Section 5

Analytical Solutions to Free and Bound Electrons

5.2 Electrons in a finite potential well

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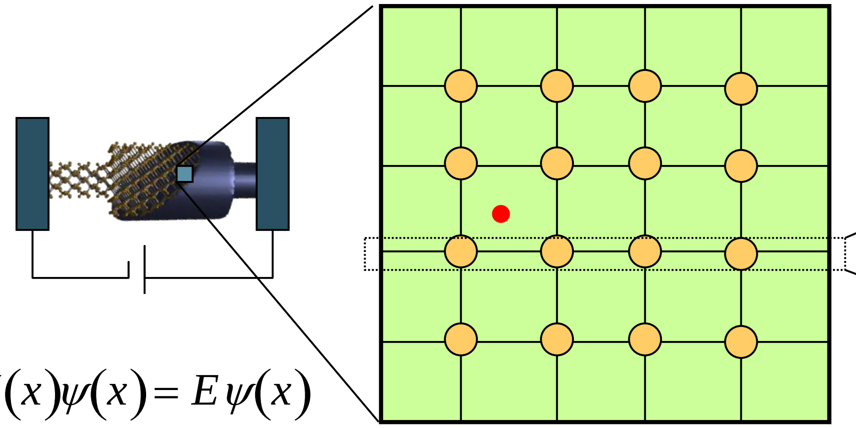
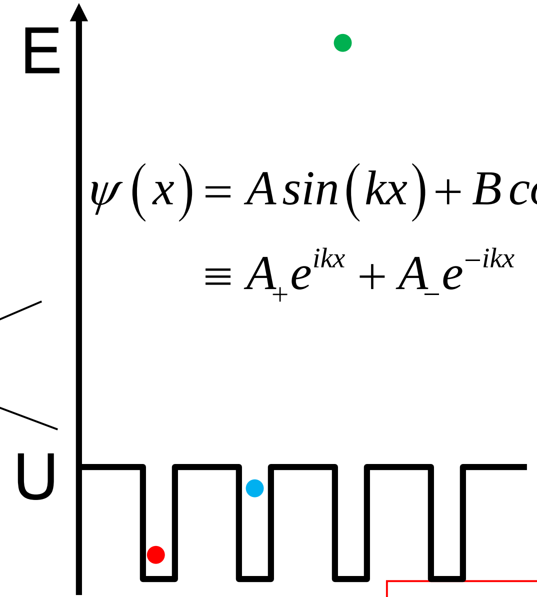
School of Electrical and Computer Engineering

Section 5
Analytical Solutions to Free and Bound Electrons

Original Problem | Periodic Structure



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



$$\psi(x)=A\sin(kx)+B\cos(kx)$$
$$\equiv A_+e^{ikx}+A_-e^{-ikx}$$

Case 1:
Free electron
E >> U

Case 3:
Electron in finite well
E < U

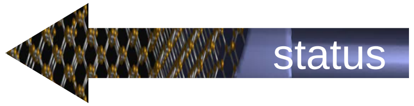
Case 2:
Electron in infinite well
E << U

- Section 5.1 – Free and Tightly Bound Electrons
  - »Time Independent Schrödinger Equation
  - »(Almost) Free Electrons
  - »Tightly bound electrons – infinite potential well

$$E_n=\frac{\hbar^2\pi^2}{2mL_x^2}n^2$$

$$\therefore \psi_n(x)=\sqrt{\frac{2}{L_x}}\sin\left(\frac{n\pi}{L_x}x\right),\quad n=1,2,3,\ldots \quad 0<x<L_x$$

- Section 5.2 - Electrons in a finite potential well

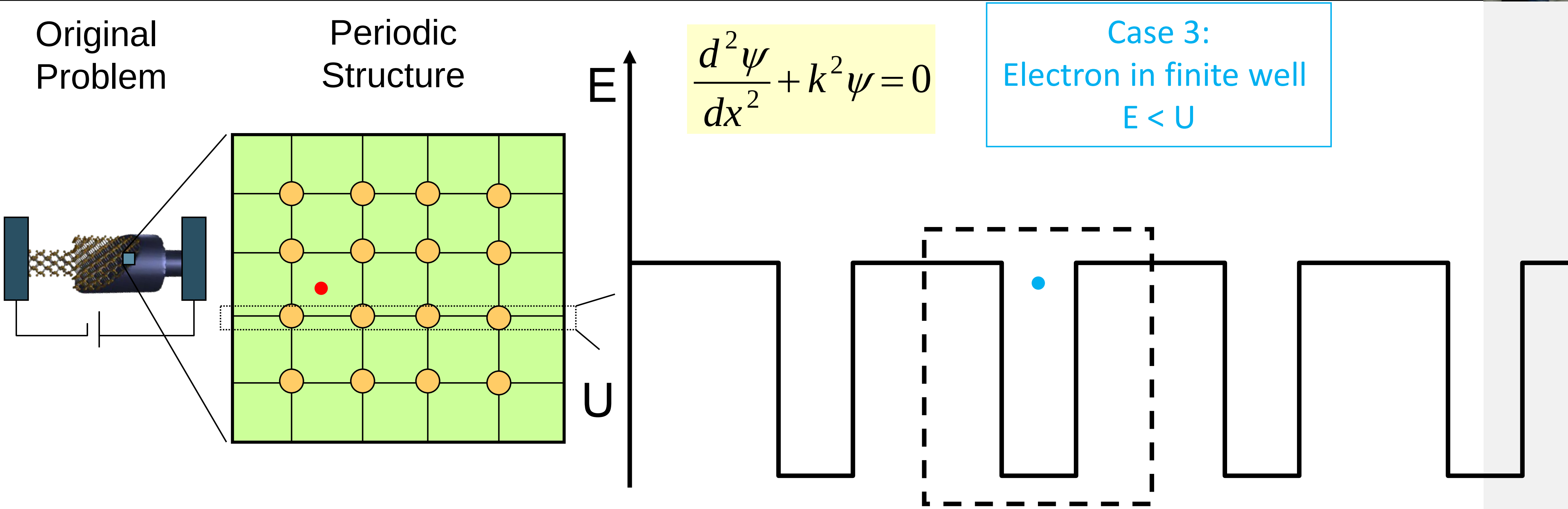


Reference: Vol. 6, Ch. 2 (pages 29-45)

One Video Segment

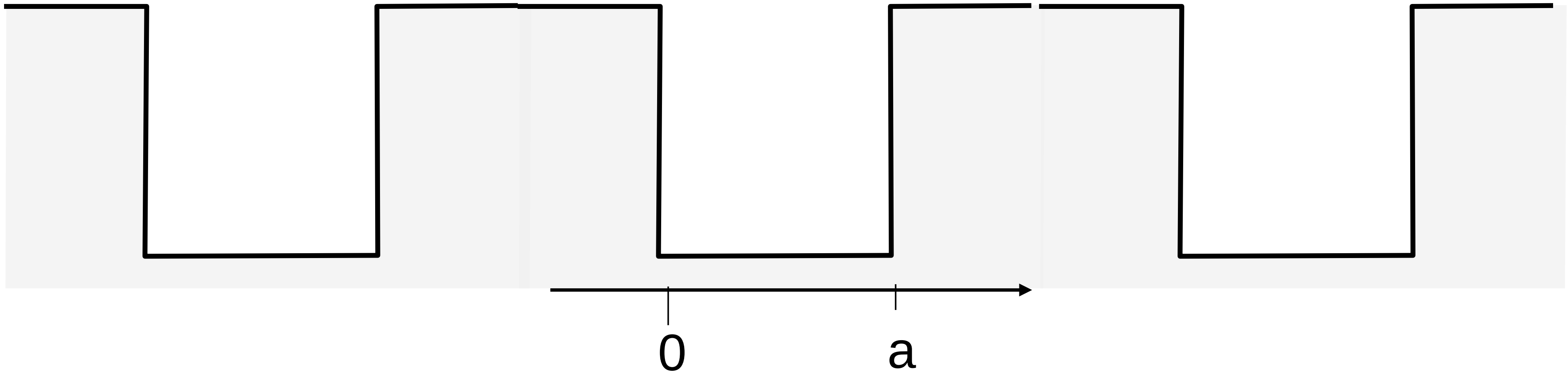
One Video Segment

Select a Single Well



$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

Case 3:
Electron in finite well
E < U

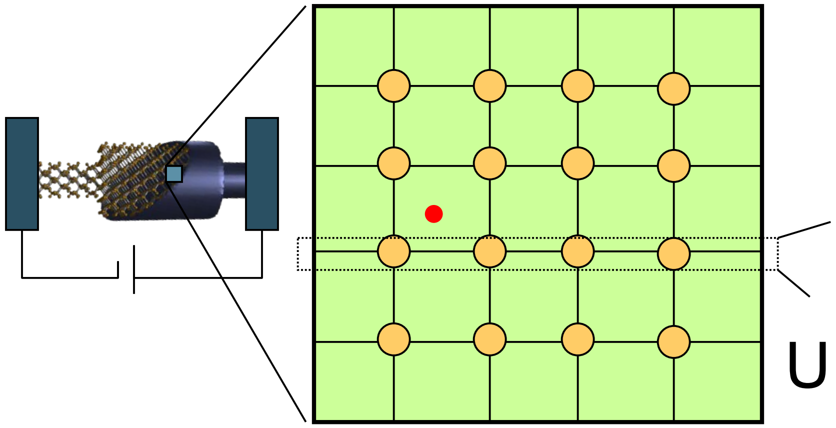


Assume Other Wells are De-Coupled

Case 3:
Electron in finite well
E < U

Original Problem

Periodic Structure



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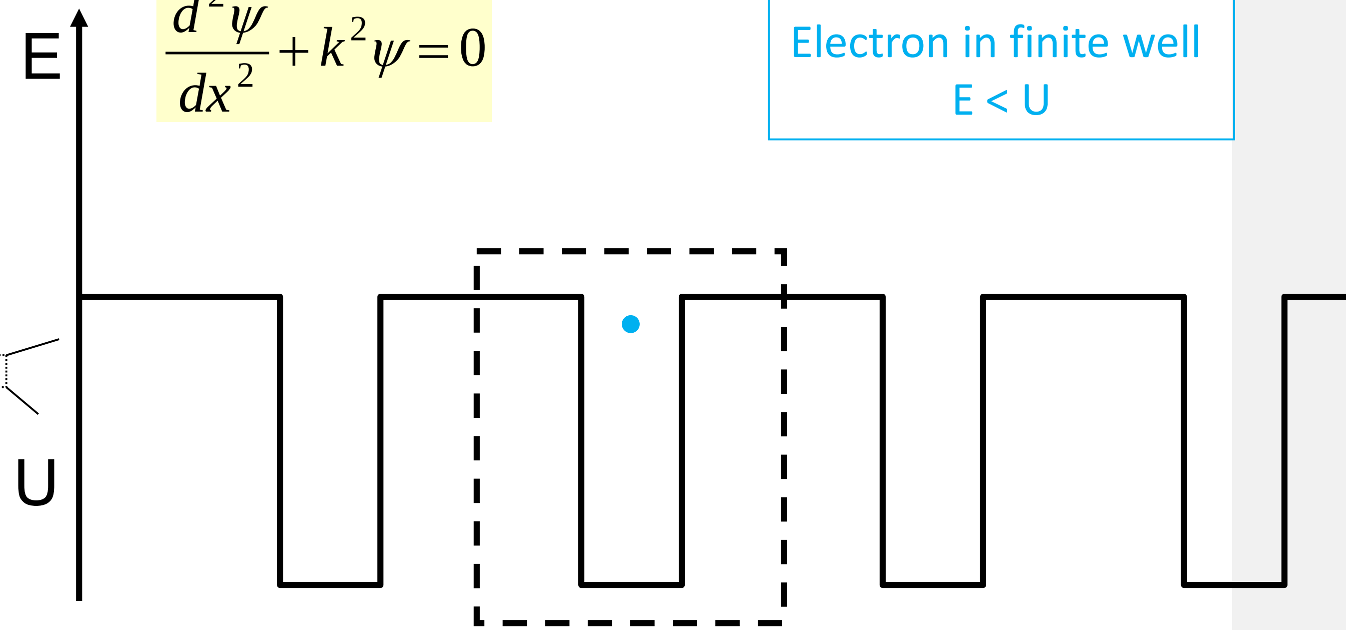
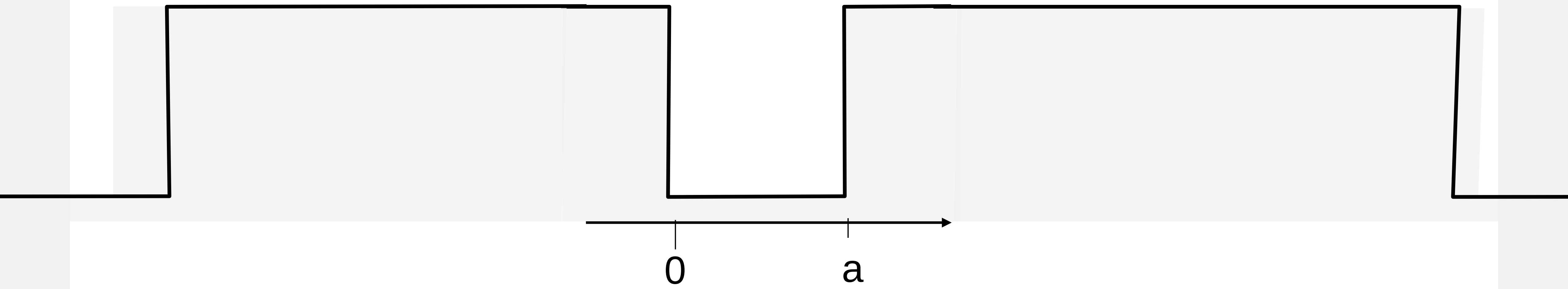
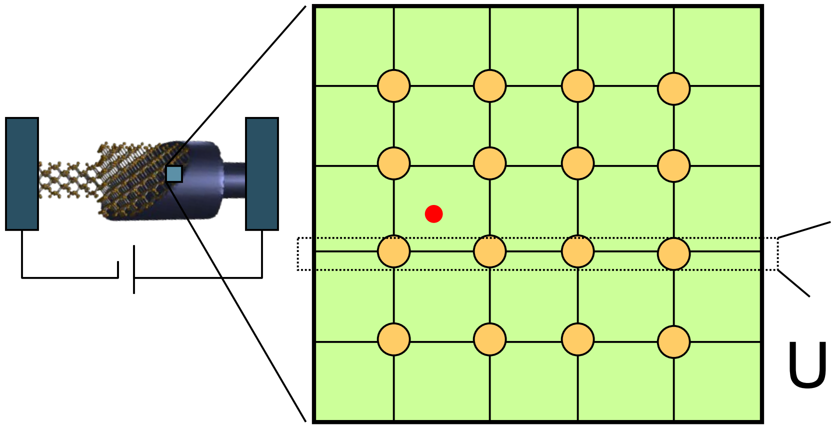


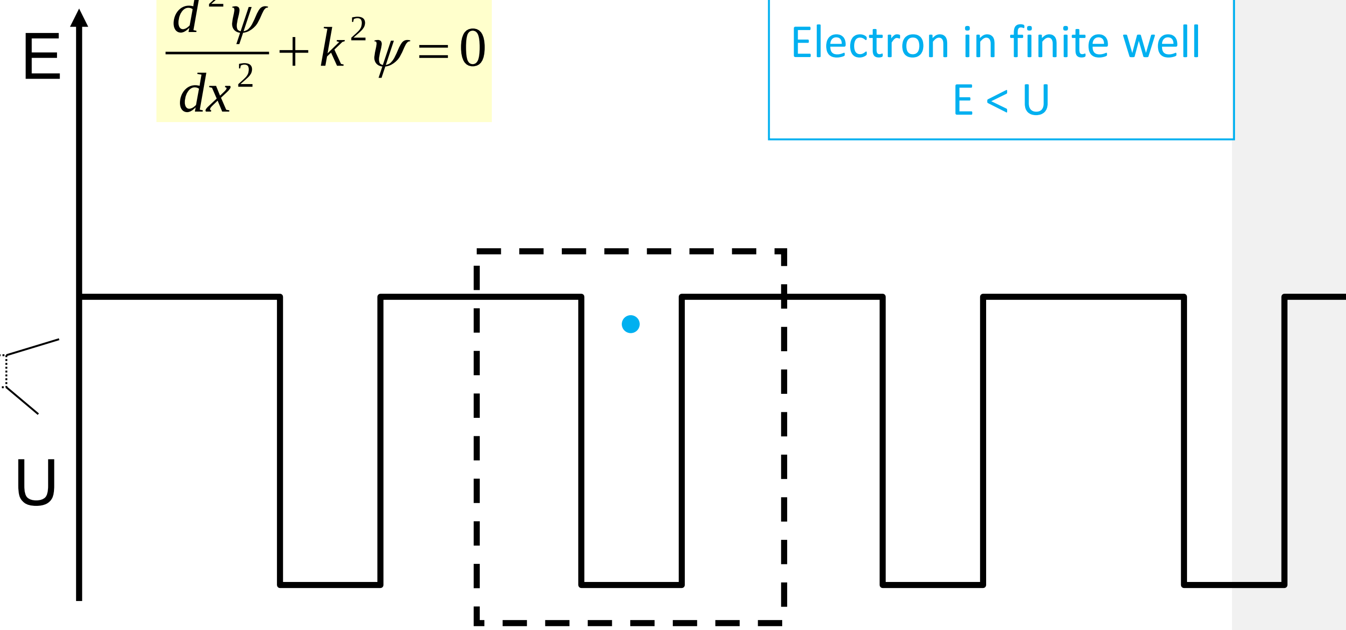
Assume the other wells are very far away



Assume a Reasonable Wavefunction Shape

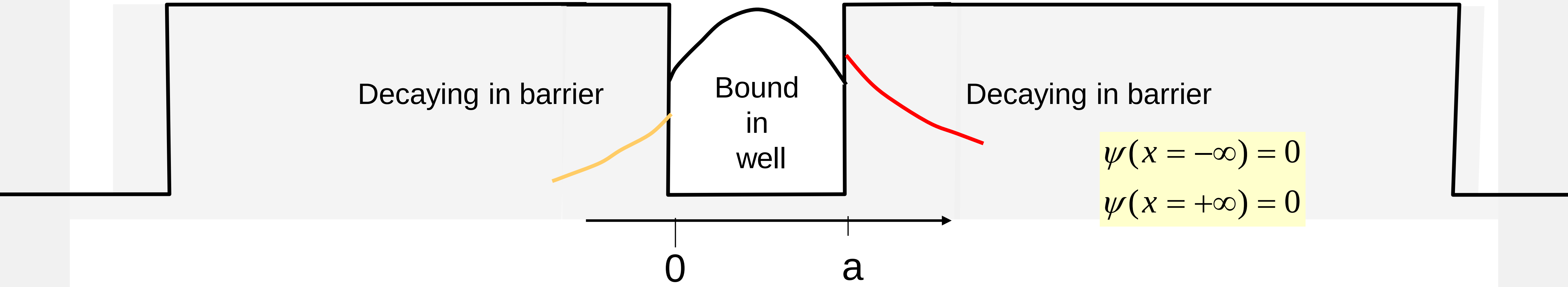


$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$



Case 3:
Electron in finite well
E < U

Assume some general shape of the wavefunction



$$\psi(x = -\infty) = 0$$
$$\psi(x = +\infty) = 0$$

Wavefunction Continuity Conditions

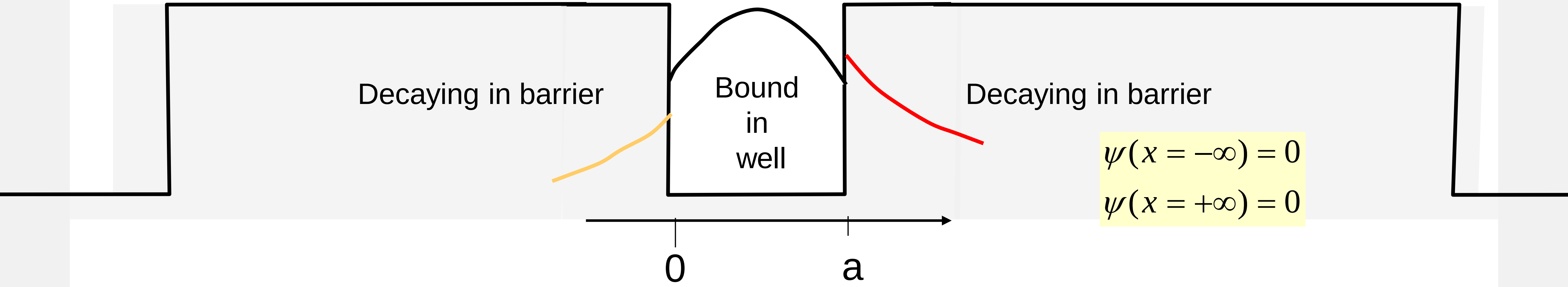
Case 3:
Electron in finite well
E < U

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

Second order differential equation
First and second order differential cannot be infinite!

Wavefunction must be continuous!
First differential must be continuous!

Assume some general shape of the wavefunction



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First Differential Must be Continuous

Case 3:
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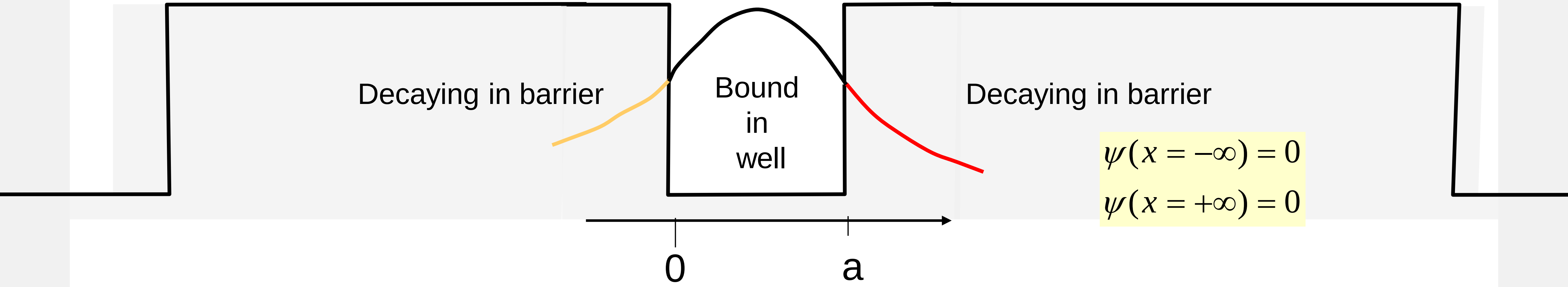
Second order differential equation
First and second order differential cannot be infinite!

Wavefunction must be continuous!
First differential must be continuous!

$$\psi\Big|_{x=x_B^-} = \psi\Big|_{x=x_B^+}$$

$$\left.\frac{d\psi}{dx}\right|_{x=x_B^-} = \left.\frac{d\psi}{dx}\right|_{x=x_B^+}$$



$$\psi(x = -\infty) = 0$$

$$\psi(x = +\infty) = 0$$

Solution Ansatz

Case 3:
Electron in finite well
E < U

$$\psi\Big|_{x=x_B^-} = \psi\Big|_{x=x_B^+}$$

$$\frac{d\psi}{dx}\Big|_{x=x_B^-} = \frac{d\psi}{dx}\Big|_{x=x_B^+}$$

$$\psi(x=-\infty)=0$$

$$\psi(x=+\infty)=0$$

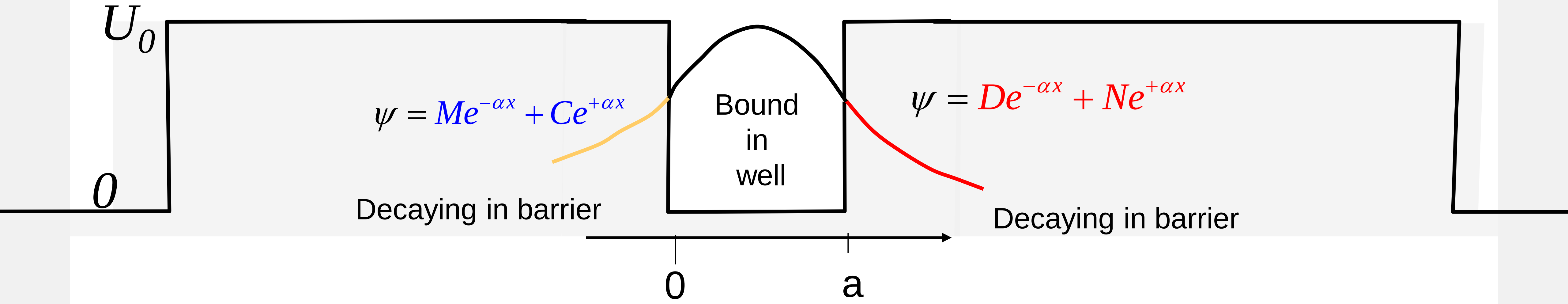
$$\frac{d^2\psi}{dx^2} - \alpha^2\psi = 0$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

$$\alpha \equiv \frac{\sqrt{2m_0[U_0-E]}}{\hbar}$$

$$k \equiv \frac{\sqrt{2m_0E}}{\hbar}$$

$$\psi = A\sin kx + B\cos kx$$



Solution Ansatz

Case 3:
Electron in finite well
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$$\psi\Big|_{x=x_B^-} = \psi\Big|_{x=x_B^+}$$

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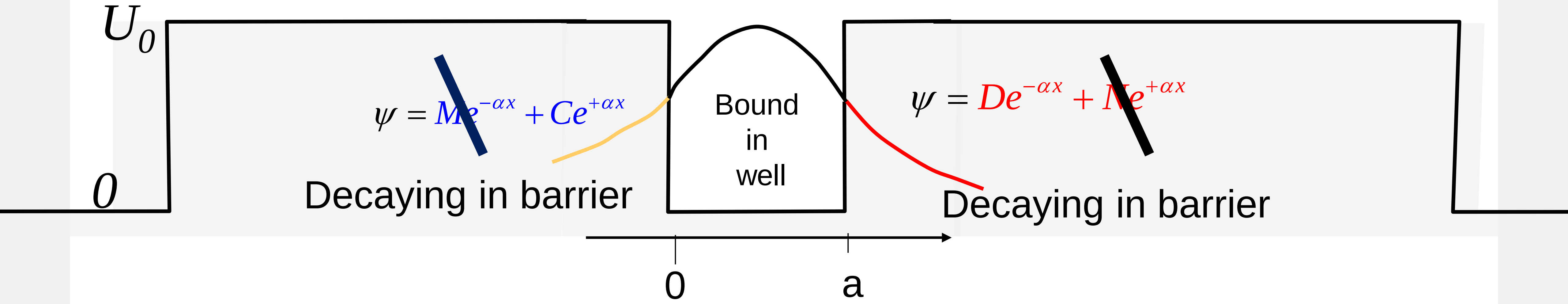


Apply Boundary Conditions at Interfaces

Case 3:
Electron in finite well
E < U

3) Boundary at each interface

$$\psi\Big|_{x=x_B^-} = \psi\Big|_{x=x_B^+}$$

$$\frac{d\psi}{dx}\Big|_{x=x_B^-} = \frac{d\psi}{dx}\Big|_{x=x_B^+}$$

$x=0$:

$$C = B$$
$$\alpha C = +kA$$

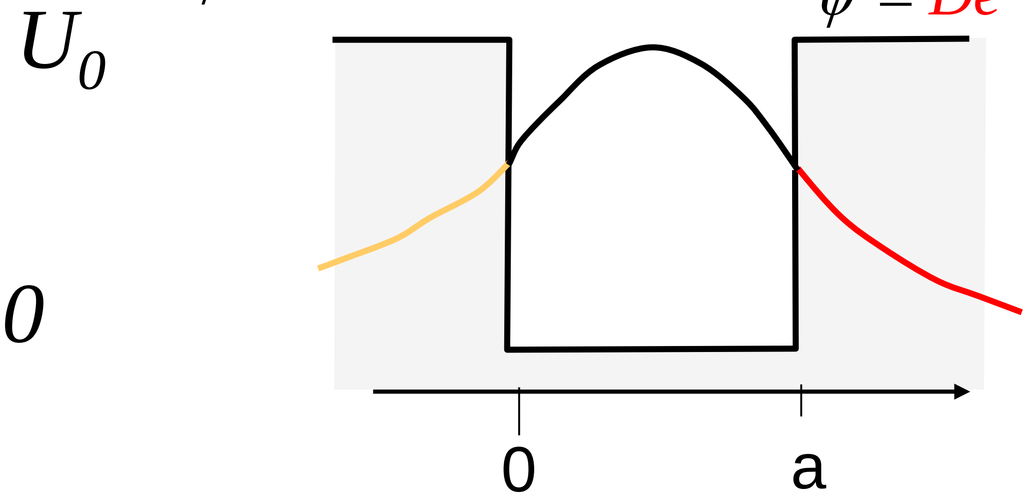
$x=a$:

$$A\sin(ka) + B\cos(ka) = De^{-\alpha a}$$
$$kA\cos(ka) - kB\sin(ka) = -\alpha De^{-\alpha a}$$

$$\psi = A\sin kx + B\cos kx$$

$$\psi = Ce^{\alpha x}$$

$$\psi = De^{-\alpha x}$$



$$\begin{pmatrix} 0 & 1 & +1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & -e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & \alpha e^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Apply Boundary Conditions at Interfaces

Case 3:
Electron in finite well
E < U

Only unknown is E

$$\tan(\alpha a\sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$

$$k \equiv \frac{\sqrt{2m_0 E}}{\hbar}$$

$$\xi \equiv \frac{E}{U_0}$$

$$\alpha \equiv \frac{\sqrt{2m_0[U_0 - E]}}{\hbar}$$

(i) Use Matlab function
(ii) Use graphical method

det (Matrix)=0

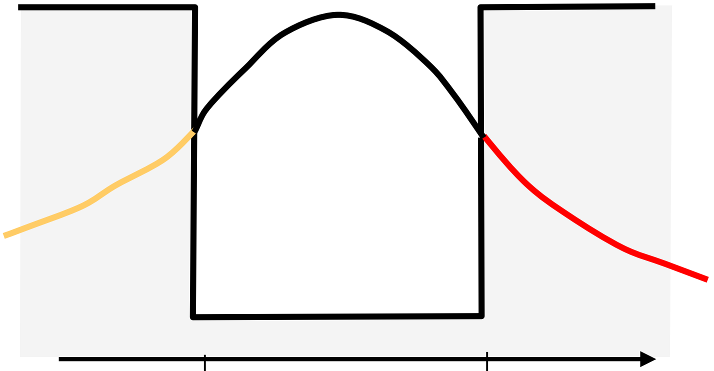
$$\psi = A\sin kx + B\cos kx$$

$$\psi = Ce^{\alpha x}$$

$$\psi = De^{-\alpha x}$$

U_0

0



0 a

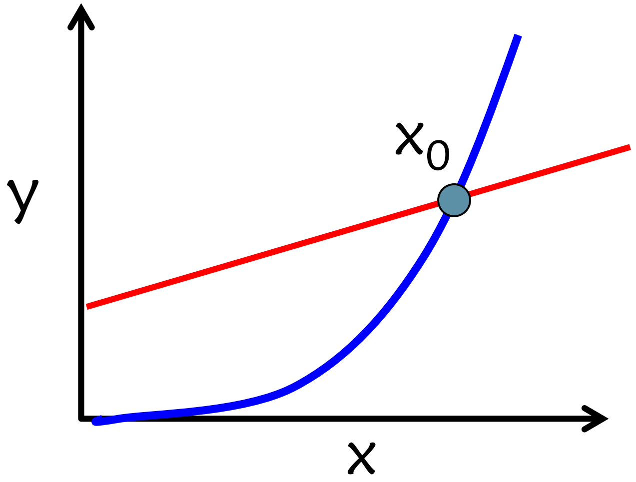
$$\begin{pmatrix} 0 & 1 & +1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & -e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & \alpha e^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Graphical Solution

Case 3:
Electron in finite well
E < U

$$x^2 = x + 5$$

$$y_1 = x^2 \quad y_2 = x + 5$$



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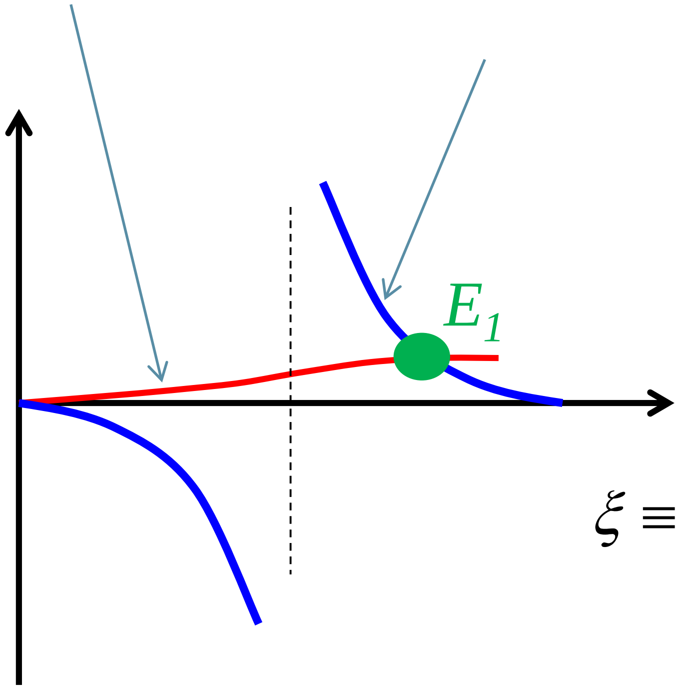

$$\xi \equiv \frac{E}{U_0}$$

Graphical Solution

Case 3:
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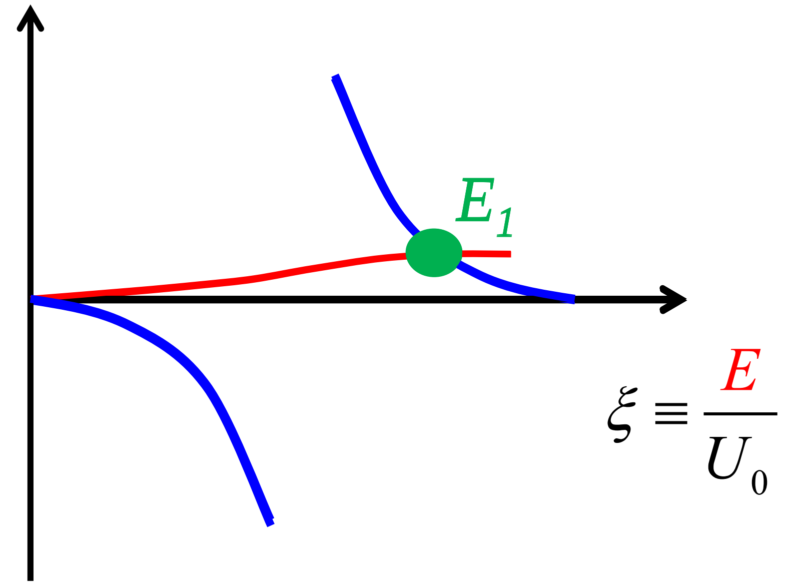
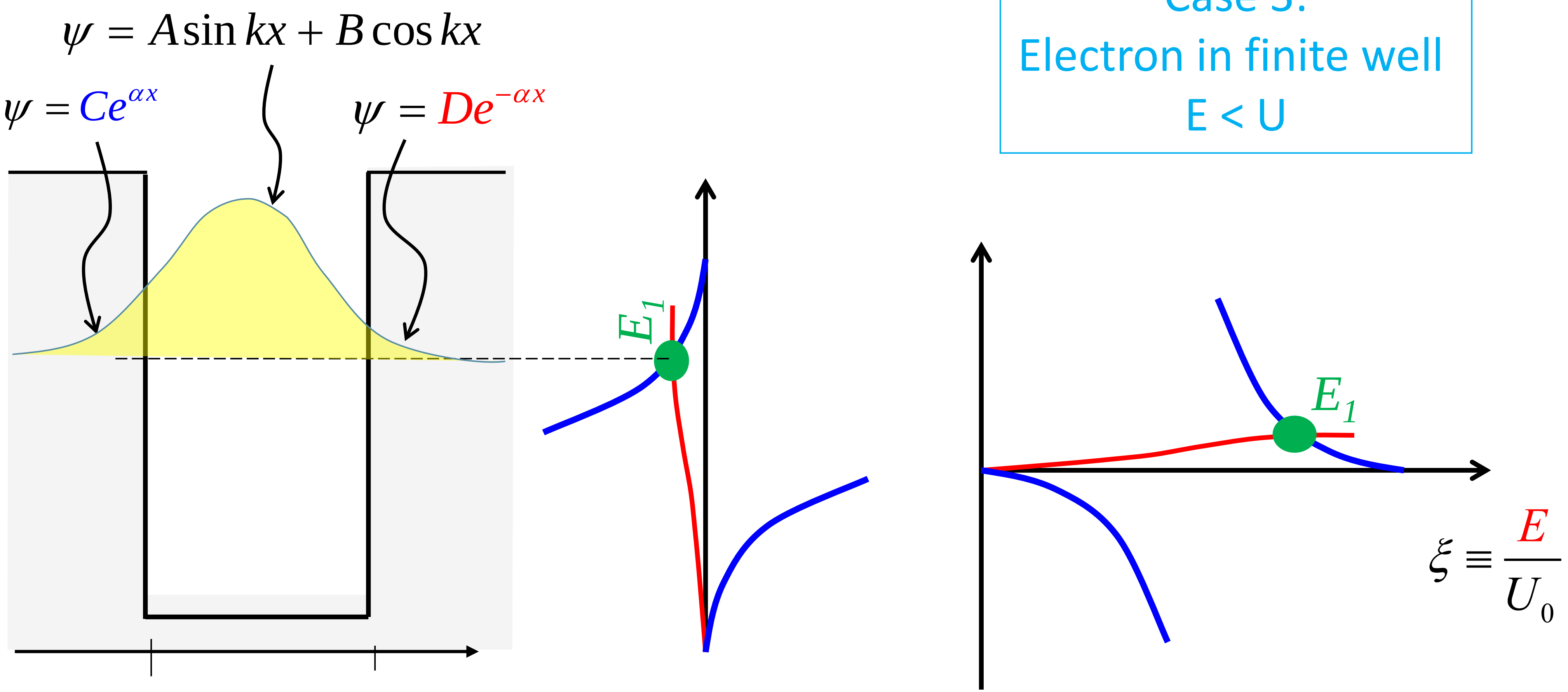


Graphical Solution



Case 3:
Electron in finite well
E < U

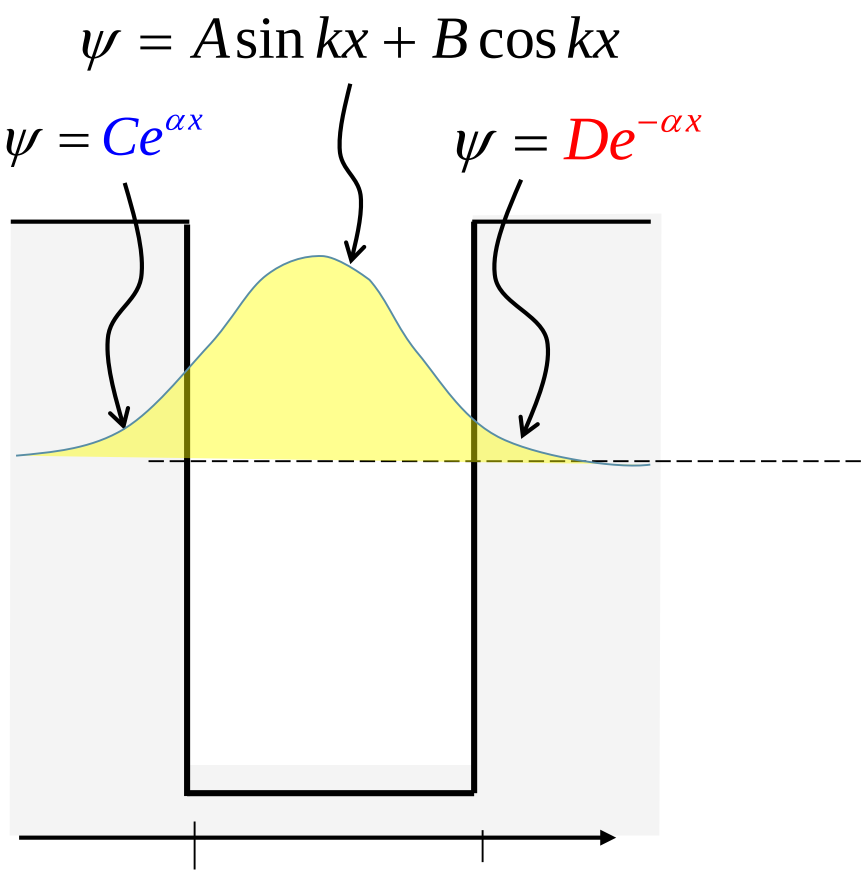
Obtained the eigenvalue => could stop here in many cases

Did not compute the explicit wavefunction yet

Wave Function Normalization

Case 3:
Electron in finite well
E < U

Need another boundary condition!



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det (Matrix)=0

=> Linear dependent system
=> Only 3 variables are unique
=> One variable is undetermined
Let's assume A can be freely Chosen => can get B,C,D

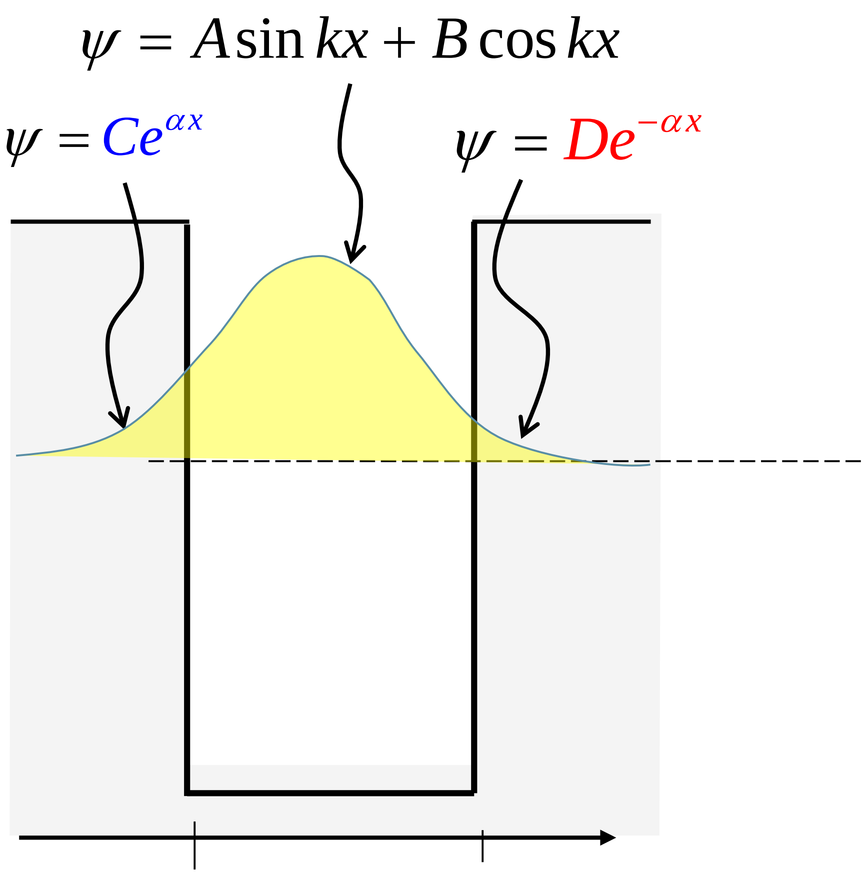
Step 5: Wave-functions

Case 3:
Electron in finite well
E < U

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \quad \Rightarrow$$

Another boundary condition!
Non-linear => no simple linear algebra expression

$$\int_{-\infty}^{0} C^2 e^{2\alpha x} dx + \int_{0}^{a} \left[A\sin(kx) + B\sin(kx) \right]^2 dx + \int_{a}^{\infty} D^2 e^{-2\alpha x} dx = 1$$



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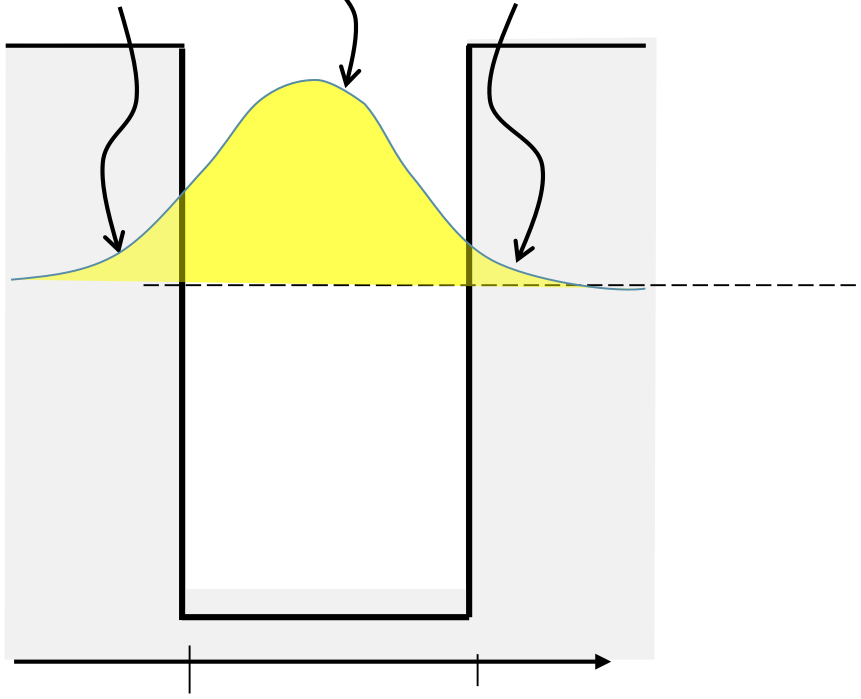
Get "*A*"

$$\psi = A\sin kx + B\cos kx$$

$$\psi = Ce^{\alpha x} \qquad \psi = De^{-\alpha x}$$



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$$\begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix} \begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

Get "*B,C,D*"

$$\begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix}^{-1} \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

Five Steps for Closed System Analytical Solution

1) $$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$ → Solution Ansatz, 2N unknowns for N regions

$$\psi(x) = A_+ e^{ikx} + A_- e^{-ikx}$$

$$\psi(x) = De^{-\alpha x} + Ee^{+\alpha x}$$

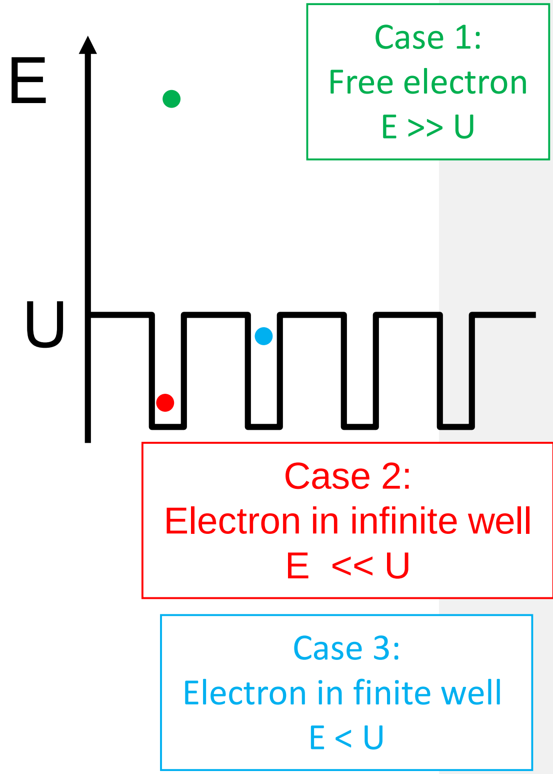
2) $$\psi(x = -\infty) = 0$$ $$\psi(x = +\infty) = 0$$ → Boundary Conditions at the edge. Reduces 2 unknowns

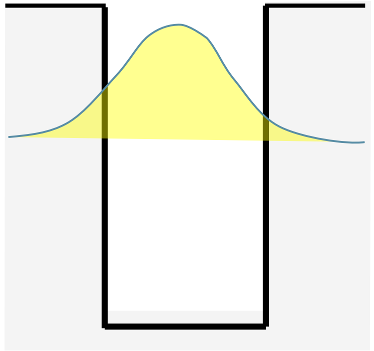
3) $$\psi\Big|_{x=x_B^-} = \psi\Big|_{x=x_B^+}$$ $$\frac{d\psi}{dx}\Big|_{x=x_B^-} = \frac{d\psi}{dx}\Big|_{x=x_B^+}$$ → Boundary Condition at each interface: Set 2N-2 equations for 2N-2 unknowns (for continuous U)

4) Det (coefficient matrix)=0
And find E by graphical or numerical solution

5) $$\int_{-\infty}^{\infty} |\psi(x,E)|^2 \, dx = 1$$

Normalization of unity probability for wave function



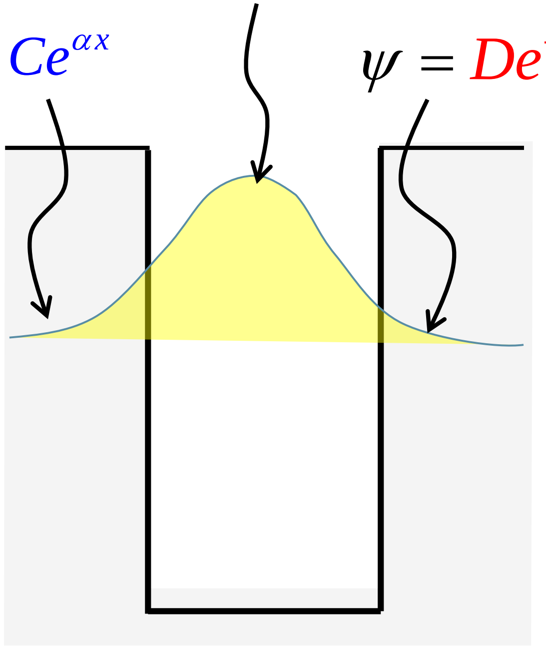


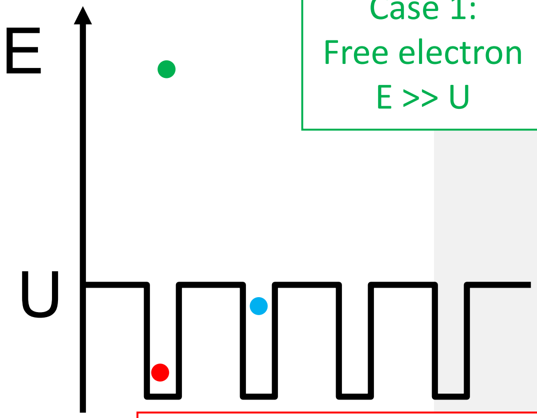
Key Summary of a Finite Quantum Well

- **Problem is analytically solvable**
- **Electron energy is quantized and wavefunction is localized**
- **In the classical world:**
  - » **Particles are not allowed inside the barriers / walls => C=D=0**
- **In the quantum world:**
  - » C **and** D **have a non-zero value!**
  - » **Electrons can tunnel inside a barrier**

$$\psi = A\sin kx + B\cos kx$$

$$\psi = Ce^{\alpha x} \qquad \psi = De^{-\alpha x}$$





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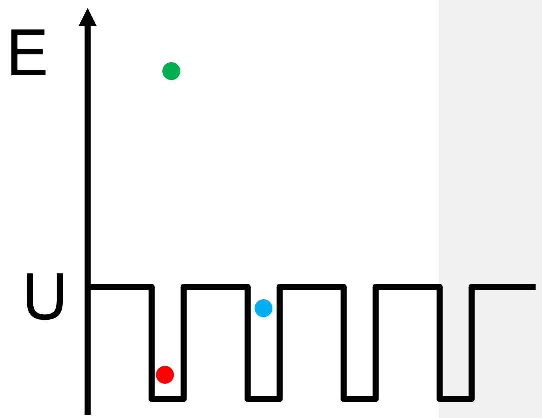
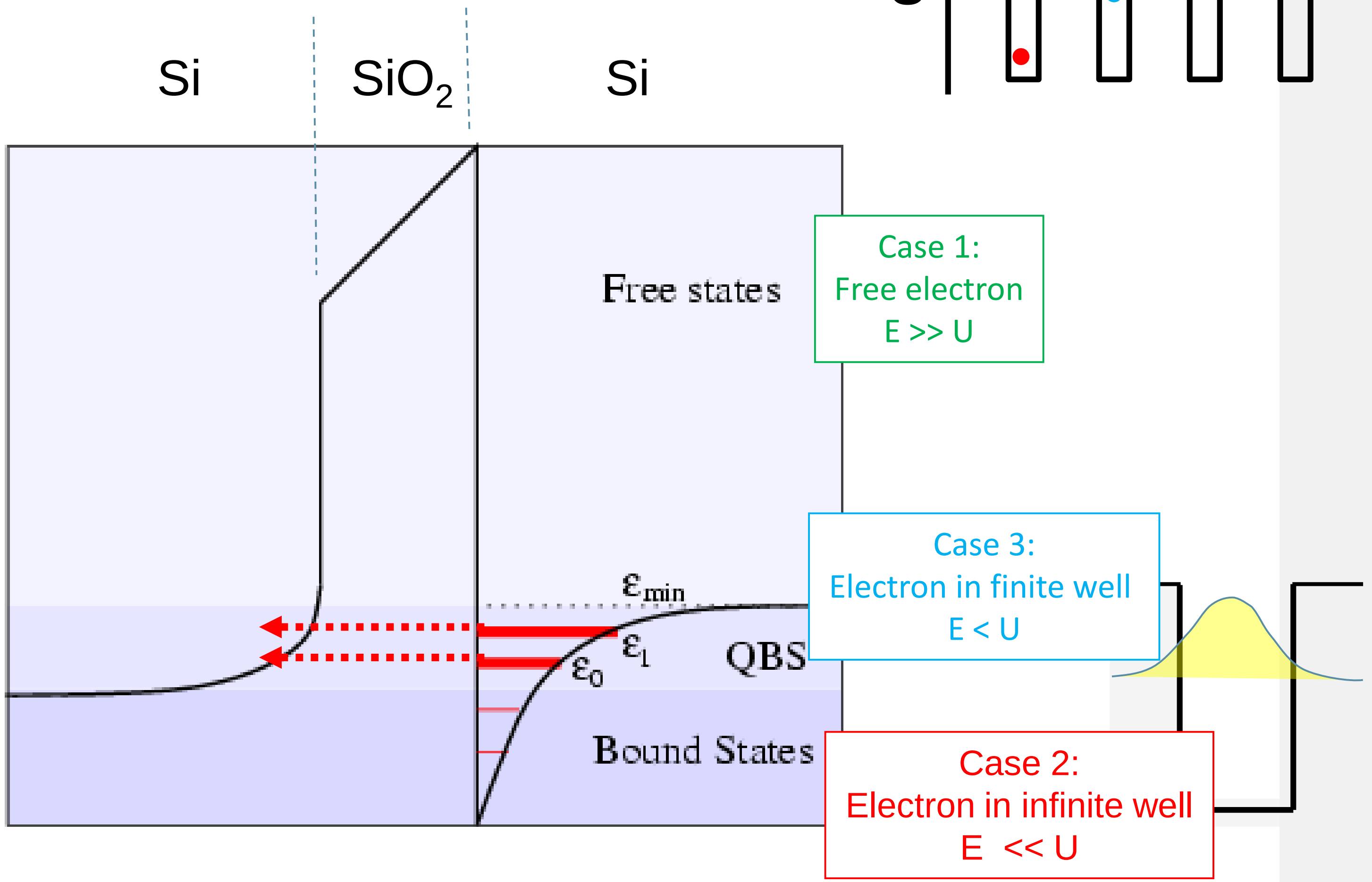


- **Problem is technically relevant**
  - » **Confinement under a gate**
  - » **Gate tunneling**
- **Heterostructures in general**
  - » **Multiple layered materials**
  - » **3D Structures**
- **Applications:**
  - » **Transistors**
  - » **Optical devices**



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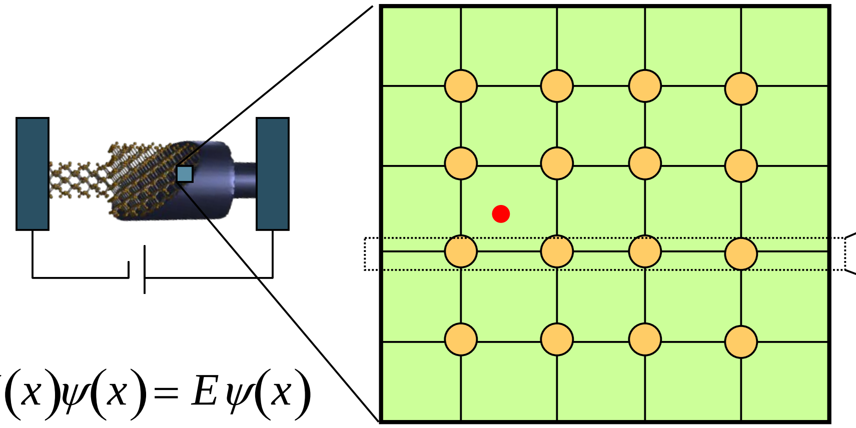
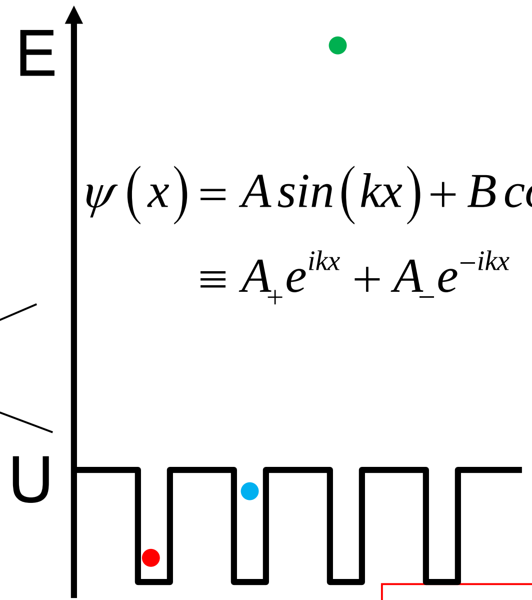
Original Problem

Periodic Structure



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



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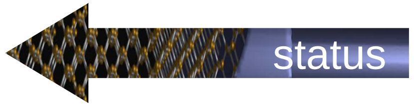
  - »Time Independent Schrödinger Equation
  - »(Almost) Free Electrons
  - »Tightly bound electrons – infinite potential well

$$E_n=\frac{\hbar^2\pi^2}{2mL_x^2}n^2$$

$$\therefore\psi_n(x)=\sqrt{\frac{2}{L_x}}\sin\left(\frac{n\pi}{L_x}x\right),\quad n=1,2,3,\ldots \quad 0<x<L_x$$

- Section 5.2 - Electrons in a finite potential well



One Video Segment

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