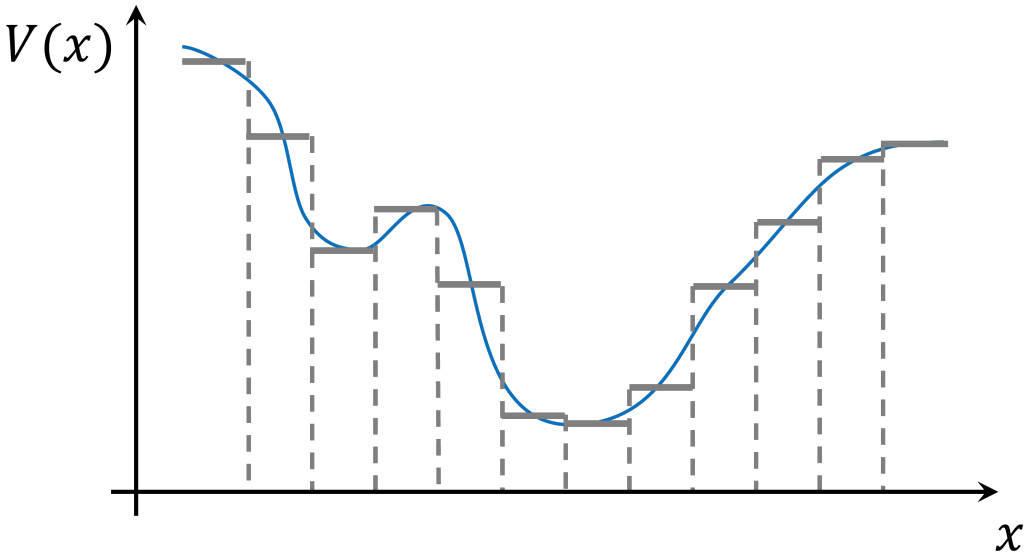




INTRO: TRANSFER MATRIX METHOD

- For 1D potential energy functions $V(x)$ (here assume 1D systems)
- Approximation of potential energy $V(x)$ by piece-wise constant V_i
- Transmission or bound states





INTRO: TRANSFER MATRIX METHOD

- For 1D potential energy functions $V(x)$ (here assume 1D systems)
- Approximation of potential energy $V(x)$ by piece-wise constant V_i
- Schrodinger equation for constant $V(x) = V$

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

- Solution depends on value of $E - V$:
- If energy is **larger than** the potential energy $E > V$, then we have propagating waves

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad k^2 = \frac{2m}{\hbar^2}(E - V)$$

INTRO: TRANSFER MATRIX METHOD

- For 1D potential energy functions $V(x)$ (here assume 1D systems)
- Approximation of potential energy $V(x)$ by piece-wise constant V_i
- Schrodinger equation for constant $V(x) = V$

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

- Solution depends on value of $E - V$:
- If energy is **less than** the potential $E < V$, then we have evanescent waves:

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x} \qquad \kappa^2 = \frac{2m}{\hbar^2}(V - E)$$

INTRO: TRANSFER MATRIX METHOD

- For 1D potential energy functions $V(x)$ (here assume 1D systems)
- Approximation of potential energy $V(x)$ by piece-wise constant V_i
- Schrodinger equation for constant $V(x) = V$

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

- Solution depends on value of $E - V$:
- If energy is the **same** as the potential energy $E = V$, then:

$$\psi(x) = A + B\,x$$

INTRO: TRANSFER MATRIX METHOD

- For 1D potential energy functions $V(x)$ (here assume 1D systems)
- Approximation of potential energy $V(x)$ by piece-wise constant V_i
- Schrodinger equation for constant $V(x) = V$

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

- Solution depends on value of $E - V$:

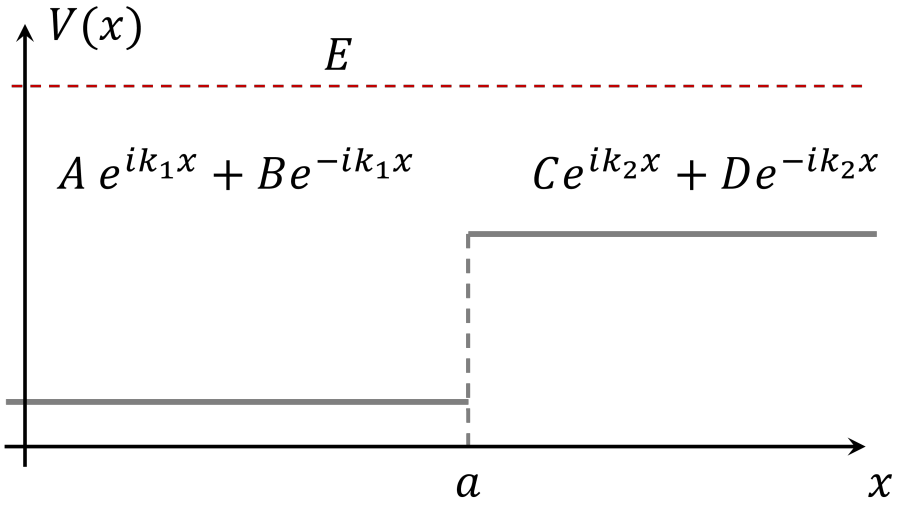
case	solutions	eigenvalue of $\hat{p}$	parameter
$E > V$	$e^{\pm ikx}$	$\pm\hbar k$	$k^2 = \frac{2m}{\hbar^2}(E - V)$
$E = V$	$1, x$	0, no e.v.	$E = V$
$E < V$	$e^{\mp\kappa x}$	$\pm i\hbar\kappa$	$\kappa^2 = \frac{2m}{\hbar^2}(V - E)$

BOUNDARY CONDITIONS ACROSS A STEP IN V(X)

- Suppose there is a step in the potential in $x = a$.
- **Boundary conditions**: Continuity of wave function $\psi(x)$ and derivative $\frac{d\psi(x)}{dx}$:

$$\psi_I(a) = \psi_{II}(a)$$
$$\frac{d\psi_I(a)}{dx} = \frac{d\psi_{II}(a)}{dx}$$

$$Ae^{ik_1 a} + Be^{-ik_1 a} = Ce^{ik_2 a} + De^{-ik_2 a}$$
$$ik_1 Ae^{ik_1 a} - ik_1 Be^{-ik_1 a} = ik_2 Ce^{ik_2 a} - ik_2 De^{-ik_2 a}$$

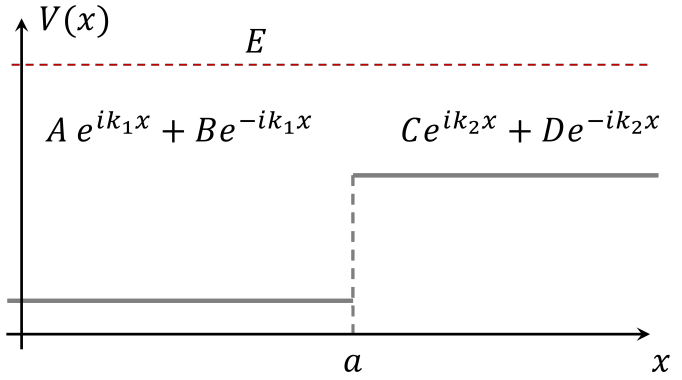


BOUNDARY CONDITIONS ACROSS A STEP IN V(X)

$$\psi_I(a) = \psi_{II}(a)$$
$$\frac{d\psi_I(a)}{dx} = \frac{d\psi_{II}(a)}{dx}$$

$$Ae^{ik_1 a} + Be^{-ik_1 a} = Ce^{ik_2 a} + De^{-ik_2 a}$$
$$ik_1 Ae^{ik_1 a} - ik_1 Be^{-ik_1 a} = ik_2 Ce^{ik_2 a} - ik_2 De^{-ik_2 a}$$

$$\begin{pmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{pmatrix} \begin{pmatrix} e^{ik_1 a} & 0 \\ 0 & e^{-ik_1 a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{pmatrix} \begin{pmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$



BOUNDARY CONDITIONS ACROSS A STEP IN V(X)

$$\begin{pmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{pmatrix} \begin{pmatrix} e^{ik_1 a} & 0 \\ 0 & e^{-ik_1 a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{pmatrix} \begin{pmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

Express coefficient A, B in C, D:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} e^{ik_1 a} & 0 \\ 0 & e^{-ik_1 a} \end{pmatrix}^{-1} \begin{pmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{pmatrix}^{-1} \times \begin{pmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{pmatrix} \begin{pmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

Rename the matrices as function of V and a:

$$\begin{pmatrix} A \\ B \end{pmatrix} = E_1^{-1}(a) K_1^{-1} K_2 E_2(a) \begin{pmatrix} C \\ D \end{pmatrix}$$

TRANSFER MATRIX FOR A SINGLE STEP

$$E_j(a) = \begin{pmatrix} e^{ik_j a} & 0 \\ 0 & e^{-ik_j a} \end{pmatrix}, \qquad K_j \begin{pmatrix} 1 & 1 \\ ik_j & -ik_j \end{pmatrix}$$

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = E_1^{-1}(a) K_1^{-1} K_2 E_2(a) \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

We can define the transfer matrix for a single step:

$$T_{12} = E_1^{-1}(a) K_1^{-1} K_2 E_2(a)$$

Connection between coefficient before/after step:

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = T_{12} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

Lecture 06: Dirac formalism

MULTIPLE POTENTIAL STEPS

Extending the relation over multiple steps:

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = T_{12} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = T_{12}\, T_{23} \begin{pmatrix} A_3 \\ B_3 \end{pmatrix}$$

In general, after N steps we obtain:

$$\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = T \begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix} = T_{01}\, T_{12}\, \ldots\, T_{N,N+1} \begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix}$$

Or renaming the indices on the left and right:

$$\begin{pmatrix} A_L \\ B_L \end{pmatrix} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} A_R \\ B_R \end{pmatrix}$$

Lecture 06: Dirac formalism

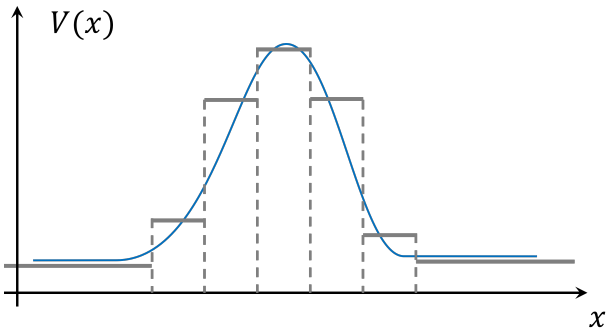
SCATTERING AND BOUND STATES

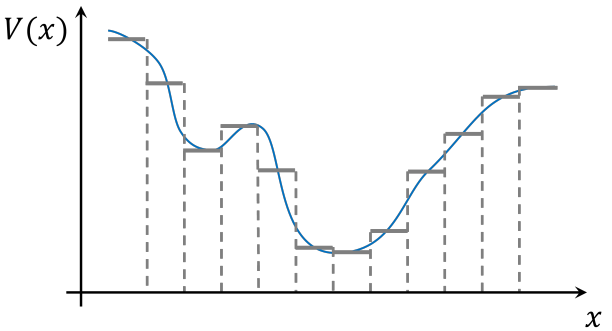
Scattering: $B_R = 0$

$$\begin{pmatrix} A_L \\ B_L \end{pmatrix} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} A_R \\ 0 \end{pmatrix}$$

Therefore the transmission and reflection coefficients become:

$$\begin{aligned} \text{Transmission} \quad & T(E) = |A_R/A_L|^2 = 1 \,/\, |t_{11}(E)|^2 \\ \text{Reflection} \quad & R(E) = |B_L/A_L|^2 = |t_{21}(E)|^2 \,/\, |t_{11}(E)|^2 \end{aligned}$$



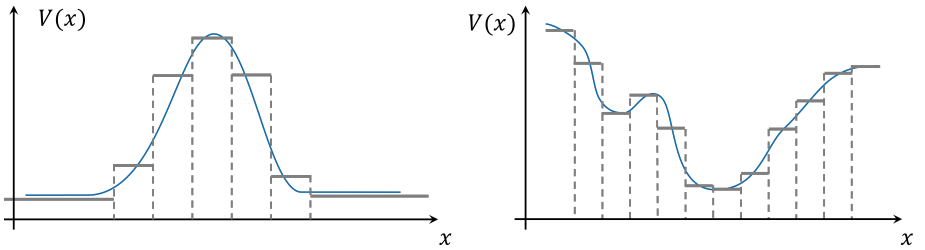


SCATTERING AND BOUND STATES

Bound states: $A_L = 0, \quad B_R = 0$

$$\begin{pmatrix} 0 \\ B_L \end{pmatrix} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} A_R \\ 0 \end{pmatrix} \Longrightarrow \begin{array}{l} A_L = t_{11}(E)\, A_R \\ B_L = t_{21}(E)\, A_R \end{array}$$

- Bound states are given by zeros of t_{11}
- The total wave function is defined upon the coefficients B_L and A_R. We can obtain these unknowns by
  - first using the second equation: $B_L = t_{21}(E)\, A_R$ to obtain B_L, and then
  - applying normalization to the whole wave function to fix A_R.



APPROXIMATIONS

	Method	Approximates?
1	Transfer matrix method	piece-wise constant $V(x)$
2	Finite basis method	limited ψ_n, E_n: Matrix-formalism
3	Finite difference method	discretizes wave function
4	Perturbation theory (stat.)	small perturbation known solutions
5	Time-dependent perturbation	small perturbation known solutions
6	Tight-binding approx.	electrons strongly bound (covalent)
7	Variational method	finding energy minima

Usage of simple examples to compare over approximations

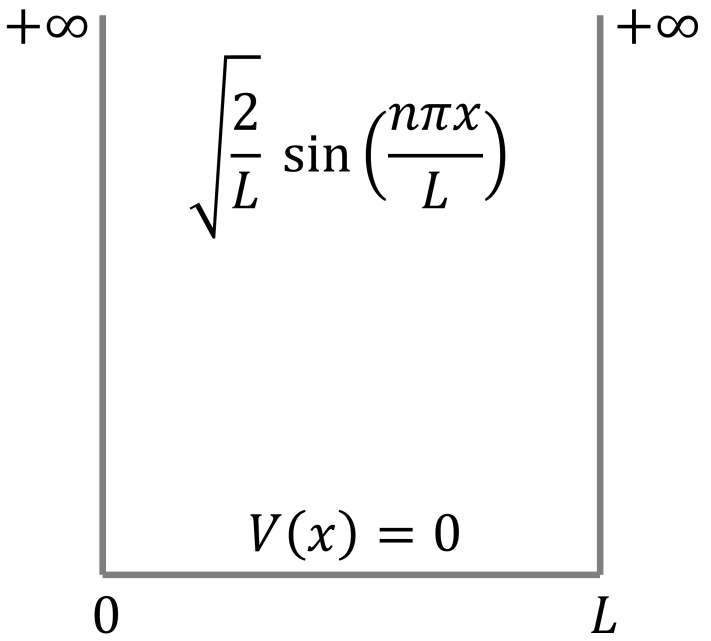
- Infinite square well with E-field (David Miller's book section 2.11)
- More on approximation methods: see Chapter 6 of David Miller's book
- Analytic solution vs. **perturbation** vs. **finite basis method** vs. **Finite difference**

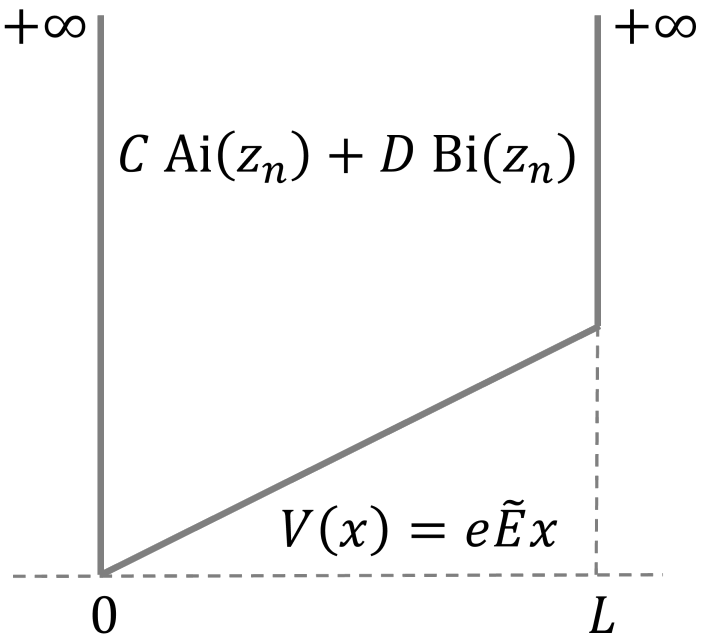
INFINITE WELL WITH E-FIELD

A CONSTANT ELECTRIC FIELD

- The potential for a constant electric field: $V(x) = e\tilde{E}\,x$
- The time-independent Schrodinger equation:

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





A CONSTANT ELECTRIC FIELD

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

Rewrite the equation to clarify its form:

$$\begin{aligned}\frac{d^2\psi(x)}{dx^2} &= \frac{2me\tilde{E}}{\hbar^2}(x - \frac{E}{e\tilde{E}})\psi(x) \\ &= c\,(x-d)\psi(x)\end{aligned}$$

Where $c = \frac{2me\tilde{E}}{\hbar^2}$ and $d = \frac{E}{e\tilde{E}}$.

This looks very much like the (solvable) Airy equation:

$$\frac{d^2 f(z)}{dz^2} = zf(z)$$

$\longrightarrow$ we need to find a suitable substitution for z

Lecture 06: Dirac formalism

SUITABLE SUBSTITUTION FOR Z(X)

Assume a linear form for $z = \alpha x + \beta$ and rewrite the Airy equation

$$\frac{d^2\psi(x)}{dx^2} = \frac{d^2 f(z)}{dz^2}\left(\frac{dz}{dx}\right)^2 = \alpha^2 z f(z) = (\alpha^3 x + \beta\alpha^2) f(z)$$

But we have also:

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

$$\Longrightarrow c(x-d) = (\alpha^3 x + \beta\alpha^2)$$

$$\Longrightarrow \alpha = c^{1/3} \qquad \beta = -c^{1/3} d$$

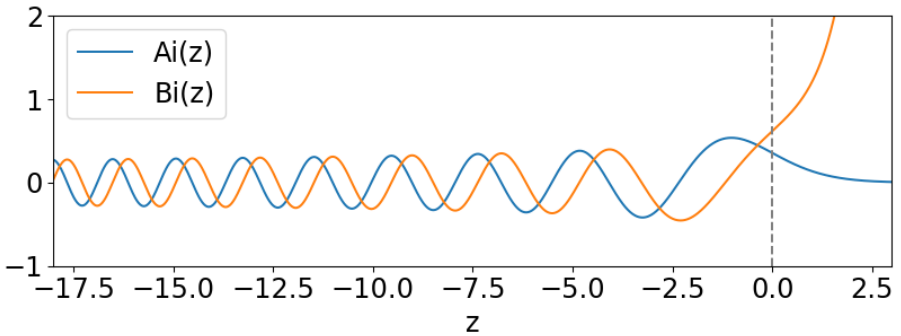
$$\Longrightarrow z = \alpha x + \beta = c^{1/3}(x-d) = \left(\frac{2me\tilde{E}}{\hbar^2}\right)^{1/3}\left(x - \frac{E}{e\tilde{E}}\right)$$

AIRY EQUATION SOLUTIONS

$$\frac{d^2 f(z)}{dz^2} = z\, f(z), \qquad \psi(x) = f(z) = C\,\mathrm{Ai}(z) + D\,\mathrm{Bi}(z)$$

$$\mathrm{Ai}(z) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{t^3}{3} + zt\right) dt$$

$$\mathrm{Bi}(z) = \frac{1}{\pi}\int_0^\infty \left[\exp\left(-\frac{t^3}{3} + zt\right) + \sin\left(\frac{t^3}{3} + zt\right)\right] dt$$



BOUNDARY CONDITIONS

$$\frac{d^2 f(z)}{dz^2} = z\, f(z), \qquad \psi(x) = f(z) = C\,\mathrm{Ai}(z) + D\,\mathrm{Bi}(z)$$

$$x = 0 \longrightarrow z_0 = -c^{1/3} d \qquad C\,\mathrm{Ai}(z_0) + D\,\mathrm{Bi}(z_0) = 0$$

$$x = L \longrightarrow z_L = c^{1/3}(L - d) \qquad C\,\mathrm{Ai}(z_L) + D\,\mathrm{Bi}(z_L) = 0$$

$$\begin{pmatrix} \mathrm{Ai}(z_0) & \mathrm{Bi}(z_0) \\ \mathrm{Ai}(z_L) & \mathrm{Bi}(z_L) \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Inverse cannot exist $\longrightarrow$ determinant is zero:

$$\det \begin{pmatrix} \mathrm{Ai}(z_0) & \mathrm{Bi}(z_0) \\ \mathrm{Ai}(z_L) & \mathrm{Bi}(z_L) \end{pmatrix} = \mathrm{Ai}(z_0)\,\mathrm{Bi}(z_L) - \mathrm{Ai}(z_L)\,\mathrm{Bi}(z_0) = 0$$

$\longrightarrow$ Numerically solutions $z_0(E)$, $z_L(E)$

Lecture 06: Dirac formalism

DIMENSIONLESS UNITS

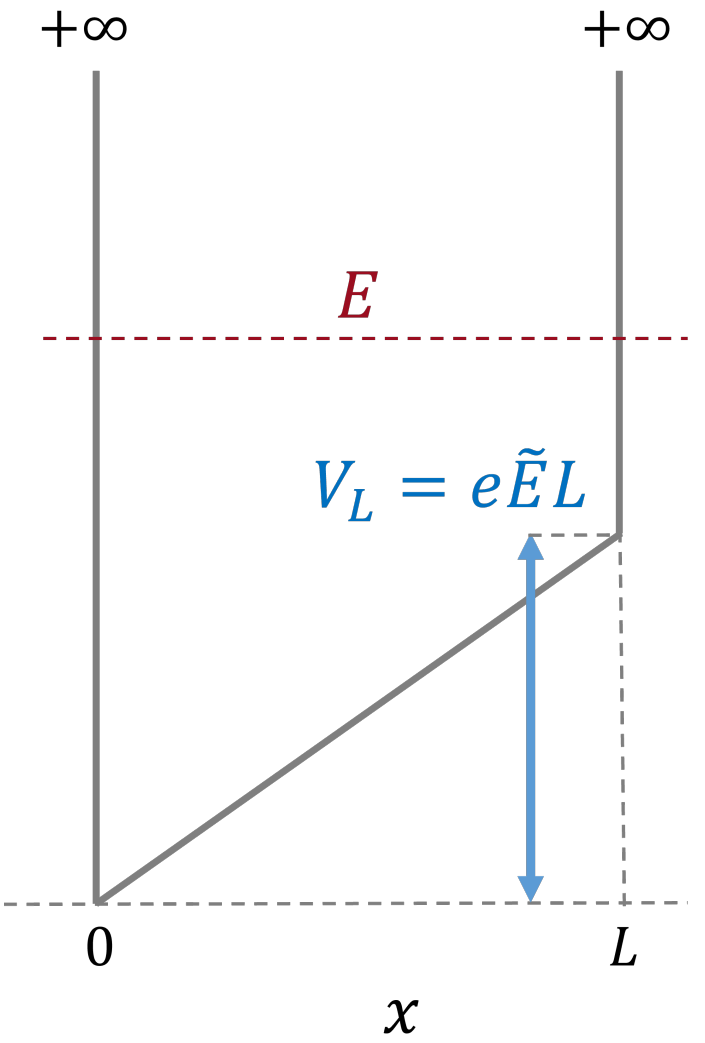
Simplify formula and units

$$\begin{cases} z_0 = -c^{1/3} d = -\left(\dfrac{2me\tilde{E}}{\hbar^2}\right)^{1/3} \dfrac{E}{e\tilde{E}} \\ z_L = c^{1/3}(L-d) = \left(\dfrac{2me\tilde{E}}{\hbar^2}\right)^{1/3} \left(L - \dfrac{E}{e\tilde{E}}\right) \end{cases}$$

In units of $E_1^\infty = \frac{\hbar^2\pi^2}{2mL^2}$,

$$\boxed{E \longrightarrow \varepsilon = \frac{E}{E_1^\infty}} \qquad \boxed{V_L \longrightarrow \nu_L = \frac{V_L}{E_1^\infty} = \frac{e\tilde{E}L}{E_1^\infty}}$$

$$\Rightarrow \boxed{z_0 = -\left(\frac{\pi}{\nu_L}\right)^{\frac{2}{3}} \varepsilon, \qquad z_L = \left(\frac{\pi}{\nu_L}\right)^{\frac{2}{3}} (\nu_L - \varepsilon)}$$



Lecture 06: Dirac formalism

CHOICE OF UNITS

For comparison with the infinite well: energy unit E_1^∞

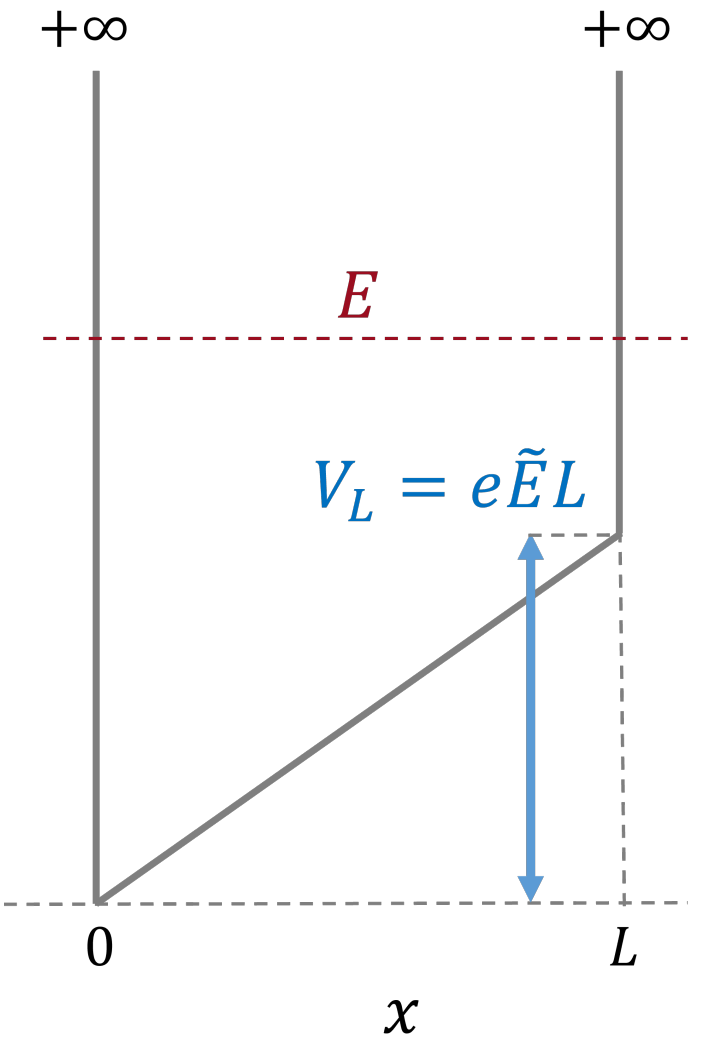
$$z_0 = -\left(\frac{\pi}{\nu_L}\right)^{\frac{2}{3}} \varepsilon, \qquad z_L = \left(\frac{\pi}{\nu_L}\right)^{\frac{2}{3}} (\nu_L - \varepsilon)$$

Alternative: energy unit ν_L

$$z_0 = -\pi^{\frac{2}{3}} \tilde{\varepsilon}, \qquad z_L = \pi^{\frac{2}{3}} (1 - \tilde{\varepsilon})$$

eigenenergies: Solve determinant equation

eigenstates: Fill in eigenenergies in boundary conditions (constants C, D)



EIGENENERGIES & EIGENSTATES

1. Numerically solve determinant equation for eigenenergies E_n,
2. Use E_n in boundary conditions to obtain $\psi_n(x)$
3. Normalize by $\int_0^L |\psi(x)|^2 dx = 1$

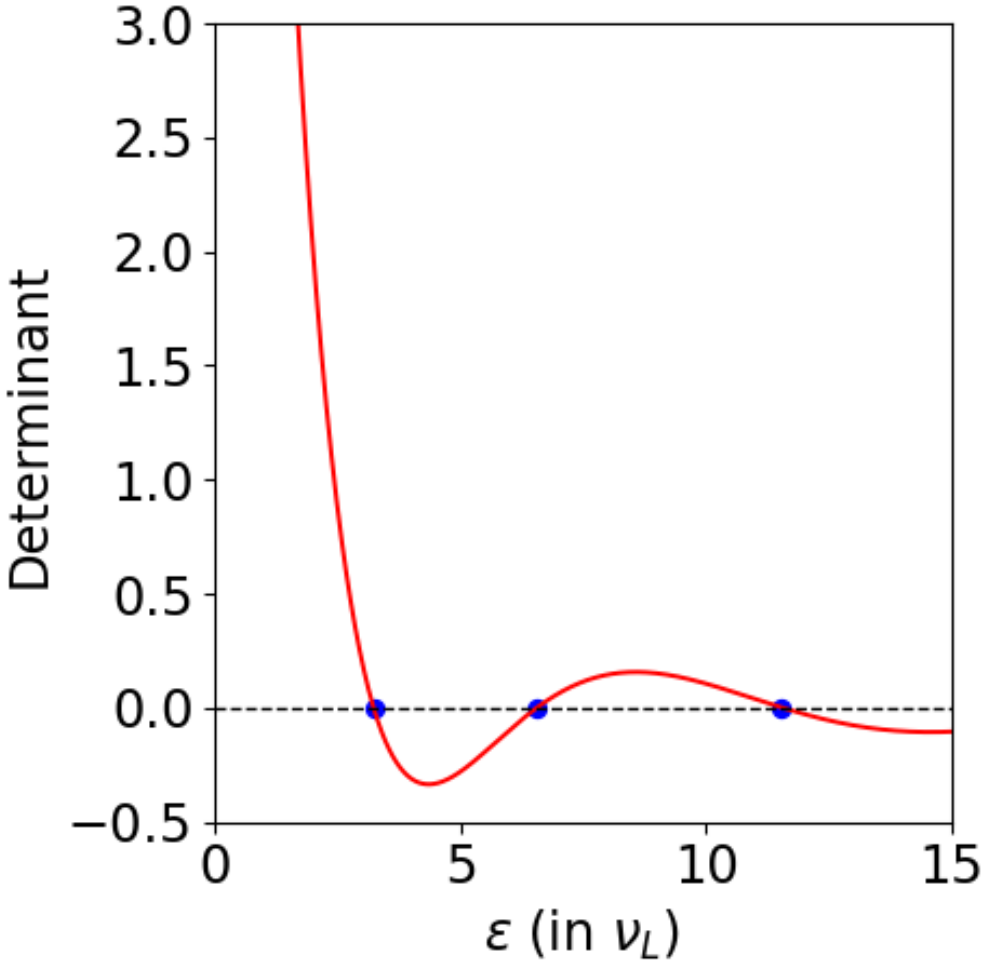
$$\text{Eigenenergies } E_n: \qquad \mathrm{Ai}(z_0)\,\mathrm{Bi}(z_L) - \mathrm{Ai}(z_L)\,\mathrm{Bi}(z_0) = 0$$

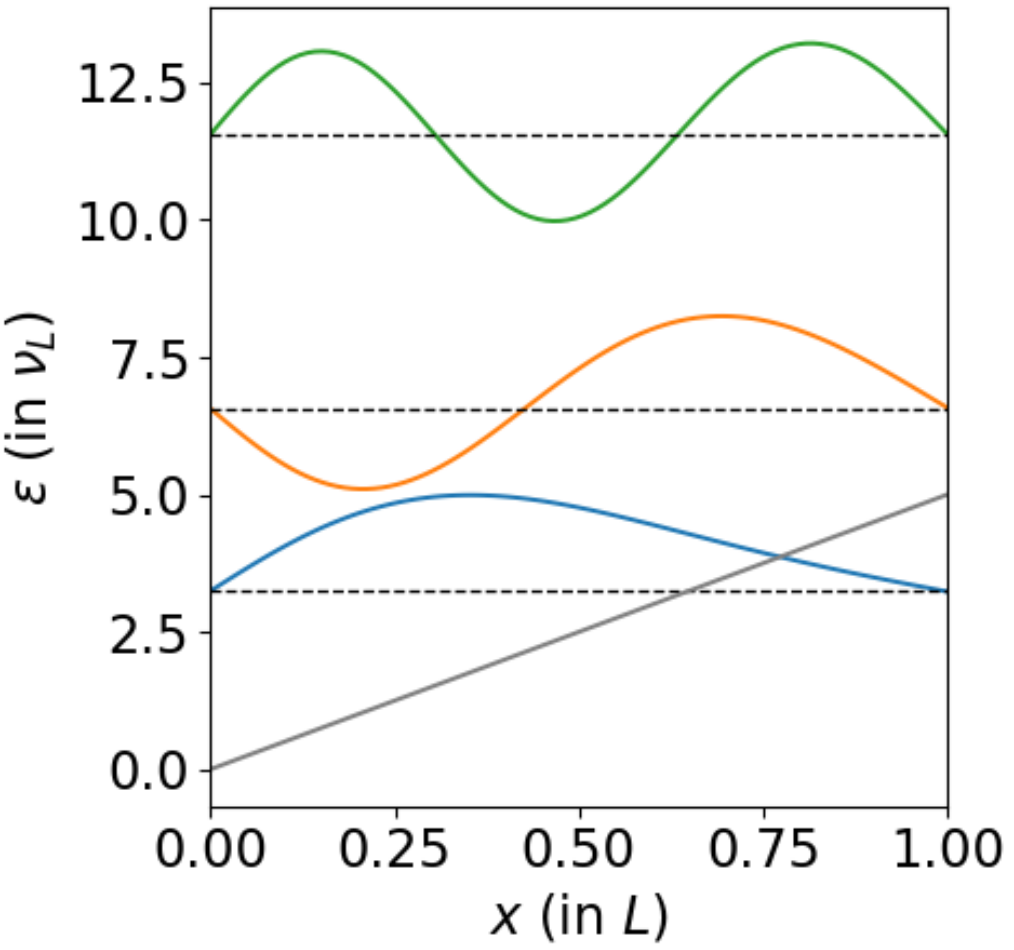
$$\text{Eigenstates } \psi_n(x) = C\,\mathrm{Ai}(z) + D\,\mathrm{Bi}(z): \qquad \frac{D}{C} = -\frac{\mathrm{Bi}(z_0)}{\mathrm{Ai}(z_0)}$$

Remember that z scales with energy

$$z = c^{1/3}(x-d) = \left(\frac{2me\tilde{E}}{\hbar^2}\right)^{1/3}\left(x - \frac{E}{e\tilde{E}}\right) = \left(\frac{\pi}{\nu_L}\right)^{\frac{2}{3}}\left(\frac{x}{L}\nu_L - \varepsilon\right)$$

FINAL SOLUTION





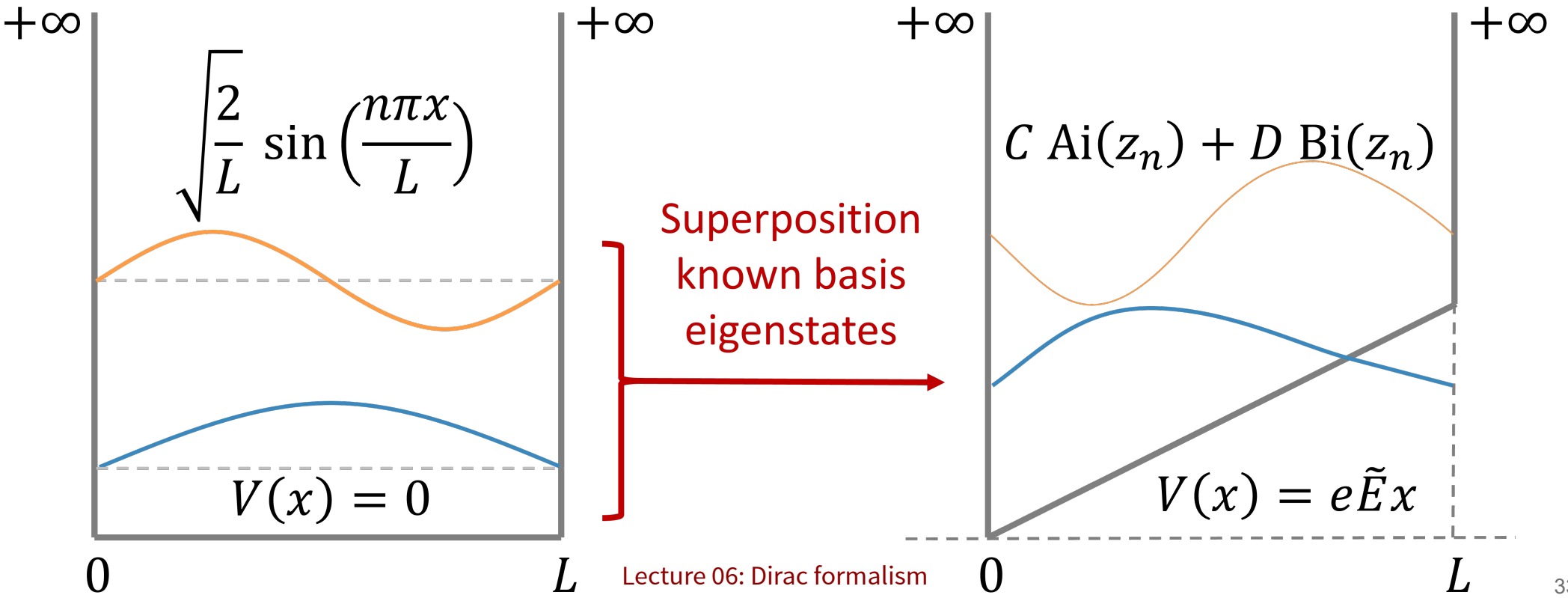
- Eigenenergies ε_n have zero determinant: find roots
- Fill in ε_n to get eigenstates $\psi_n(x)$ Lecture 06: Dirac formalism

FINITE BASIS APPROXIMATION

FINITE BASIS APPROXIMATION

Steps to reach to the solutions:

1. Expand the solution in a known basis
2. Limit the amount of energy levels $\longrightarrow$ matrix algebra
3. Solve the eigenvalue equations for **eigenenergies** & **eigenstates**



DIMENSIONLESS HAMILTONIAN

The dimensionless Hamiltonian for infinite well is obtained by:

- $z = x/L, E \longrightarrow E/E_1^{\infty}$,
- electric field ν_L in units of V_L/E_1^{∞}

$$\hat{H} = -\frac{1}{\pi^2}\frac{d^2}{dz^2} + \nu_L\,(z - 1/2) \quad \text{with} \quad \hat{H}_0 = -\frac{1}{\pi^2}\frac{d^2}{dz^2}$$

Compute the elements of the Hamiltonian (matrix)

$$H_{mn} = -\frac{1}{\pi^2}\int \psi_m(z)\frac{d^2}{dz^2}\psi_n(z)dz \; + \; \int \nu_L\,(z - 1/2)\psi_m(z)\psi_n(z)dz,$$

With $\psi_n(z) = \sqrt{2}\sin(n\pi z)$

HAMILTONIAN: OVERLAP INTEGRALS

$$H_{mn} = \langle \psi_m | \hat{H} | \psi_n \rangle = -\frac{1}{\pi^2} \int \psi_m(z) \frac{d^2}{dz^2} \psi_n(z) dz \; + \; \int \nu_L \left(z - \frac{1}{2}\right) \psi_m(z) \psi_n(z) dz,$$

With the eigenstates $\psi_n(z) = \sqrt{2} \sin(n\pi z)$

$$\begin{aligned} H_{mn} &= -\frac{1}{\pi^2} \int_0^1 \psi_m(z) \frac{d^2}{dz^2} \psi_n(z) dz \; + \; \int_0^1 \nu_L \left(z - 1/2\right) \psi_m(z) \psi_n(z) dz, \\ &= n^2 \delta_{mn} \; + \; \nu_L \int_0^1 (z - 1/2) \sin(m\pi z) \sin(n\pi z) dz, \end{aligned}$$

The second integral can be calculated:

$$\int_0^1 (z - 1/2) \sin(m\pi z) \sin(n\pi z) dz = \begin{cases} \dfrac{4nm}{\pi^2 (m^2 - n^2)^2} & \text{if } \; m+n \; \text{ is odd} \\ 0 & \text{if } \; m+n \; \text{ is even} \end{cases}$$

HAMILTONIAN: OVERLAP INTEGRALS

We see that the integral has two different contributions:

- Diagonal elements H_{nn} are defined by $\hat{H}_0$ with $E_n = n^2\, E_1^\infty$
- Other elements $H_{n,m\neq n}$ determined by perturbing potential $\hat{H}_p = \hat{H} - \hat{H}_0$

$$H_{nn} = n^2 \qquad \begin{cases} H_{mn} = -\nu_L \dfrac{4nm}{\pi^2(m^2-n^2)^2} & \text{if } \; n = m \pm 1, m \pm 3, \ldots \\ \\ H_{mn} = 0 & \text{if } \; n = m \pm 2, m \pm 4, \ldots \end{cases}$$

- The Hamiltonian gives contributions of eigenstates $\psi_n(z) = \sqrt{2}\sin(n\pi z)$
- Eigenenergies E_n and potential ν_L are in units of $E_1^\infty = \frac{\hbar^2\pi^2}{2mL^2}$

SOLVING THE EIGENVALUE EQUATION

The eigenvalue equation is:

$$\hat{H}\psi_n(z) = E_n\psi_n(z)$$

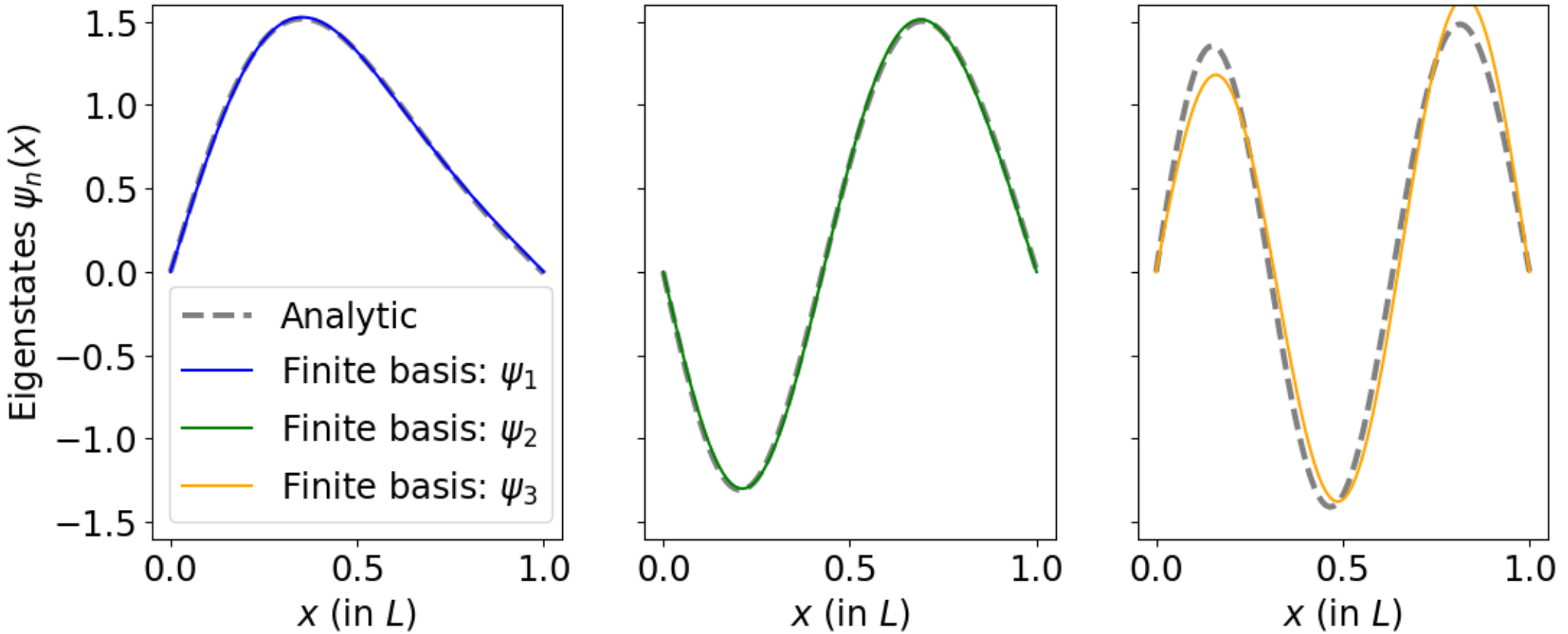
If we numerically calculate the overlap integrals:

$$H_{mn} = \begin{pmatrix} 1 & -0.54 & 0 \\ -0.54 & 4 & -0.584 \\ 0 & -0.584 & 9 \end{pmatrix}$$

When comparing resulting eigenvalues:

Eigenvalues	E_1	E_2	E_3
Finite basis approx.	0.90437	4.0279	9.068
Analytical solution	0.90419	4.0275	9.017

COMPARING EIGENSTATES



From the plot

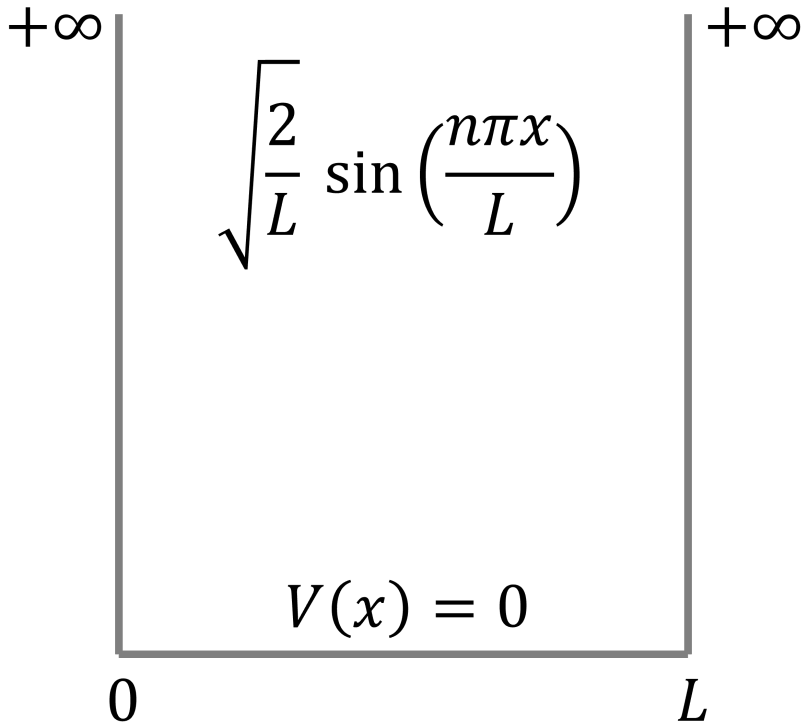
Finite basis method gives good results for lower eigenenergies/eigenstates

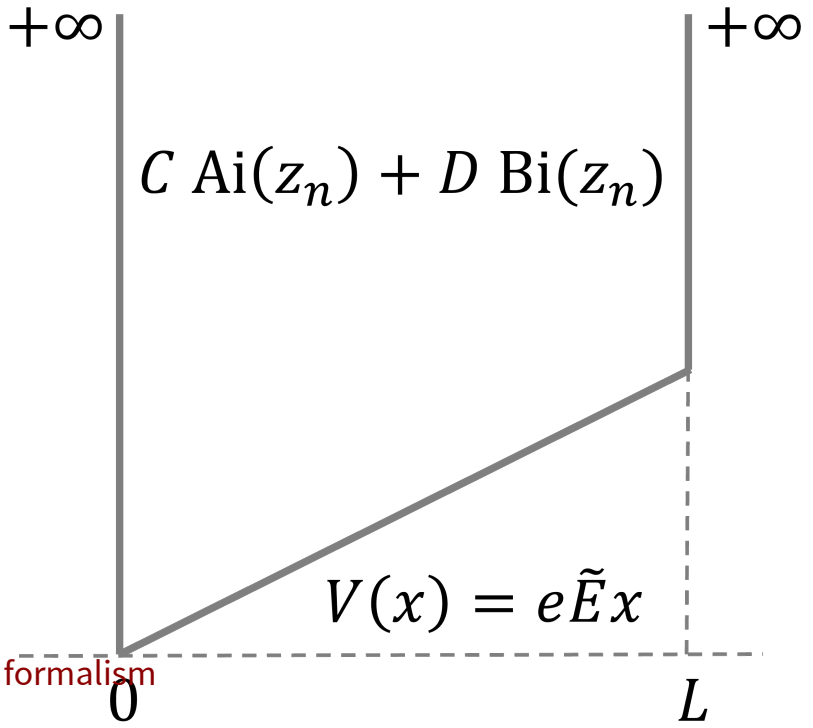
FINITE DIFFERENCE APPROXIMATION

FINITE DIFFERENCE APPROXIMATION

Steps to reach to the solutions:

1. Discretize the wave function (finite basis)
2. Finite Difference Method to discretize the Schr"odinger equation
3. Limited discrete points $\longrightarrow$ matrix algebra (Requires finite **box**)
4. Solve the eigenvalue equations for **eigenenergies** & **eigenstates**

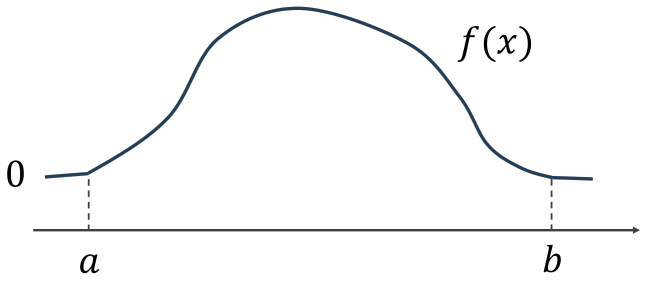


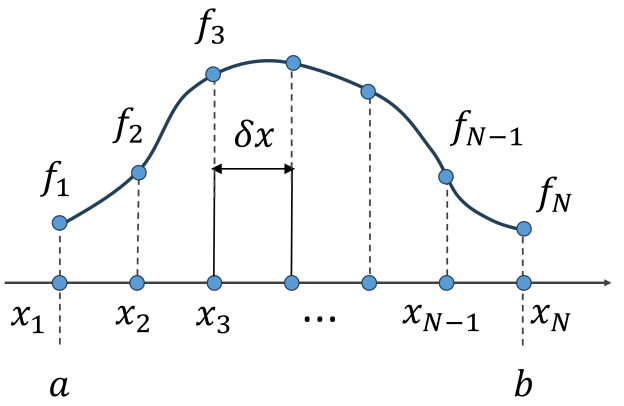


DISCRETIZING A FUNCTION

- A function on a computer as a vector:

$$f(x) = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_N) \end{pmatrix} \longrightarrow \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix}$$





A NORMALIZED STATE

- A normalized state requires: $\langle f|f\rangle = 1$
- If we define the normalized state as ket and bra:

$$|f\rangle = |f(x_j)\sqrt{\delta x}\rangle = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_N) \end{pmatrix} \longrightarrow \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix}$$

$$\langle f| = \langle f^*(x_j)\sqrt{\delta x}| \longrightarrow \begin{pmatrix} f_1^*\sqrt{\delta x} & f_2^*\sqrt{\delta x} & \cdots & f_N^*\sqrt{\delta x} \end{pmatrix}$$

And the inner product is:

$$\langle f|f\rangle = \langle f(x)|f(x)\rangle\delta x = \sum_{j=1}^{N} |f_j|^2 \delta x \quad \longleftrightarrow \quad \int_a^b |f(x)|^2 dx$$

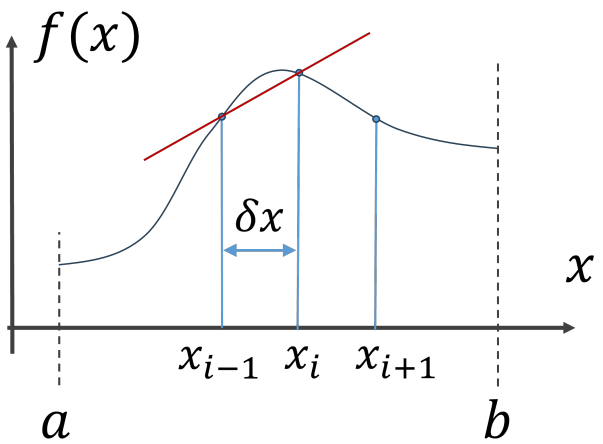
Lecture 06: Dirac formalism

FINITE DIFFERENCES

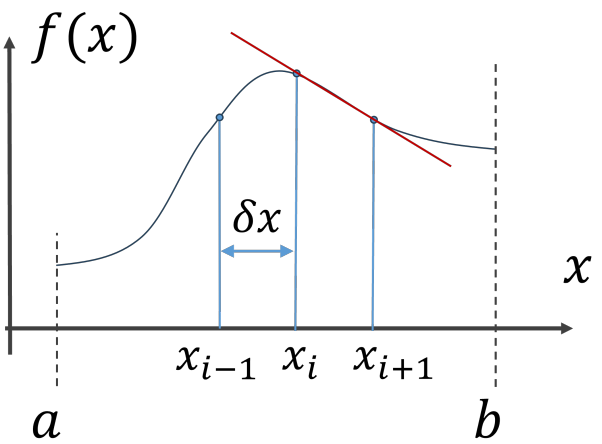
- Hamiltonian contains second derivative
- Derivative of a discrete function?

$$\text{Central difference scheme:} \quad \frac{df(x)}{dx} \longrightarrow \frac{\delta f(x)}{\delta x} = \frac{f_{i+1} - f(i-1)}{2\delta x}$$

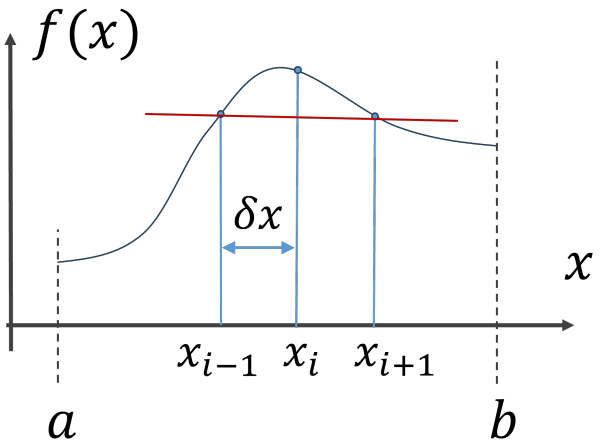
Backward difference



Forward difference



Central difference



SECOND DERIVATIVE

- Hamiltonian contains second derivative
- Derivative of a discrete function?

$$\text{Central difference scheme:} \quad \frac{df(x)}{dx} \longrightarrow \frac{\delta f(x)}{\delta x} = \frac{f_{i+1} - f(i-1)}{2\delta x}$$

- Second derivative by using central difference scheme with $\delta/2$

$$\frac{d^2 f(x)}{dx^2} \longrightarrow \frac{\frac{f_{i+1}-f_i}{\delta x} - \frac{f_i - f_{i-1}}{\delta x}}{\delta x} = \frac{f_{i+1} + f_{i-1} - 2f_i}{\delta x^2}$$

- Discrete potential function $V_i = V(x_i)$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \quad \longrightarrow \quad -\frac{\hbar^2}{2m}\frac{f_{i+1} + f_{i-1} - 2f_i}{\delta x^2} + V_i$$

Lecture 06: Dirac formalism

MATRIX FORM

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \quad \longrightarrow \quad -\frac{\hbar^2}{2m}\frac{f_{i+1} + f_{i-1} - 2f_i}{\delta x^2} + V_i$$

- The Hamiltonian can be written as a matrix operator

$$\hat{H} = -\frac{\hbar^2}{2m\,\delta x^2}\begin{pmatrix} 1 & 0 & & & & & \\ 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 1 & -2 & 1 & \\ & & & & 1 & -2 & 1 \\ & & & & & 0 & 1 \end{pmatrix} + V(x)1$$

MATRIX FORM (DIMENSIONLESS)

$$\hat{H} = -\frac{1}{\pi^2}\frac{d^2}{dx^2} + V(x) \quad \longrightarrow \quad -\frac{1}{\pi^2}\frac{f_{i+1} + f_{i-1} - 2f_i}{\delta x^2} + \nu_L\left(\frac{i}{N} - \frac{1}{2}\right)$$

- The Hamiltonian can be written as a matrix operator (E, ν_L in units of E_1^∞)

$$-\frac{1}{\pi^2\,\delta x^2}\begin{pmatrix} 1 & 0 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 0 & 1 \end{pmatrix} + \begin{pmatrix} V_1 & & & & \\ & V_2 & & & \\ & & \ddots & & \\ & & & V_{N-1} & \\ & & & & V_N \end{pmatrix}$$

MATRIX FORM (DIMENSIONLESS)

$$\hat{H} = -\frac{1}{\pi^2}\frac{d^2}{dx^2} + V(x) \quad \longrightarrow \quad -\frac{1}{\pi^2}\frac{f_{i+1} + f_{i-1} - 2f_i}{\delta x^2} + \nu_L\left(\frac{i}{N} - \frac{1}{2}\right)$$

- The Hamiltonian can be written as a matrix operator (E, ν_L in units of E_1^∞)

$$-\frac{1}{\pi^2\,\delta x^2}\begin{pmatrix} 1 & 0 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 0 & 1 \end{pmatrix} + \frac{\nu_L}{2N}\begin{pmatrix} -N & & & & \\ & -N+2 & & & \\ & & \ddots & & \\ & & & N-2 & \\ & & & & N \end{pmatrix}$$

$\longrightarrow$ Solve the eigenvalue equation: $\hat{H}|\psi_n\rangle = E_n|\psi_n$

Lecture 06: Dirac formalism

SOLVING LARGE MATRIX EQUATIONS

```python
import numpy as np
from scipy.sparse import diags_array
from scipy.sparse.linalg import eigsh, LaplacianNd

# Parameters
n = 500; L = 1.0; dx = L/(n-1)
x = np.linspace(0, L, n)
V = 5 * (x - L/2)

# Calculate E_n, Psi_n
lap = LaplacianNd(
  grid_shape=(n, ), boundary_conditions='dirichlet'
).tosparse().astype(np.float64)
Vmat = diags_array([V], offsets=[0]).toarray()
E_n, Psi_n = eigsh(-lap/np.pi**2/dx**2 + Vmat, k=3, which="SM")
print("Eigenvalues E1, E2, E3:\n\t\t" + str(np.round(E_n, 3)))
```

```
Eigenvalues E1, E2, E3:
        [0.729 4.038 8.976]
```

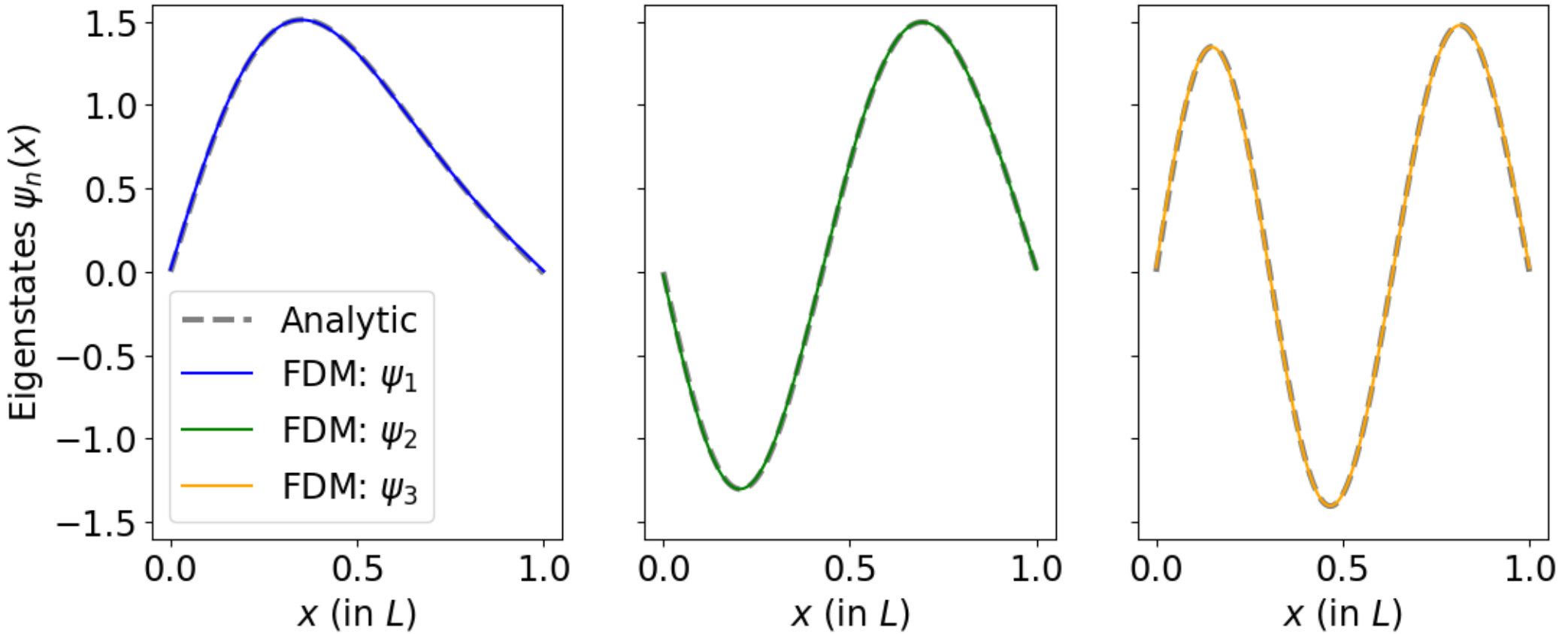
INFINITE WELL WITH ELECTRIC FIELD

$$\hat{H} = -\frac{1}{\pi^2}\frac{d^2}{dz^2} + \nu_L\,(z - 1/2) \quad \text{with} \quad \hat{H}_0 = -\frac{1}{\pi^2}\frac{d^2}{dz^2}$$

Eigenvalues	E_1	E_2	E_3
Finite difference	0.7293	4.0382	8.976
Finite basis approx.	0.9044	4.0279	9.068
Analytical solution	0.9042	4.0275	9.017

- Choosing initial basis functions not necessary
- Accurate potential $V(x)$ (δx dependent)
- *BAD* eigenenergies accuracy? Wave function accuracy *GOOD*?

WAVE FUNCTION COMPARISON

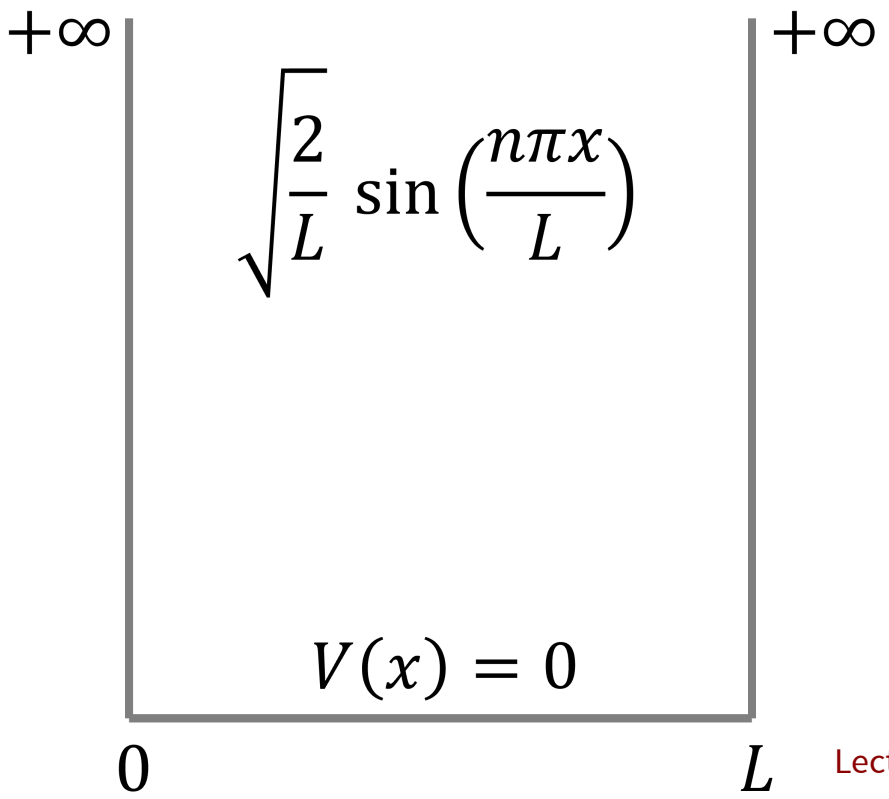


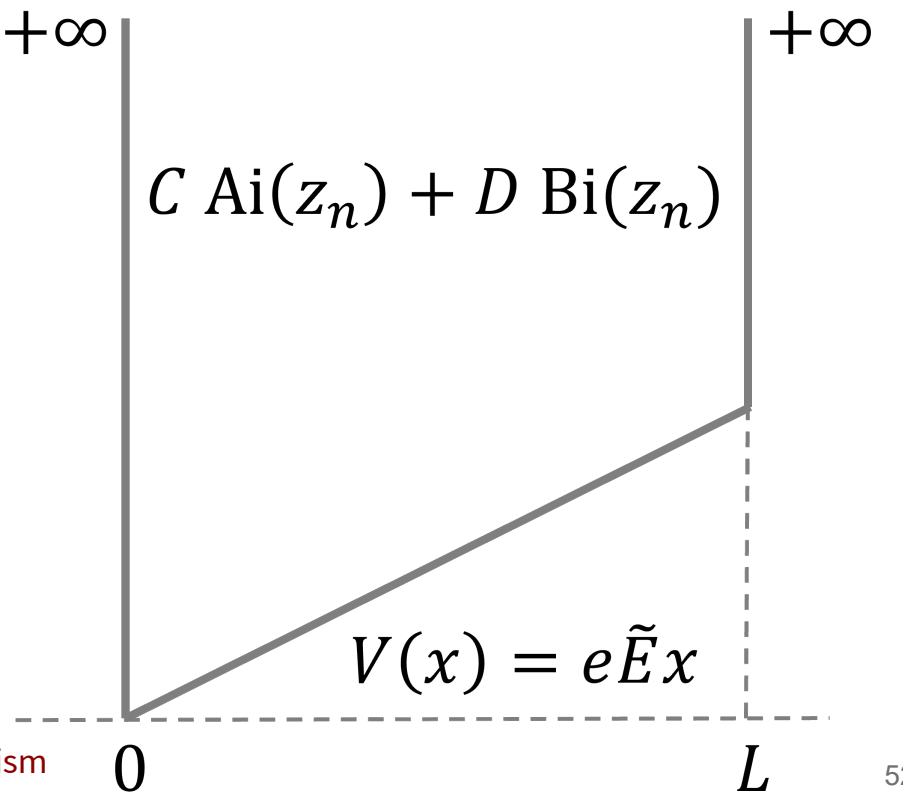
TIME-INDEPENDENT PERTURBATION THEORY

PERTURBATION THEORY

Steps to reach to the solutions:

1. $\hat{H} = \hat{H}_0 + \gamma \hat{H}_p$ Assume the perturbation to be small
2. Expand both the **eigenenergies** & **eigenstates** into power series in γ
3. Recursive relations for **eigenenergies** & **eigenstates**



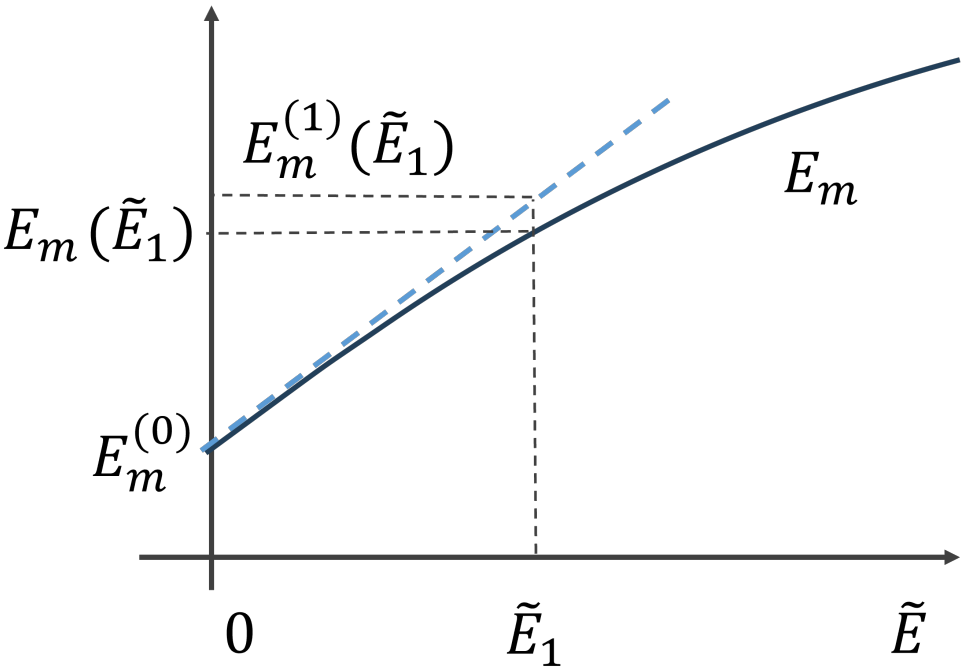


EXAMPLE OF STANDARD PERTURBATION

- Putting on a “small” electric field
- Approximating the effect of $V(x) = e\tilde{E}(x - L/2) \equiv \varepsilon z$ by power series:

$$E_m = E_m^{(0)} + \alpha_1 \varepsilon + \alpha_2 \varepsilon^2 + \ldots$$

- Eigenstates $|\psi_m\rangle$ extracted from E_m
- $\varepsilon \ll 1 \longrightarrow$ higher orders zero
- Can we generalize perturbations?



PERTURBATION PART OF HAMILTONIAN

- Independent of the actual perturbation form
- Known solutions for the unperturbed part $\hat{H}_0$

$$\hat{H}_0|\psi_n\rangle = E_n|\psi_n\rangle$$

- Perturbation of $\hat{H}_0$ by “small” perturbing part $\hat{H}_p$:

$$\hat{H} = \hat{H}_0 + \gamma\hat{H}_p$$

- We can express the eigenenergies E and eigenstates $|\phi\rangle$:

$$\hat{H}|\phi\rangle = (\hat{H}_0 + \gamma\hat{H}_p)|\phi\rangle = E|\phi\rangle$$

POWER SERIES EXPANSION

$$\hat{H}|\phi\rangle = (\hat{H}_0 + \gamma \hat{H}_p)|\phi\rangle = E|\phi\rangle$$

Expand E and $|\phi\rangle$ as power series in γ:

$$E = E^{(0)} + \gamma E^{(1)} + \gamma^2 E^{(2)} + \gamma^3 E^{(3)} + \gamma^4 E^{(4)} + \dots$$

$$|\phi\rangle = |\phi^{(0)}\rangle + \gamma|\phi^{(1)}\rangle + \gamma^2|\phi^{(2)}\rangle + \gamma^3|\phi^{(3)}\rangle + \gamma^4|\phi^{(4)}\rangle + \dots$$

Schrodinger equation becomes:

$$(\hat{H}_0 + \gamma \hat{H}_p)\left(|\phi^{(0)}\rangle + \gamma|\phi^{(1)}\rangle + \gamma^2|\phi^{(2)}\rangle + \dots\right) =$$
$$\left(E^{(0)} + \gamma E^{(1)} + \gamma^2 E^{(2)} + \dots\right)\left(|\phi^{(0)}\rangle + \gamma|\phi^{(1)}\rangle + \gamma^2|\phi^{(2)}\rangle + \dots\right)$$

$\longrightarrow$ Equate coefficients of same order in γ

ZEROTH ORDER PERTURBATION

$$(\hat{H}_0 + \gamma \hat{H}_p)\left(|\phi^{(0)}\rangle + \gamma|\phi^{(1)}\rangle + \gamma^2|\phi^{(2)}\rangle + \ldots\right) =$$
$$\left(E^{(0)} + \gamma E^{(1)} + \gamma^2 E^{(2)} + \ldots\right)\left(|\phi^{(0)}\rangle + \gamma|\phi^{(1)}\rangle + \gamma^2|\phi^{(2)}\rangle + \ldots\right)$$

- zeroth order in γ:

$$\hat{H}_0|\phi^{(0)}\rangle = E^{(0)}|\phi^{(0)}\rangle \quad \longrightarrow \quad |\psi_m\rangle \equiv |\phi^{(0)}\rangle, \quad E_m \equiv E^{(0)}$$

- These are the solutions of the unperturbed Hamiltonian

MATCHING ORDERS

$$(\hat{H}_0 + \gamma \hat{H}_p)\left(|\psi_m\rangle + \gamma|\phi^{(1)}\rangle + \gamma^2|\phi^{(2)}\rangle + \ldots\right) =$$
$$\left(E_m + \gamma E^{(1)} + \gamma^2 E^{(2)} + \ldots\right)\left(|\psi_m\rangle + \gamma|\phi^{(1)}\rangle + \gamma^2|\phi^{(2)}\rangle + \ldots\right)$$

Matching orders in γ

$$\hat{H}_0|\psi_m\rangle = E_m|\psi_m\rangle$$

$$\hat{H}_0|\phi^{(1)}\rangle + \hat{H}_p|\psi_m\rangle = E_m|\phi^{(1)}\rangle + E^{(1)}|\psi_m\rangle$$

$$\hat{H}_0|\phi^{(2)}\rangle + \hat{H}_p|\phi^{(1)}\rangle = E_m|\phi^{(2)}\rangle + E^{(1)}|\phi^{(1)}\rangle + E^{(2)}|\psi_m\rangle$$

MATCHING ORDERS CTU'D

$$\hat{H}_0|\psi_m\rangle = E_m|\psi_m\rangle$$
$$\hat{H}_0|\phi^{(1)}\rangle + \hat{H}_p|\psi_m\rangle = E_m|\phi^{(1)}\rangle + E^{(1)}|\psi_m\rangle$$
$$\hat{H}_0|\phi^{(2)}\rangle + \hat{H}_p|\phi^{(1)}\rangle = E_m|\phi^{(2)}\rangle + E^{(1)}|\phi^{(1)}\rangle + E^{(2)}|\psi_m\rangle$$

Rewrite highest order state to the left-hand-side:

$$(\hat{H}_0 - E_m)|\psi_m\rangle = 0$$
$$(\hat{H}_0 - E_m)|\phi^{(1)}\rangle = (E^{(1)} - \hat{H}_p)|\psi_m\rangle$$
$$(\hat{H}_0 - E_m)|\phi^{(2)}\rangle = (E^{(1)} - \hat{H}_p)|\phi^{(1)}\rangle + E^{(2)}|\psi_m\rangle$$

FIRST ORDER PERTURBATION THEORY

$$
\begin{aligned}
(\hat{H}_0 - E_m)|\psi_m\rangle &= 0 \\
(\hat{H}_0 - E_m)|\phi^{(1)}\rangle &= (E^{(1)} - \hat{H}_p)|\psi_m\rangle \\
(\hat{H}_0 - E_m)|\phi^{(2)}\rangle &= (E^{(1)} - \hat{H}_p)|\phi^{(1)}\rangle + E^{(2)}|\psi_m\rangle
\end{aligned}
$$

Left-multiply by the bra $\langle\psi_m|$

$$
\begin{aligned}
\text{left-hand-side:} \quad & \langle\psi_m|(\hat{H}_0 - E_m)|\phi^{(1)}\rangle = \langle\psi_m|(E_m - E_m)|\phi^{(1)}\rangle = 0 \\
\text{right-hand-side:} \quad & \langle\psi_m|(E^{(1)} - \hat{H}_p)|\psi_m\rangle = E^{(1)} - \langle\psi_m|\hat{H}_p|\psi_m\rangle
\end{aligned}
$$

$$
\implies E^{(1)} = \langle\psi_m|\hat{H}_p|\psi_m\rangle
$$

- First order correction to the eigenenergy: $E_m + E^{(1)}$

FIRST ORDER EIGENSTATE

- Expand first order correction eigenstate: $|\phi^{(1)}\rangle = \sum_n a_n^{(1)} |\psi_n\rangle$
- Filling in:

$$(\hat{H}_0 - E_m)|\phi^{(1)}\rangle = (E^{(1)} - \hat{H}_p)|\psi_m\rangle$$

$$\text{left-hand-side:} \quad \langle\psi_i|(\hat{H}_0 - E_m)|\phi^{(1)}\rangle = (E_i - E_m)\langle\psi_i|\phi^{(1)}\rangle = (E_i - E_m)a_i^{(1)}$$

$$\text{right-hand-side:} \quad \langle\psi_i|(E^{(1)} - \hat{H}_p)|\psi_m\rangle = E^{(1)}\langle\psi_i|\psi_m\rangle - \langle\psi_i|\hat{H}_p|\psi_m\rangle$$

$$\implies \qquad a_i^{(1)} = \frac{\langle\psi_i|\hat{H}_p|\psi_m\rangle}{E_m - E_i}$$

$$\implies \qquad |\phi^{(1)}\rangle = \sum_{n\neq m} \frac{\langle\psi_n|\hat{H}_p|\psi_m\rangle}{E_m - E_n}|\psi_n\rangle$$

ELECTRIC FIELD AS PERTURBATION

Up to first order we have:

$$|\psi_m\rangle \longrightarrow |\psi_m\rangle + |\phi_m^{(1)}\rangle = |\psi_m\rangle + \sum_{n\neq m} \frac{\langle\psi_n|\hat{H}_p|\psi_m\rangle}{E_m - E_n}|\psi_n\rangle$$

$$E_m \longrightarrow \quad E_m + E^{(1)} = E_m + \langle\psi_m|\hat{H}_p|\psi_m\rangle$$

The Hamiltonian in dimensionless units:

$$\hat{H} = -\frac{1}{\pi^2}\frac{d^2}{dz^2} + \nu_L\,(z - 1/2) \quad \text{with} \quad \hat{H}_0 = -\frac{1}{\pi^2}\frac{d^2}{dz^2}$$

- The Hamiltonian gives contributions of eigenstates $\psi_n(z) = \sqrt{2}\sin(n\pi z)$
- Eigenenergies E_n and potential ν_L are in units of $E_1^\infty = \frac{\hbar^2\pi^2}{2mL^2}$

FIRST ORDER CORRECTION

The correction in the energies is zero (no change):

$$\begin{aligned} E_m + E_m^{(1)} &= E_m + \langle \psi_m | \hat{H}_p | \psi_m \rangle \\ &= m^2 \ + \ \nu_L \int_0^1 (z - 1/2) \sin^2(m\pi z) dz, \\ &= m^2 + 0 = m^2 \end{aligned}$$

$$\begin{aligned} |\psi_m\rangle + |\phi_m^{(1)}\rangle &= |\psi_m\rangle + \sum_{n \neq m} \frac{\langle \psi_n | \hat{H}_p | \psi_m \rangle}{E_m - E_n} |\psi_n\rangle \\ &= |\psi_m\rangle \ - \sum_{n \neq m} \frac{2\nu_L}{m^2 - n^2} \int_0^1 (z - 1/2) \sin(m\pi z) \sin(n\pi z) dz \ |\psi_n\rangle \\ &= |\psi_m\rangle \ - \sum_{n = m \pm 1, \pm 3, \ldots} \frac{2\nu_L}{m^2 - n^2} \ \frac{4nm}{\pi^2 (m^2 - n^2)^2} \ |\psi_n\rangle \end{aligned}$$

FIRST ORDER CORRECTION CTU'D

Where the second integral was obtained from:

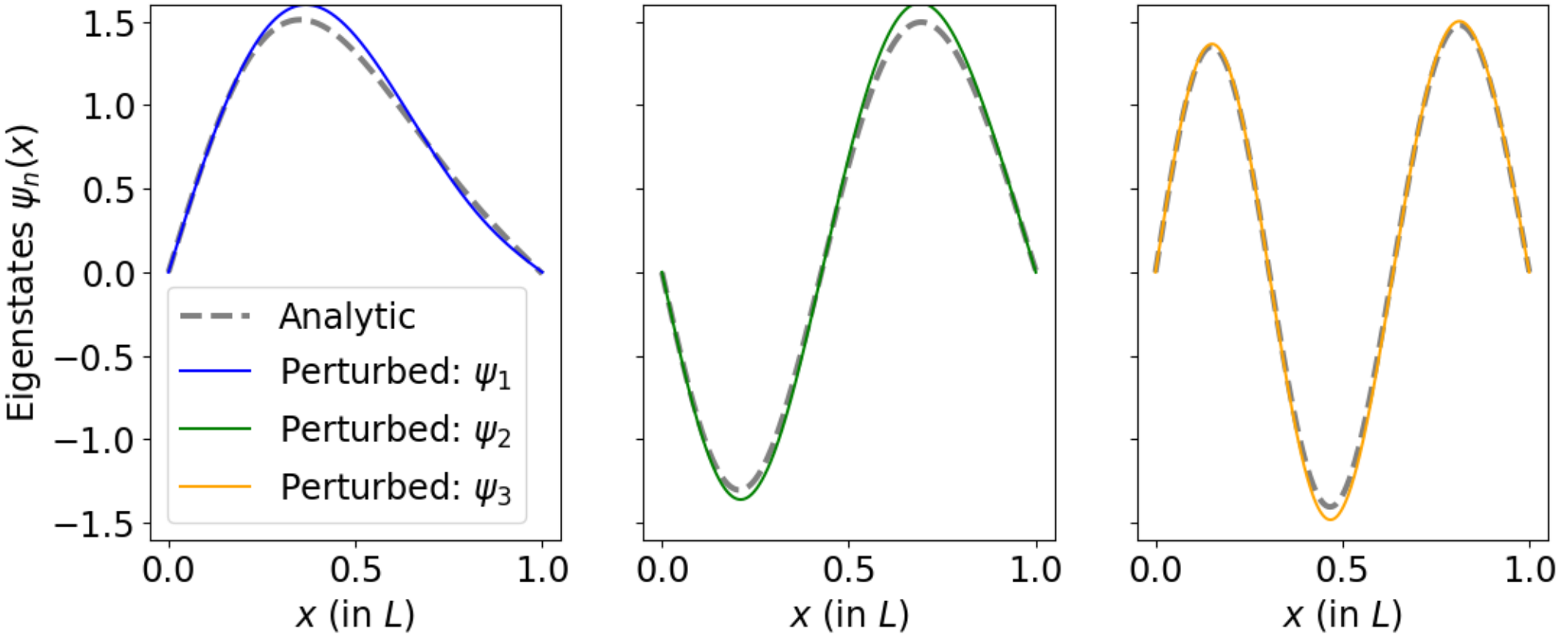
$$\int_0^1 (z-1/2)\sin(m\pi z)\sin(n\pi z)dz = \begin{cases} \dfrac{4nm}{\pi^2(m^2-n^2)^2} & \text{if } m+n \text{ is odd} \\ 0 & \text{if } m+n \text{ is even} \end{cases}$$

So we have for eigenenergies and eigenstates:

$$E_m + E_m^{(1)} = m^2$$

$$|\psi_m\rangle + |\psi_m^{(1)}\rangle = \sqrt{2}\sin(m\pi z) \; + \sum_{n=m\pm 1,\pm 3,\ldots} \frac{8nm\nu_L\sqrt{2}}{\pi^2(m^2-n^2)^3}\sin(n\pi z)$$

WAVE FUNCTION COMPARISON



For 2nd order perturbation theory: see Chapter 6 of David Miller's book