Unit 2: Quantum Mechanics

Lecture 2.2: Quantum confinement

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Time-independent wave equation

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

The probability of finding an electron between *x* and *x* + *dx* is:

$$P(x)dx=\psi^*(x)\psi(x)dx$$

Electron energy > potential energy

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E - U_0\right]\psi(x) = 0$$

$$E > U_0 \qquad k^2 = \frac{2m}{\hbar^2}\left[E - U_0\right] \qquad \frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

Solution: $\psi(x) = Ae^{\pm ikx}$

Or: $\psi(x) = A\sin(kx) + B\cos(kx)$

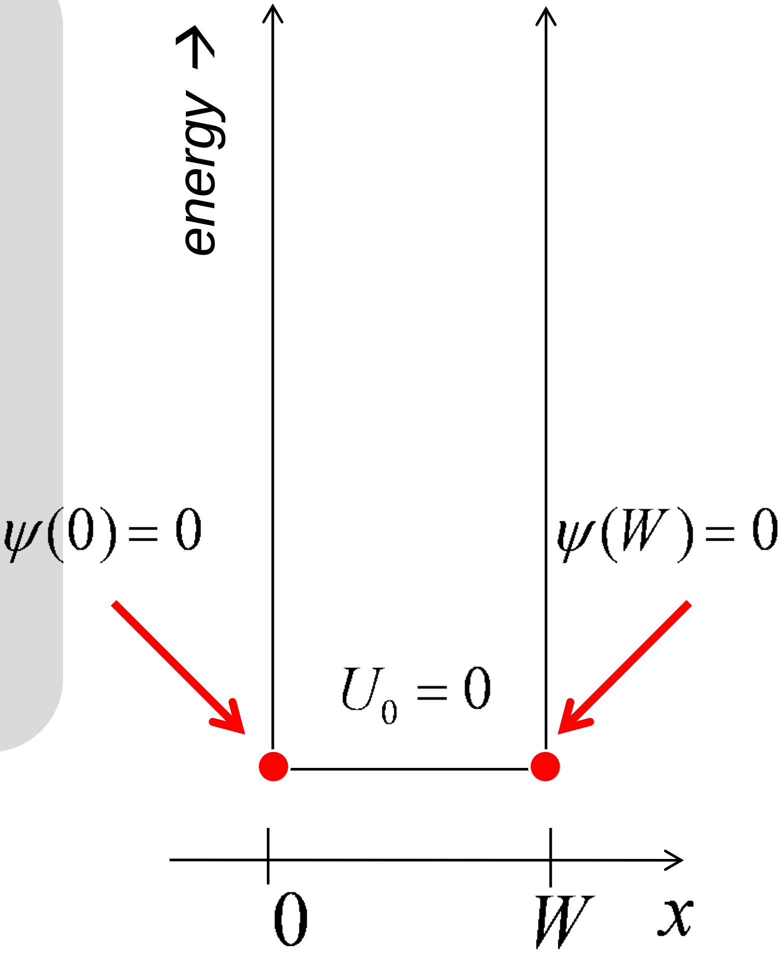
1D particle in a box

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0 \qquad k^2 = \frac{2mE}{\hbar^2}$$

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

boundary conditions:

$$\psi(x=0) = \psi(x=W) = 0$$



Satisfying the boundary conditions

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0 \qquad k^2 = \frac{2mE}{\hbar^2}$$

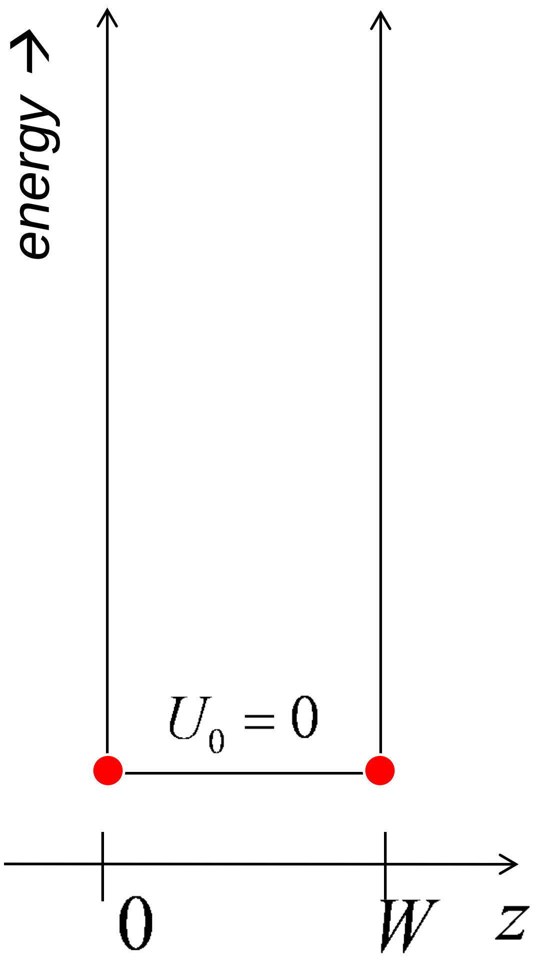
$$\psi(x) = A\sin kx$$

$$\psi(0) = 0 \quad ✓$$

$$\psi(W) = A\sin(kW) = 0$$

$$kW = j\pi \quad j = 1,2,3...$$

$$k_j = j\frac{\pi}{W} \quad j = 1,2,3... \quad ✓$$



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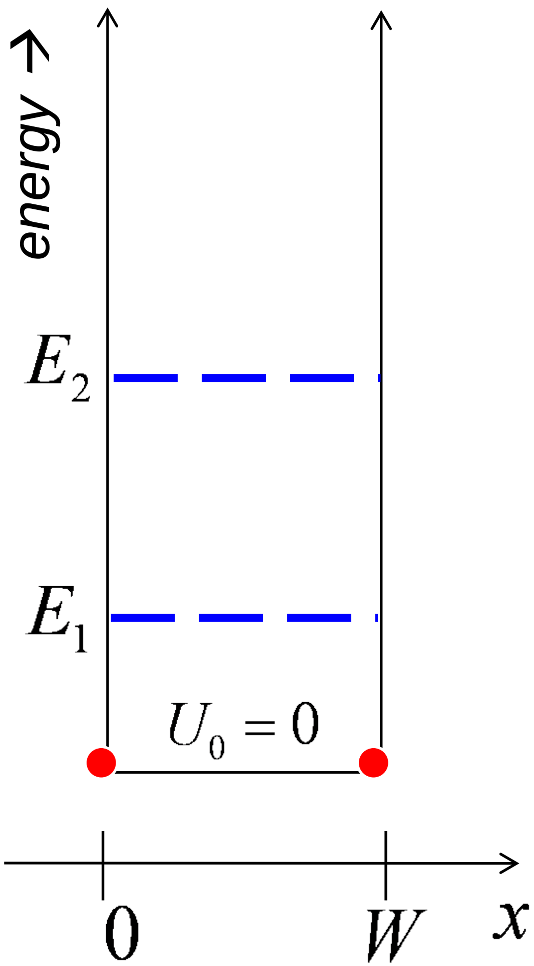
Energy is quantized

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0 \qquad k^2 = \frac{2mE}{\hbar^2}$$

$$\psi(x) = \sin k_j x$$

$$k_j = \frac{\pi}{W} j \qquad j = 1, 2, 3 \ldots$$

$$E_j = \frac{\hbar^2 k_j^2}{2m} = \frac{\hbar^2 j^2 \pi^2}{2mW^2}$$

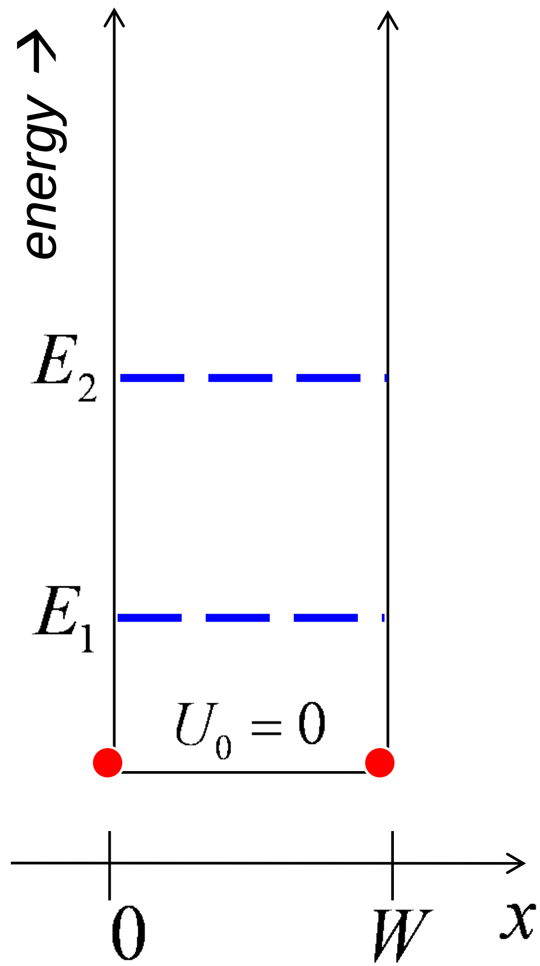


1D QW summary

$$\psi(x) = A \sin k_j x \qquad k_j = \frac{\pi}{W} j \qquad j = 1,2,3\ldots$$

$$k^2 = \frac{2mE}{\hbar^2} \qquad E_j = \frac{\hbar^2 k_j^2}{2m} = \frac{\hbar^2 j^2 \pi^2}{2mW^2}$$

- Confined electrons have quantized energies.
- Tighter confinement (smaller *W* leads to higher energies.
- Lighter masses leads to higher energies.



Normalization of the wavefunction

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0 \qquad k^2 = \frac{2mE}{\hbar^2}$$

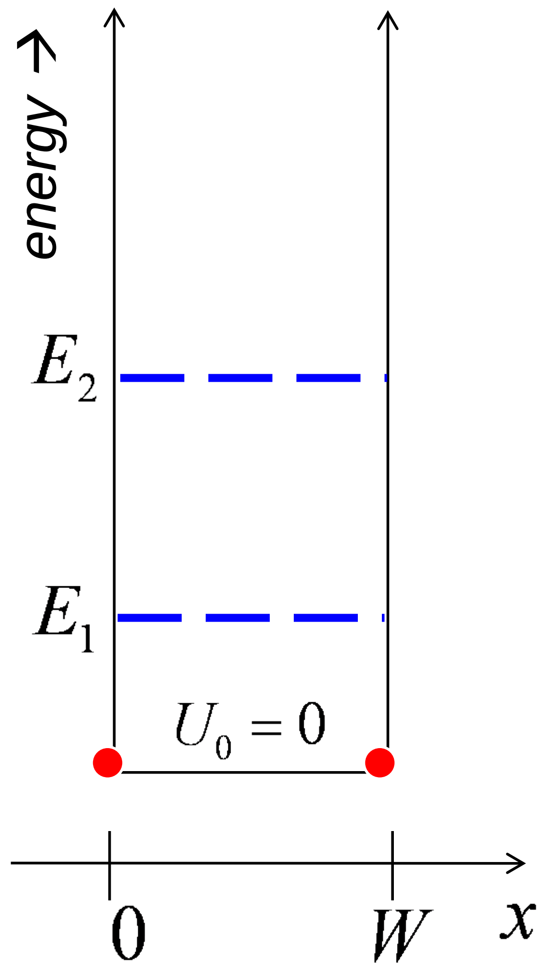
$$\psi(x) = A\sin k_j x \qquad k_j = \frac{\pi}{W} j \qquad j = 1, 2, 3\ldots$$

$$\int_0^W \psi^*(x)\psi(x)dx = 1$$

$$A^2 \int_0^W \sin^2\left(k_j x\right)dx = 1$$

$$A = \sqrt{2/W}$$

$$\boxed{\psi(x) = \sqrt{\frac{2}{W}}\sin k_j x}$$

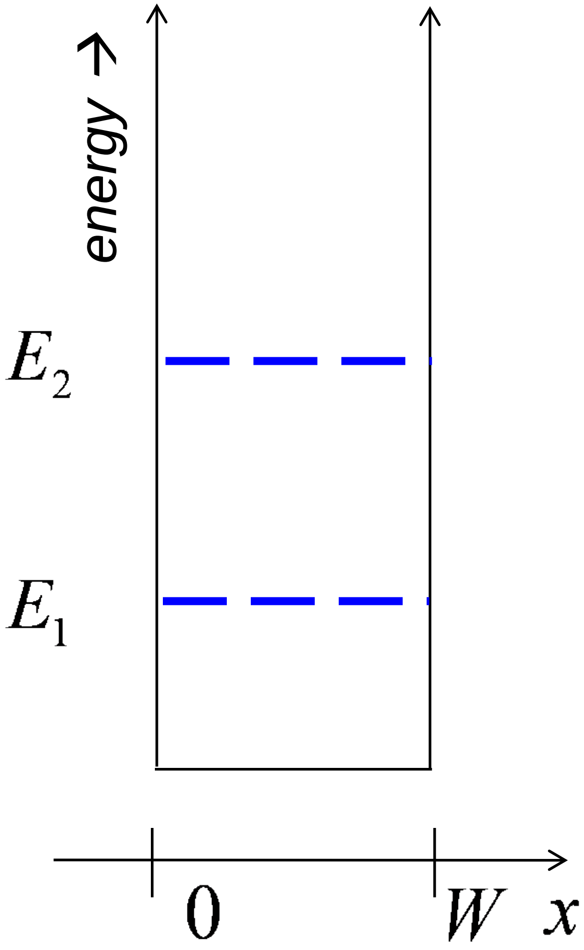


Carrier densities in quantum wells

$$n(x) \propto \psi^*(x)\psi(x)$$

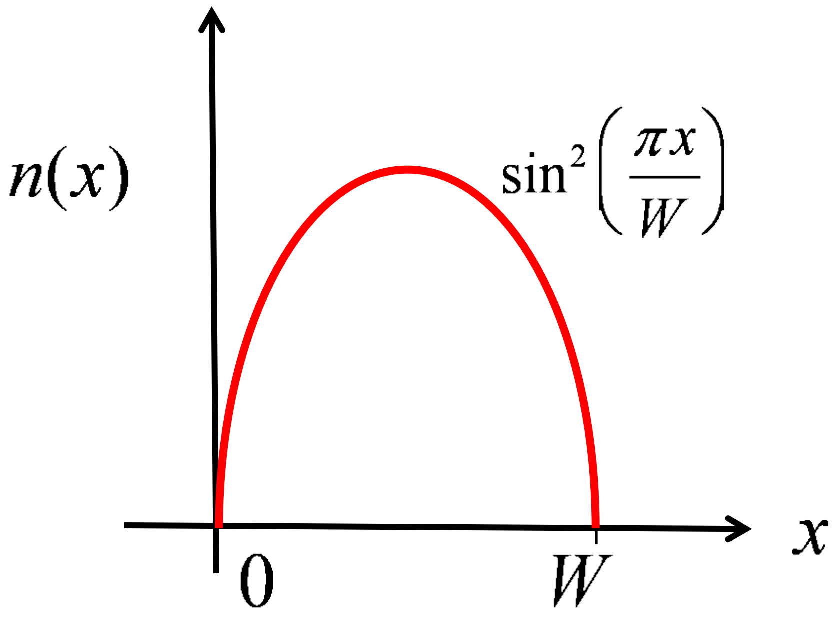
$$n(x) \propto \sin^2 k_j x$$

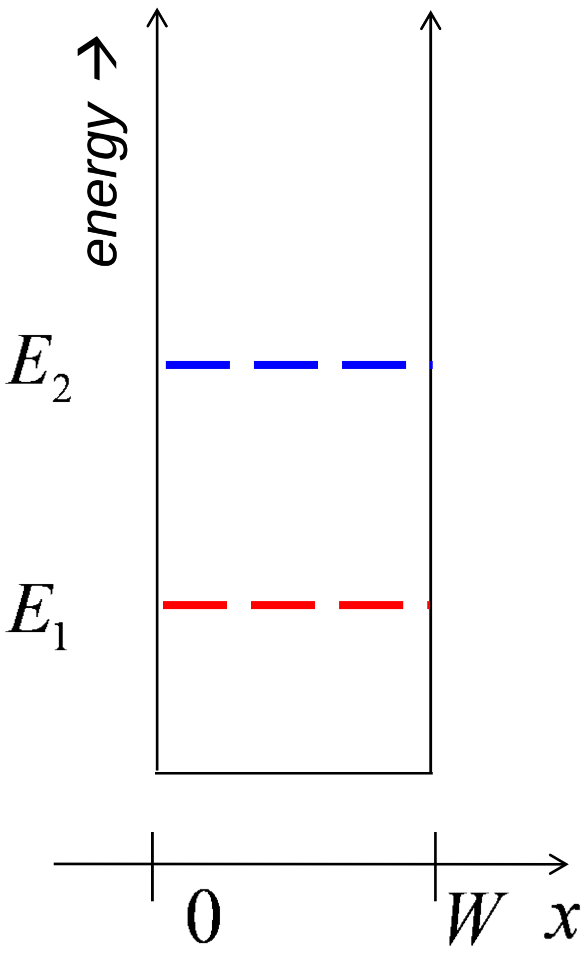
$$n(x) \propto \sin^2\left(j\pi \frac{x}{W} \right)$$



Carrier density in subband 1

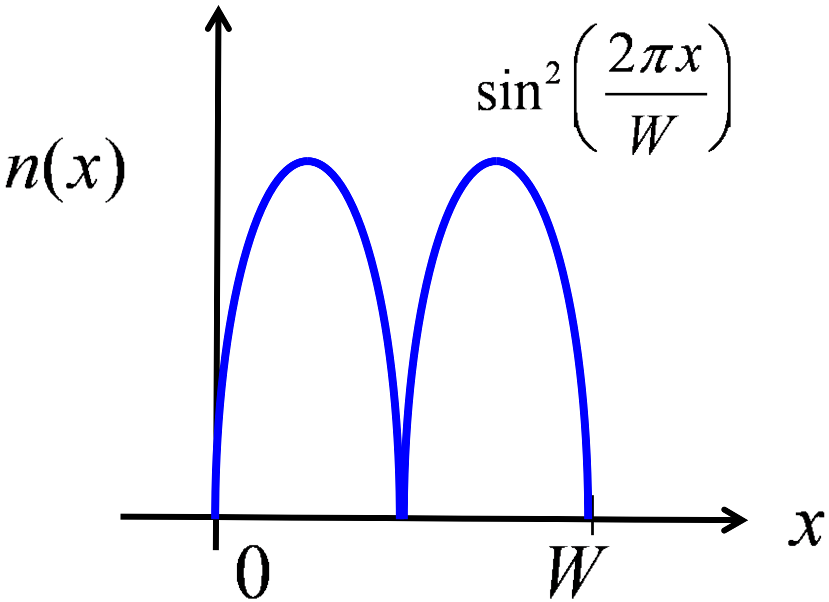
$$n(x) \propto \sin^2\left(j\pi \frac{x}{W} \right)$$

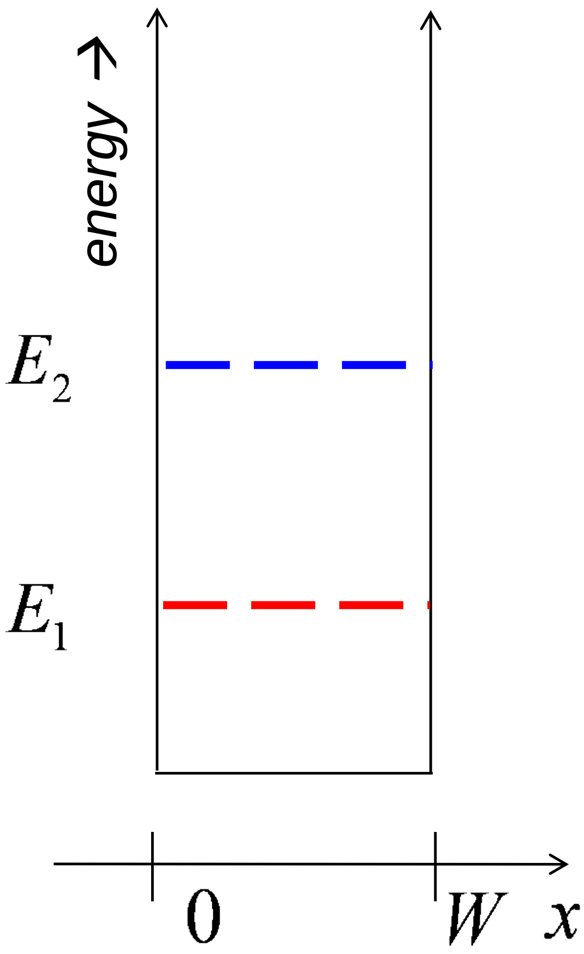




Carrier density in subband 2

$$n(x) \propto \sin^2\left(j\pi \frac{x}{W} \right)$$





Question

How narrow does the quantum well need to be in order to observe quantum effects?

Answer: When we confine electrons on the scale of their wavelength, we should expect quantum effects.

de Broglie Wavelength

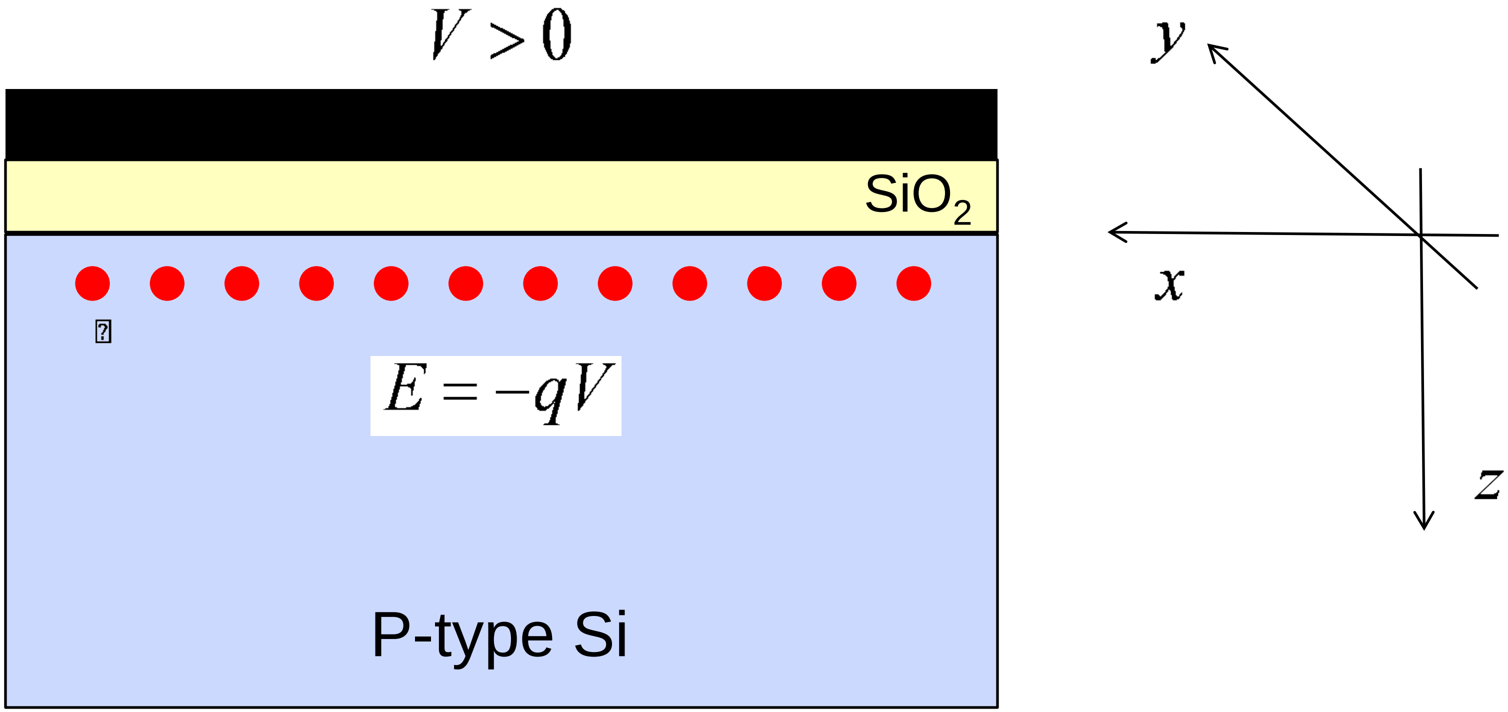
What is the wavelength of a free (mobile) electron?

$$p = \hbar k = \hbar \frac{2\pi}{\lambda_B} \qquad E = \frac{p^2}{2m} \approx \frac{3}{2} k_B T \qquad \lambda_B = \sqrt{\frac{4\pi^2 \hbar^2}{3 m k_B T}}$$

About 10 nm for electrons in silicon at room temperature

For lighter masses, confinement is felt in wider wells.

One way to produce a quantum well



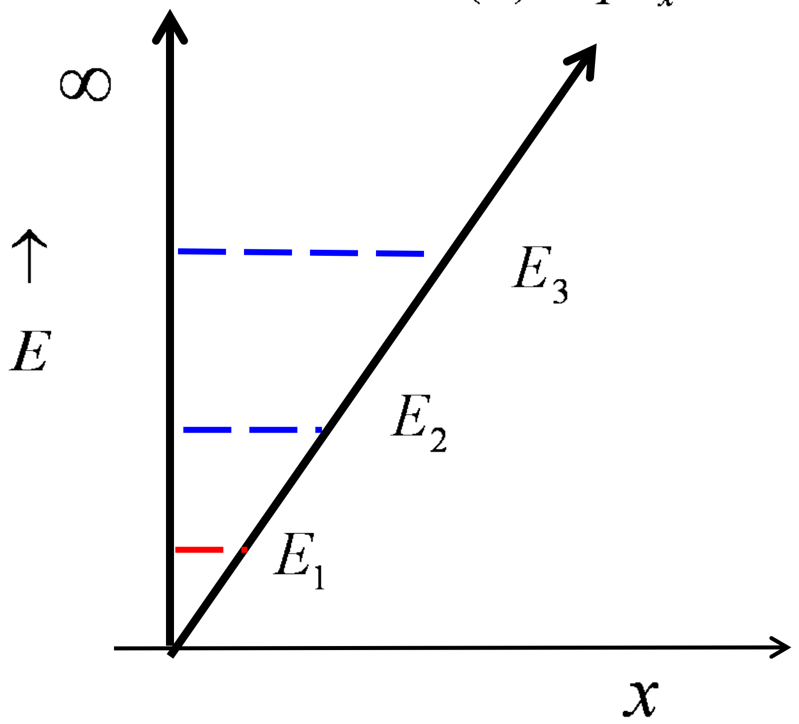
Electrons are confined in the z-direction, but free to move in the x-y plane.

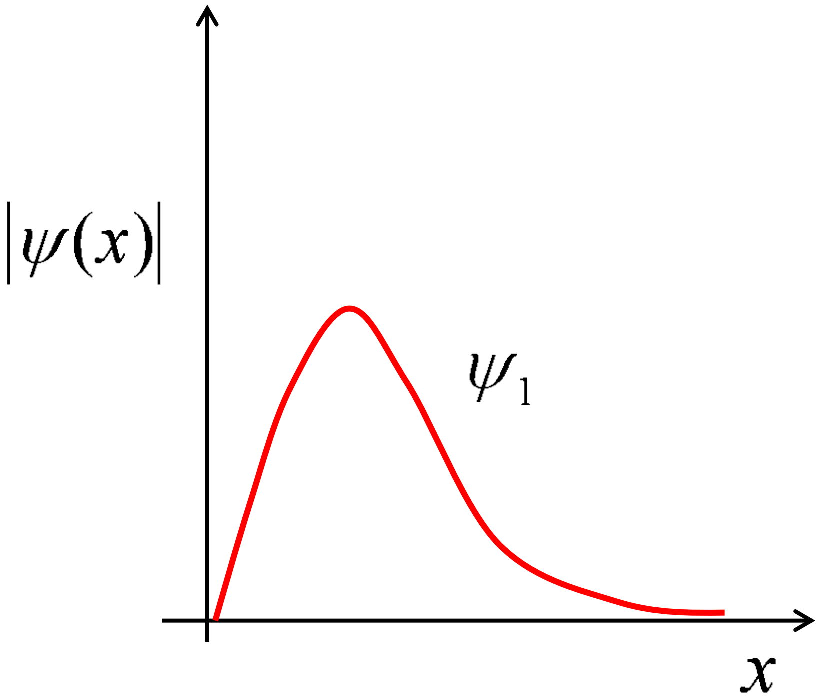
"electrostatic confinement"

Triangular quantum well

$U(x) = q\mathcal{E}_x x$

$\psi(x)$: Airy functions

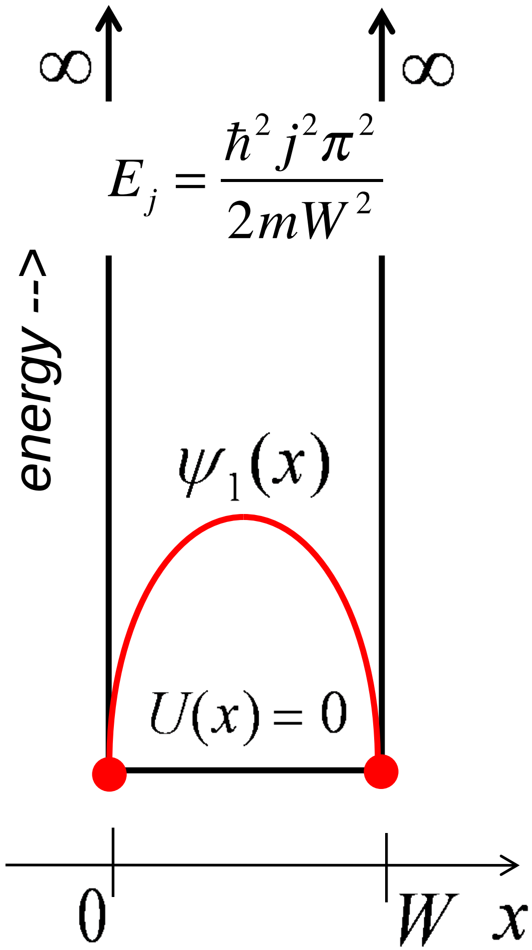




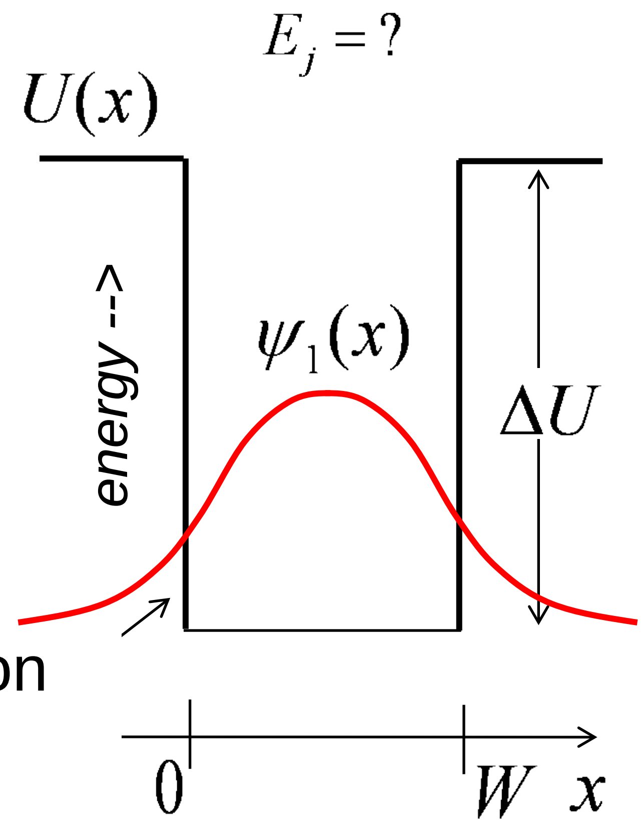
$$E_j = \left[\frac{3hq\mathcal{E}_x}{4\sqrt{2m^*}}\left(j+3/4\right)\right]^{2/3} \qquad j = 1,2,3,\ldots$$

$$\langle x \rangle = \frac{2E_i}{3q\mathcal{E}}$$

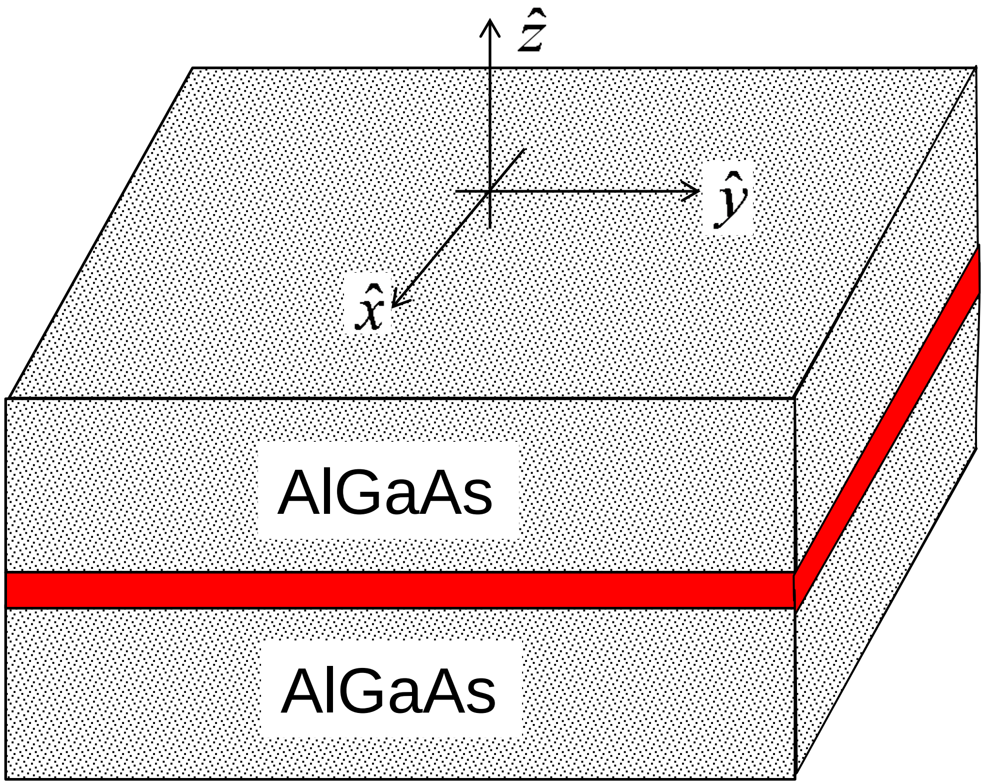
Infinite vs. finite quantum well



"wave function penetration"



Quantum confinement with heterostrucrures



GaAs

"GaAs quantum well"

Electrons are confined in the z-direction, but free to move in the x-y plane.

$$\psi(x,y,z) = ?$$

Wave function

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

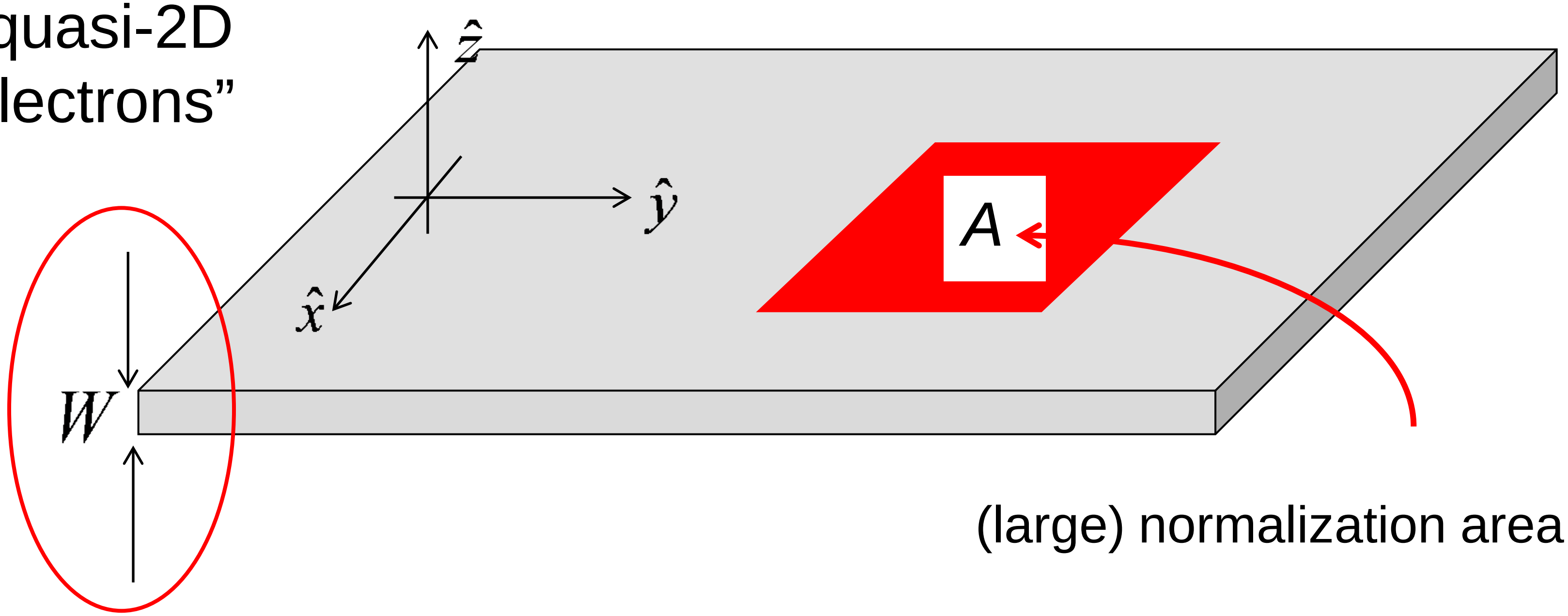
$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z)+U(z)\psi(x,y,z)=E\psi(x,y,z)$$

$$\psi(x,y,z)=X(x)Y(y)Z(z)$$

$$\psi(x,y,z)\propto e^{\pm ik_x x}e^{\pm ik_y y}\phi(z) \qquad \psi(x,y,z)\propto e^{\pm i\vec{k}_{\parallel}\bullet\vec{\rho}}\phi(z)$$

2D electrons

“quasi-2D electrons”

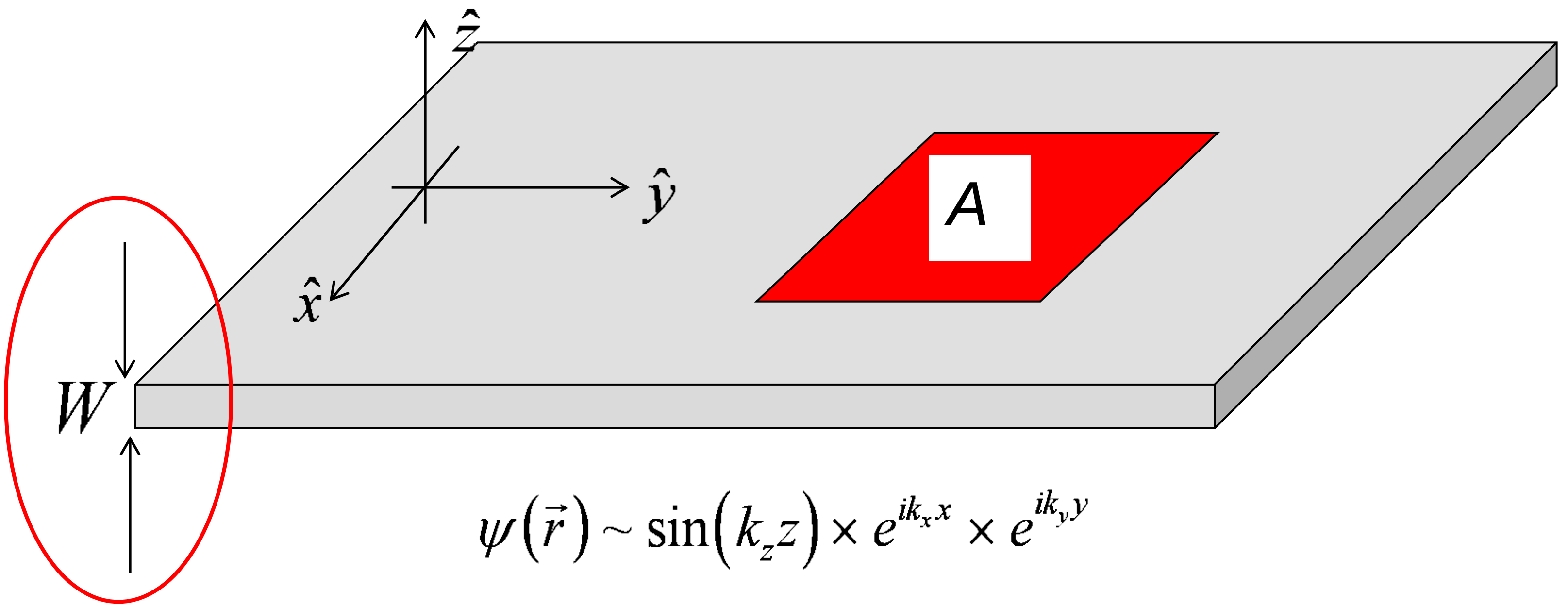


Semi-infinite in the x-y plane, but very thin in the z-direction.

$$\psi(\vec{r}) \sim e^{i\vec{k}\cdot\vec{r}} \rightarrow \sin(k_z z) \times e^{ik_x x} \times e^{ik_y y}$$

$$\psi(\vec{r}) = \sqrt{2/W}\,\sin(k_z z) \times 1/\sqrt{A}\, e^{i(k_x x + k_y y)}$$

2D electrons: subbands

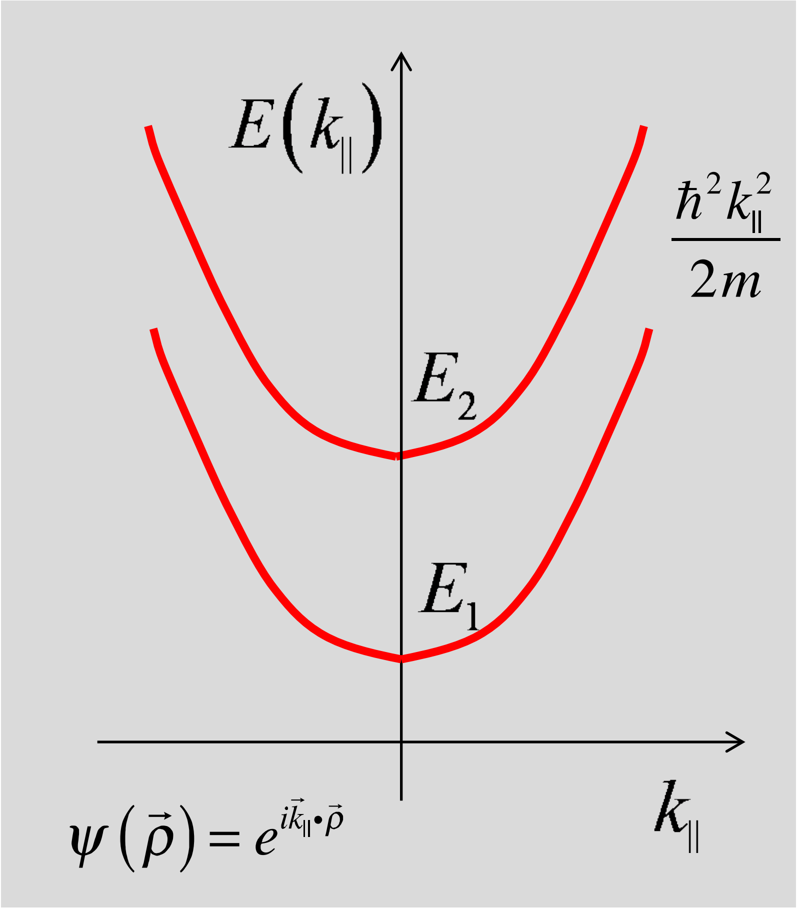


$$\psi(\vec{r}) \sim \sin(k_z z) \times e^{ik_x x} \times e^{ik_y y}$$

$$k_{zj} = j\frac{\pi}{W} \qquad E_j = \frac{\hbar^2 j^2 \pi^2}{2mW^2} \qquad E = E_j + \frac{\hbar^2 k_\parallel^2}{2m}$$

j is the subband index

Subbands



$$E_j = \frac{\hbar^2 j^2 \pi^2}{2mW^2}$$

$$k_\parallel = \sqrt{k_x^2 + k_y^2}$$

$$E = E_j + \frac{\hbar^2 k_\parallel^2}{2m}$$

Summary

When electrons are confined, their energy is quantized and their wave functions change.

Quantum confinement can be produced in 3D materials with electric fields or by epitaxial growth.

Quantum confinement leads to “subbands”.

Specifics depend on the shape of the quantum well but the general features can be understood by analogy with the particle in a box solution.