Ch. 5. Quantum Mechanics

Erwin Schrödinger
(1887-1961)

Schrödinger's Equation

$$\frac{p^2}{2m} + U(x,y,z,t) = H$$

$$\hat{\mathbf{p}} = -i\hbar\vec{\nabla} \qquad \hat{H} = i\hbar\frac{\partial}{\partial t}$$

$$\frac{\hat{\mathbf{p}}^2}{2m}\Psi(x,y,z,t) + U(x,y,z,t)\Psi(x,y,z,t) = \hat{H}\Psi(x,y,z,t)$$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(x,y,z,t) + U(x,y,z,t)\Psi(x,y,z,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,y,z,t)$$

One-Dimensional Schrödinger's Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)+U(x,t)\Psi(x,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

We consider the case of time-independent potential energy only. $U(x,t)=U(x)$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)+U(x)\Psi(x,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

Time-Independent Schrödinger's Equation

$$\text{Try} \quad \Psi(x,t) = \psi(x)\phi(t).$$

$$\text{Then,} \quad \phi(t) = e^{-i\frac{E}{\hbar}t}.$$

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

Wave Functions

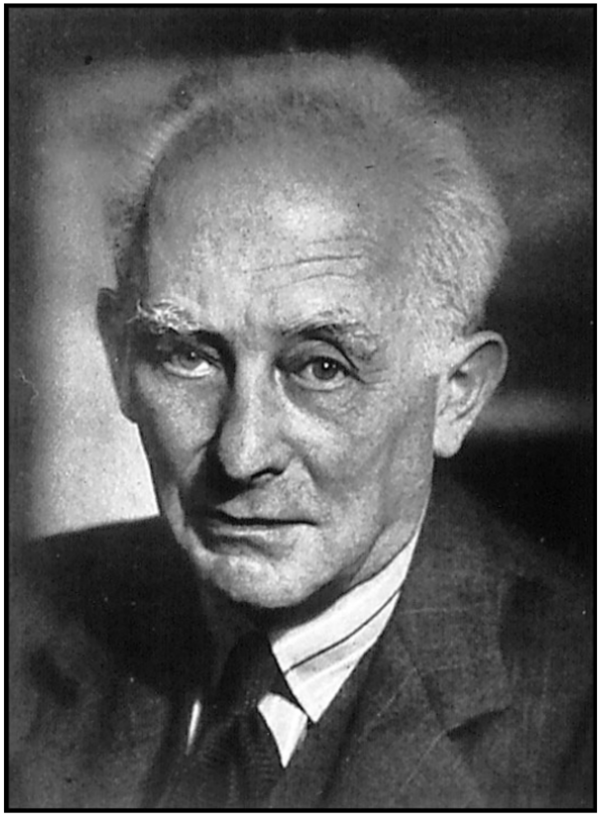
Finite and single-valued

Normalized (except for the case of considering plane waves)

Continuous

First-order spatial derivative should be continuous
(except for the case of infinite potential energy)

Waves of What?

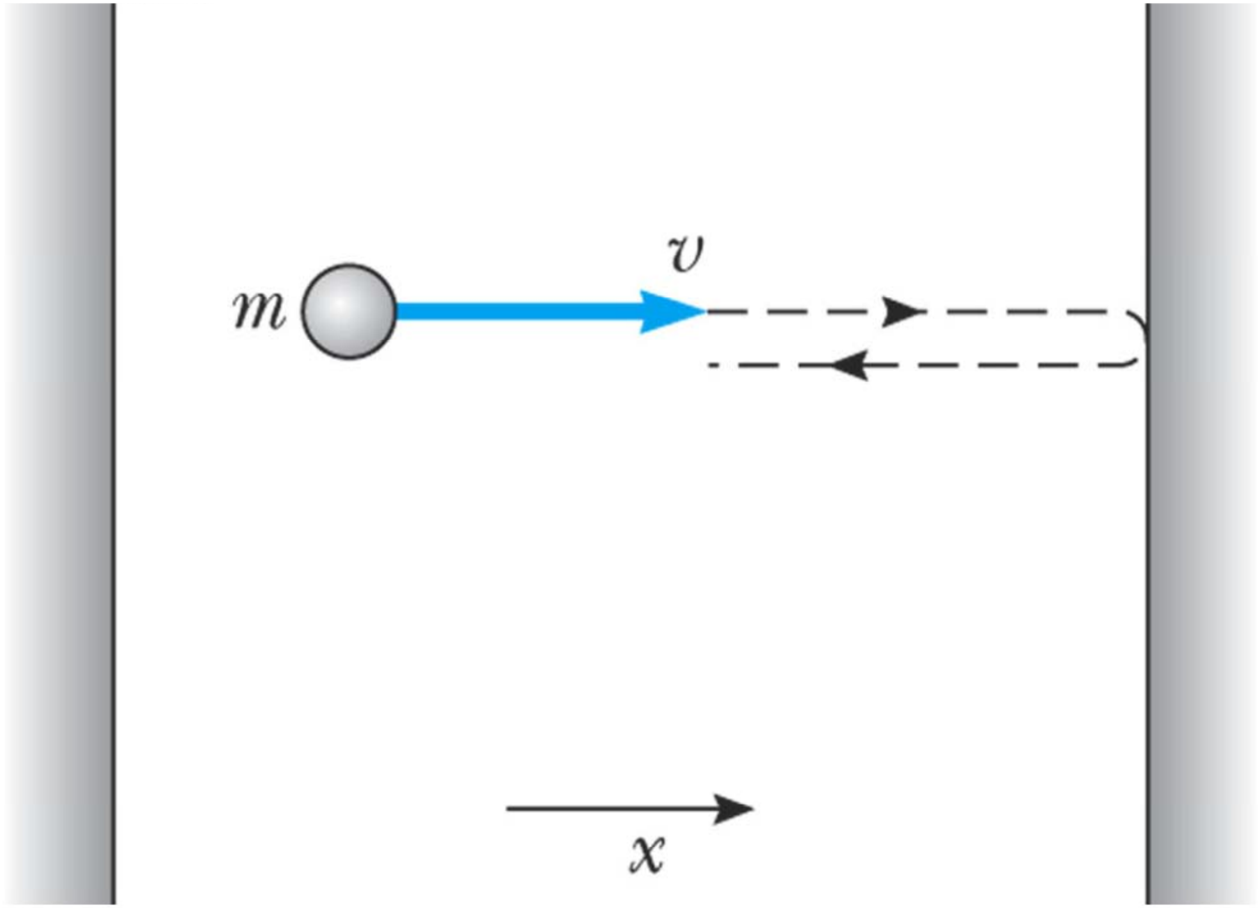


Max Born (1882-1970)

Waves of probability

$$|\Psi(x,y,z,t)|^2 \qquad \text{probability density function}$$

One-Dimensional Quantum Well



One-Dimensional Quantum Well

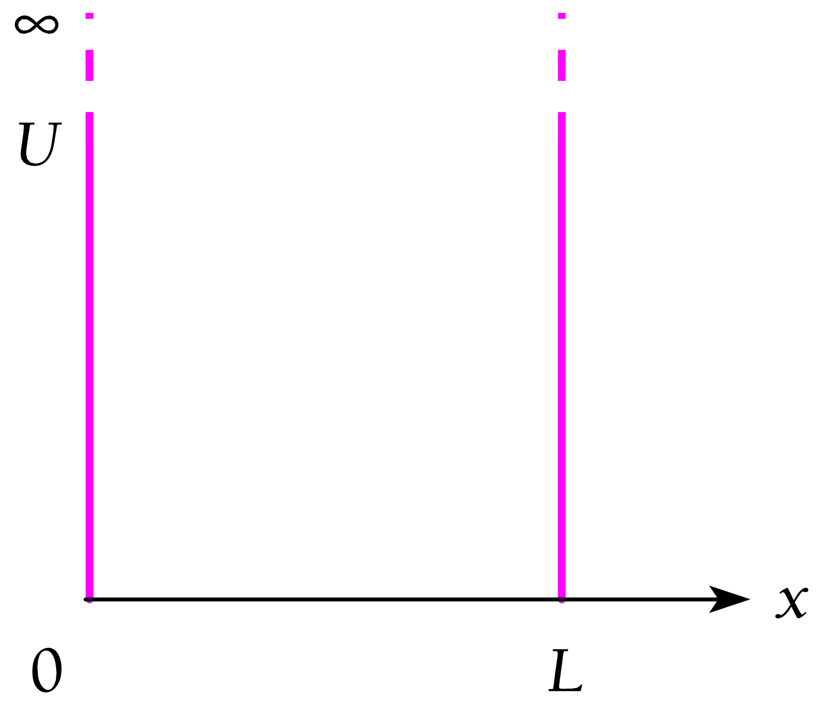


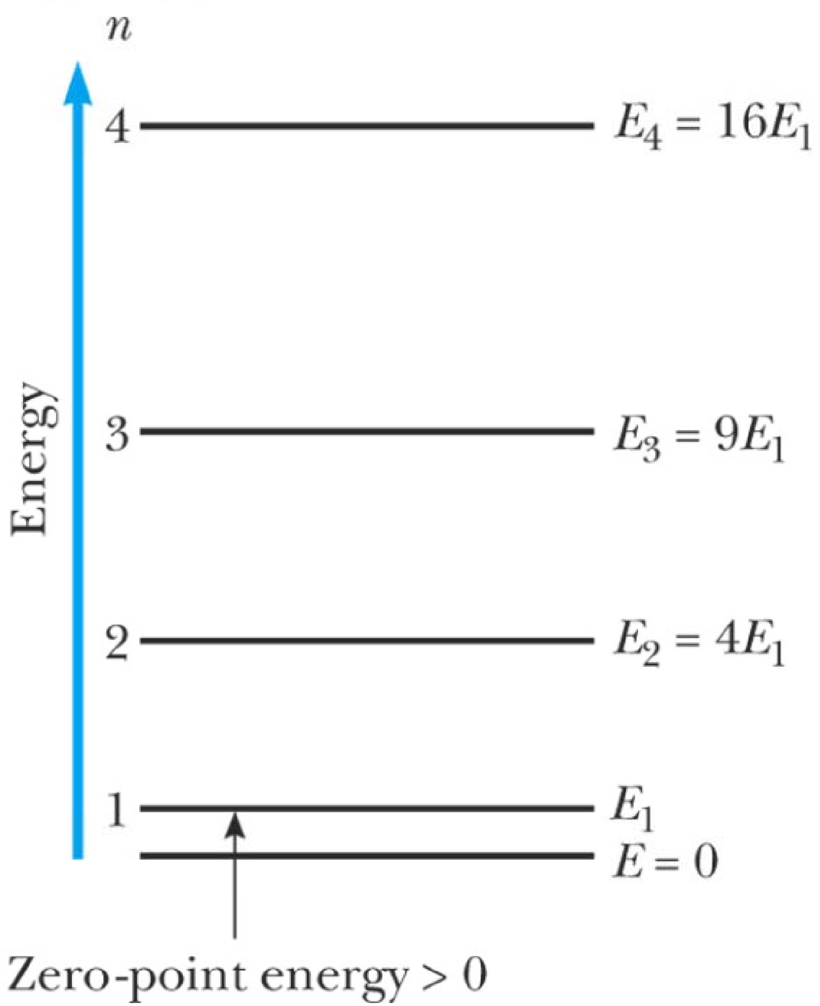
그림 5.4 무한히 딱딱한 벽을 가진 상자에 해당하는 양끝에서 무한히 높은 장벽을 가진 네모 퍼텐셜 우물.

One-Dimensional Quantum Well

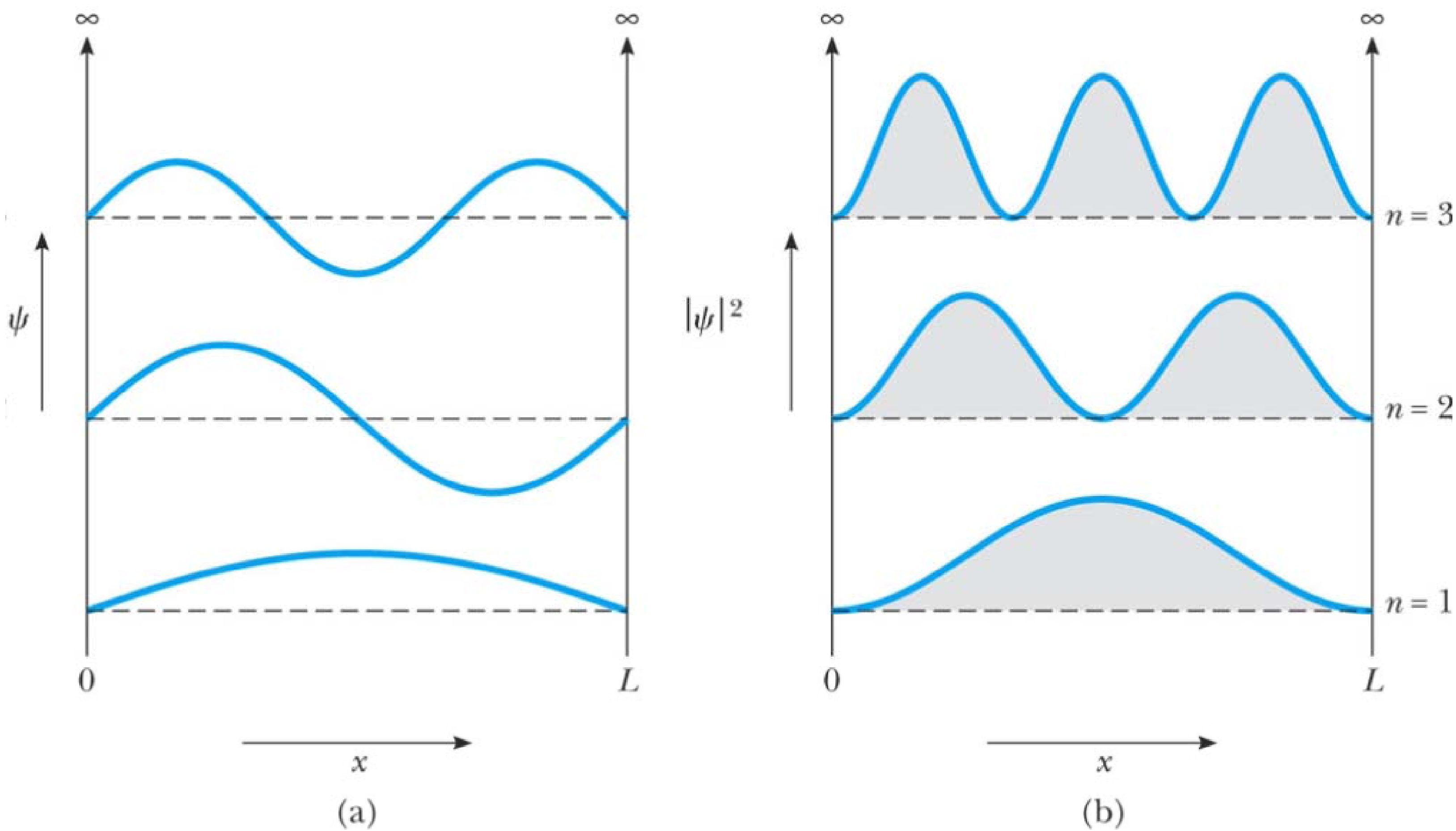
$$k = \frac{n\pi}{L}, \qquad n = 1, 2, 3, \cdots$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad \text{for} \quad 0 < x < L$$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$



One-Dimensional Quantum Well



One-Dimensional Quantum Well – General Solutions

$$\Psi_n(x,t)=\psi_n(x)\phi_n(t)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-i\frac{E_n}{\hbar}t},\qquad n=1,2,3,\cdots$$

$$E_n=\frac{\hbar^2k^2}{2m}=\frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$\Psi(x,t)=\sum_{n=1}^{\infty}C_n\Psi_n(x,t)=\sum_{n=1}^{\infty}C_n\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-i\frac{E_n}{\hbar}t}$$

where $\sum_{n=1}^{\infty}\left|C_n\right|^2=1.$

Operators

표 5.1 몇가지 관측가능량에 대한 연산자

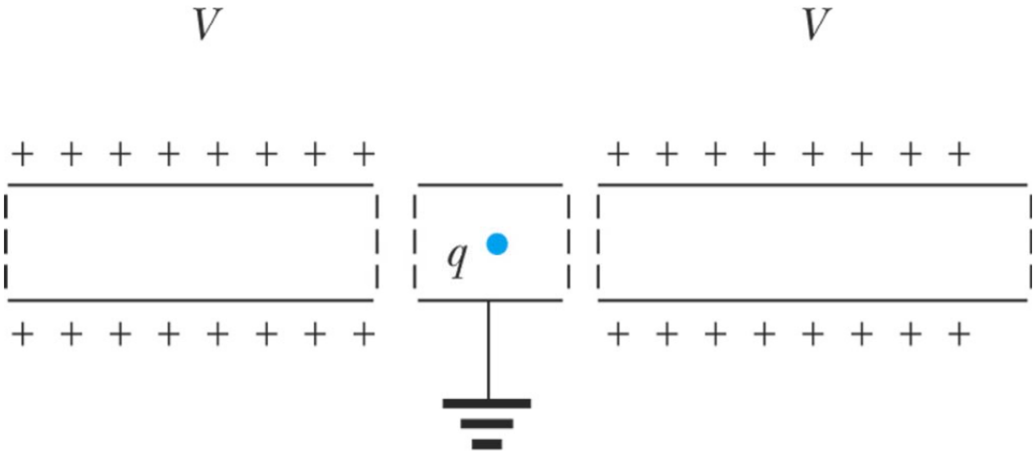
물리량	연산자
위치, x	x
선운동량, p	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
퍼텐셜 에너지, $U(x)$	$U(x)$
운동 에너지, $\mathrm{KE} = \frac{p^2}{2m}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
총 에너지, E	$i\hbar\frac{\partial}{\partial t}$
총 에너지(Hamilton의 모양), H	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)$

Operators and Observables

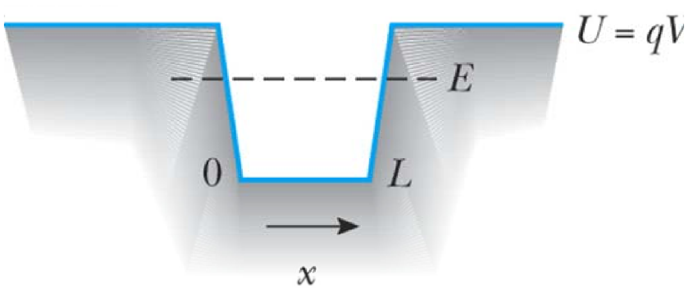
모든 물리량에는 해당하는 **Hermitian Operator**가 있고 그 고유치**(eigenvalue)**는 실수이며, 그 물리량을 측정할 때 측정될 수 있는 값들은 그 고유치들이다.

기대치

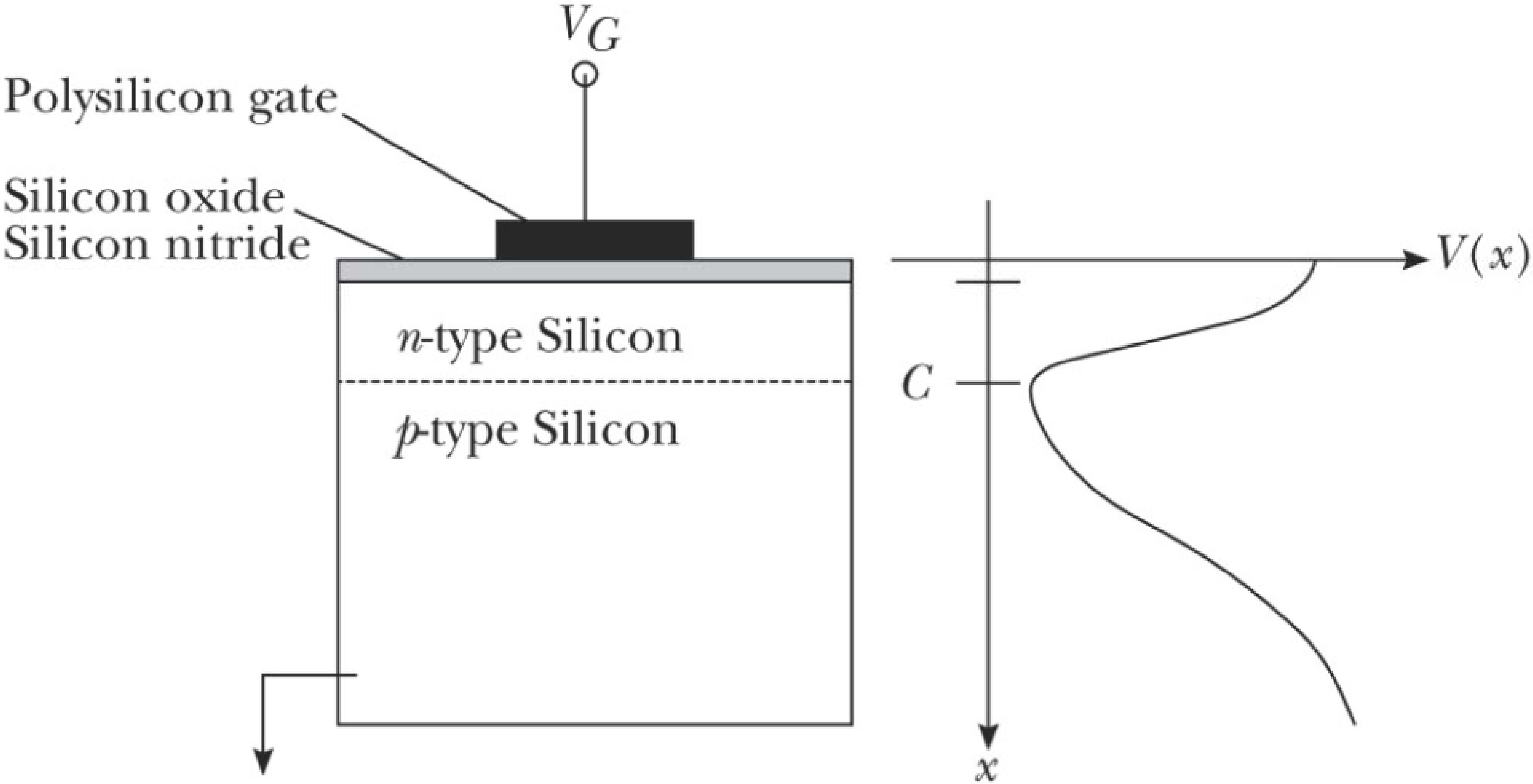
$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{Q} \Psi dx$$



(a)

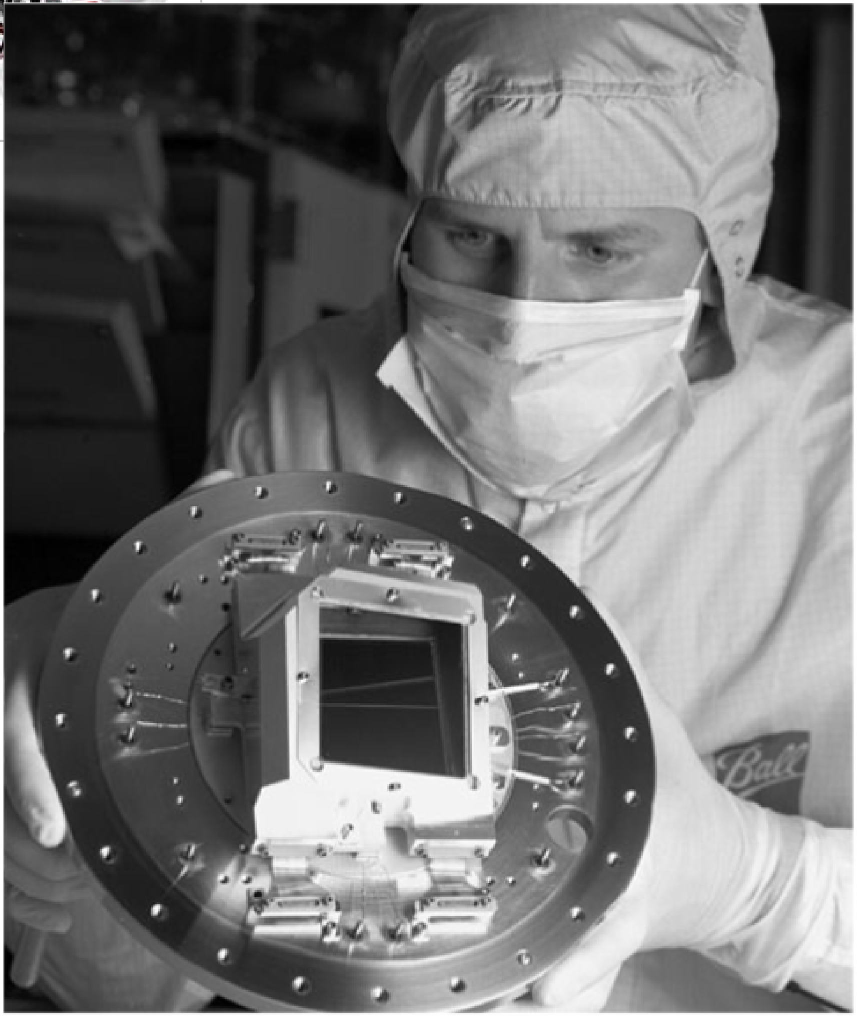


(b)

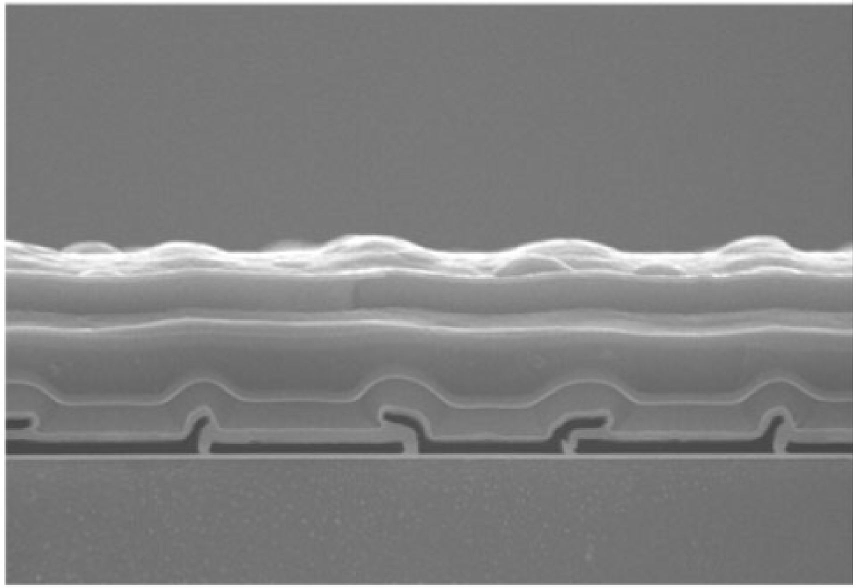


V_G
Polysilicon gate
Silicon oxide
Silicon nitride
n-type Silicon
p-type Silicon
C
V(x)
x


a
b
c
d
e
f
OUTPUT REGISTER
BURIED CHANNEL
PIXEL
PIXEL



(a)



(b)

Finite Potential Well

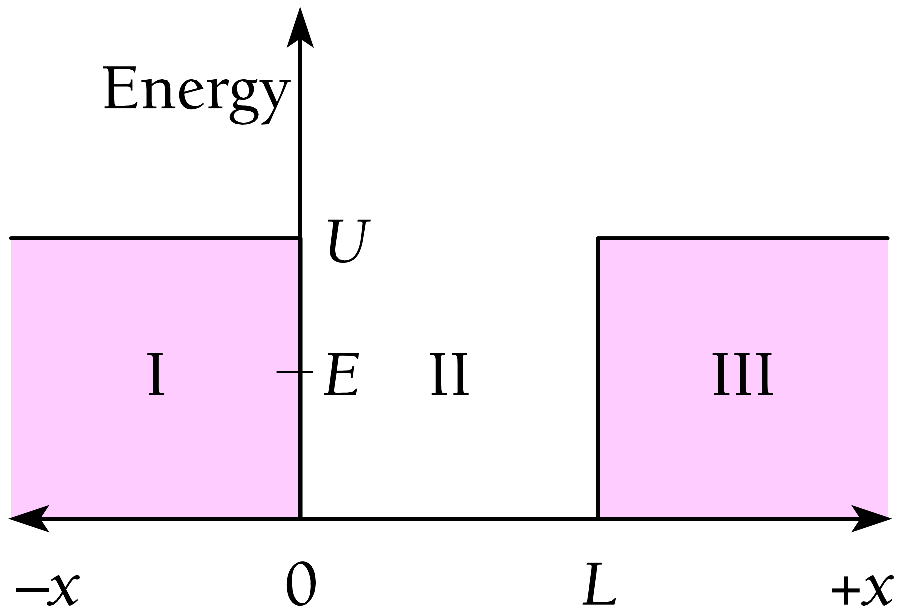
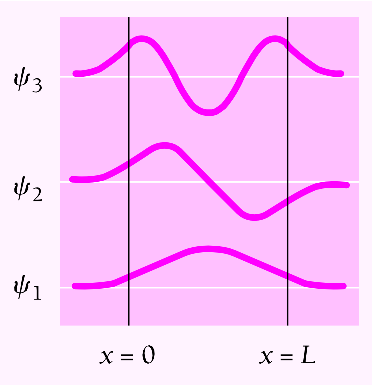


그림 5.7 유한한 장벽을 가진 네모 퍼텐셜 우물. 갇혀 있는 입자의 에너지 E가 장벽 높이 U보다 작다.

Finite Potential Well



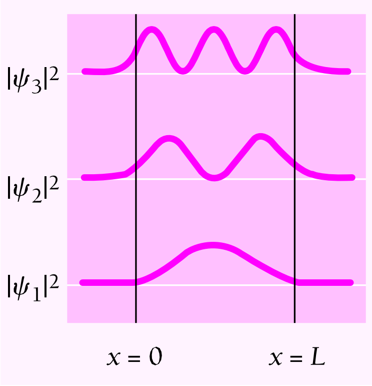
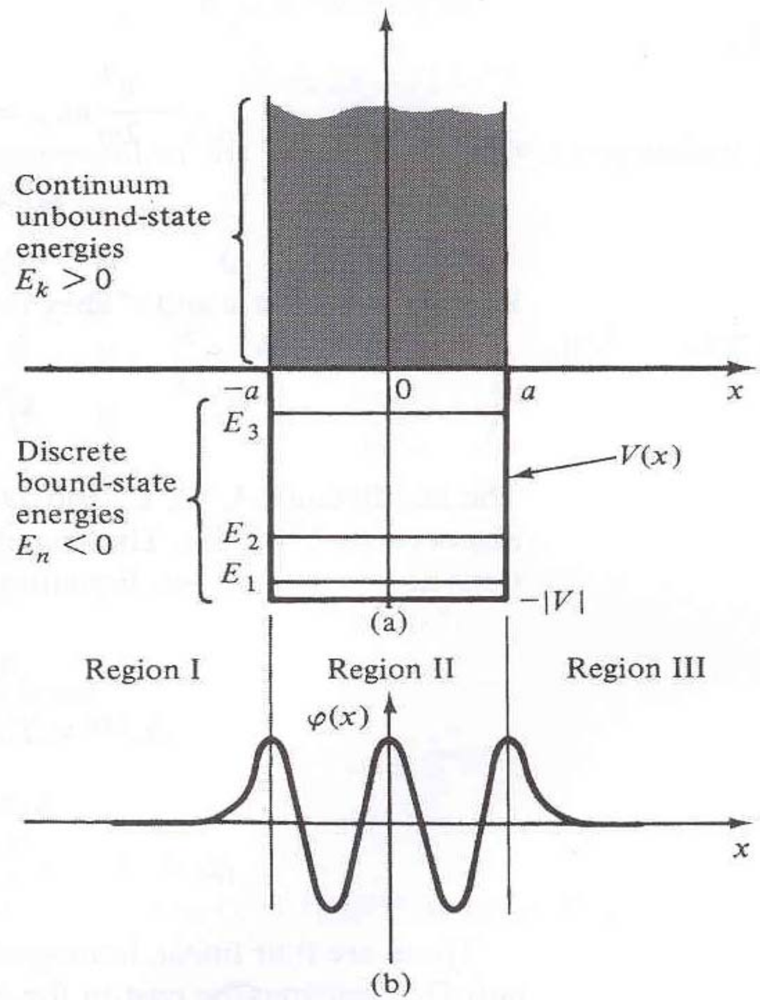
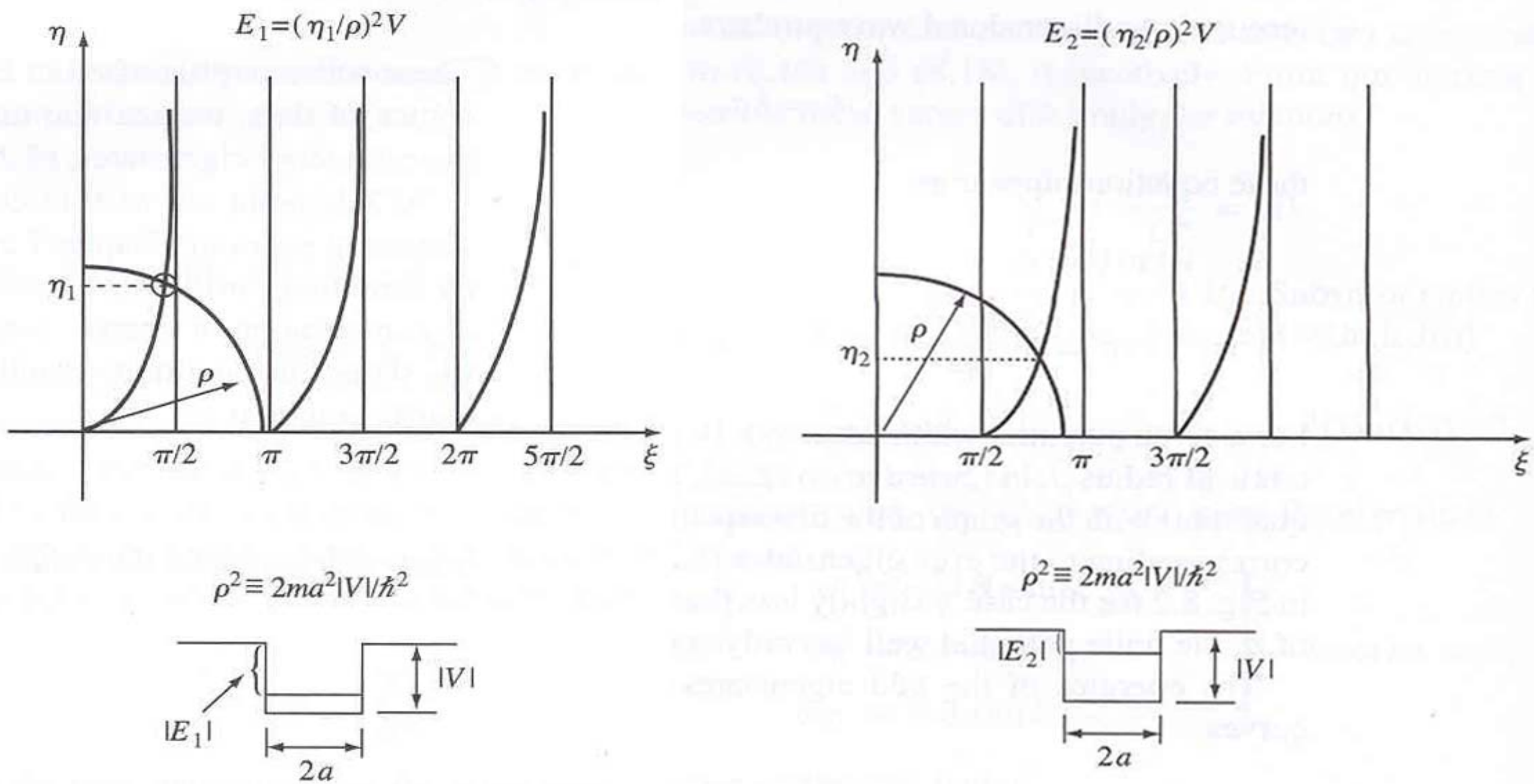


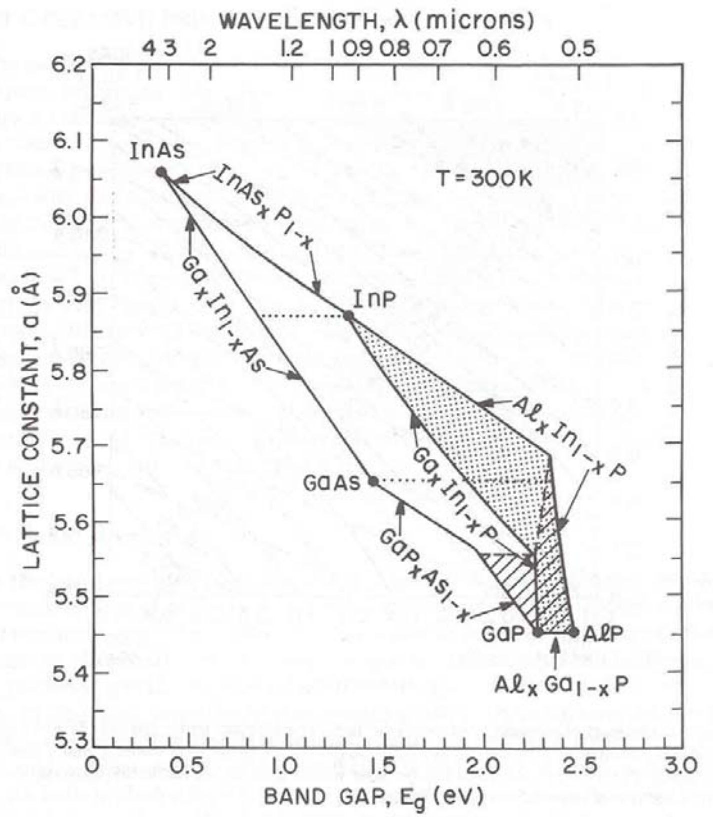
그림 5.8 유한 퍼텐셜 우물에서의 파동함수와 확률밀도. 입자는 우물 바깥에서도 발견될 일정한 확률을 가진다.


Continuum
unbound-state
energies
$E_k > 0$
$-a$
0
a
x
E_3
Discrete
bound-state
energies
$E_n < 0$
E_2
E_1
$V(x)$
$-|V|$
(a)
Region I
Region II
Region III
$\varphi(x)$
x
(b)

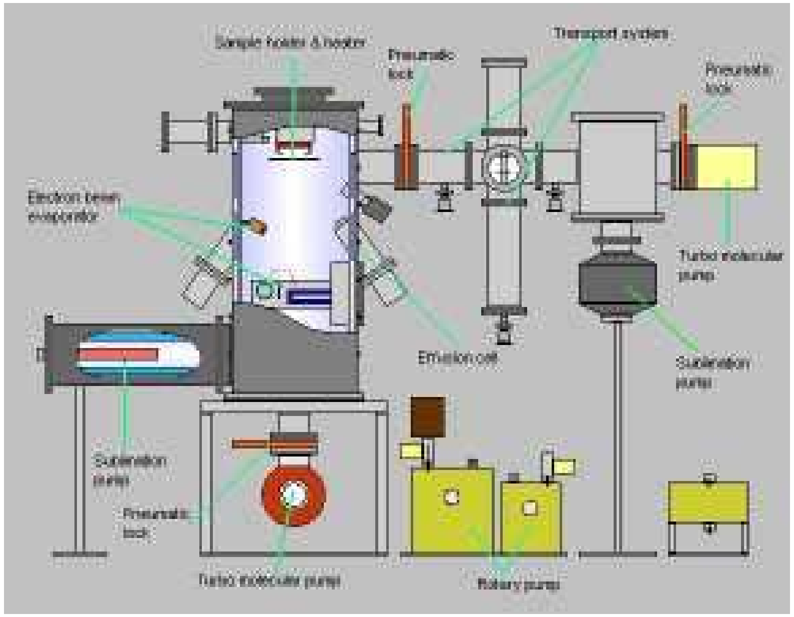


$E_1=(\eta_1/\rho)^2V$
η
η_1
ρ
$\pi/2$ π $3\pi/2$ 2π $5\pi/2$ ξ
$\rho^2 \equiv 2ma^2|V|/\hbar^2$
$|E_1|$
$|V|$
$2a$
$E_2=(\eta_2/\rho)^2V$
η
η_2
ρ
$\pi/2$ π $3\pi/2$ ξ
$\rho^2 \equiv 2ma^2|V|/\hbar^2$
$|E_2|$
$|V|$
$2a$

Bandgap Engineering

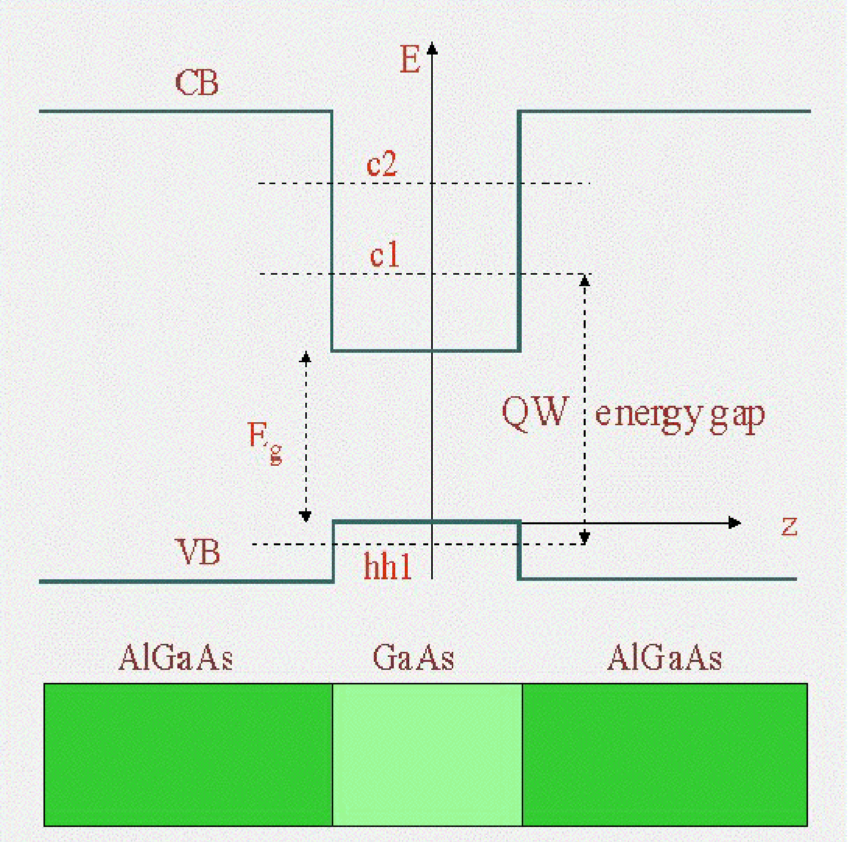


MBE (Molecular Beam Epitaxy)

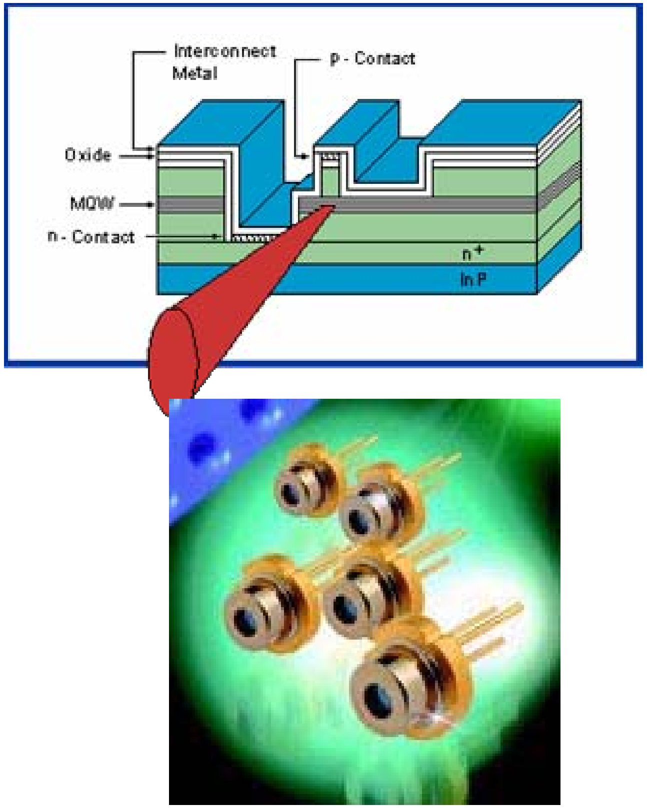


http://people.deas.harvard.edu/~jones/ap216/images/bandgap_engineering/bandgap_engineering.html

Quantum Well Devices

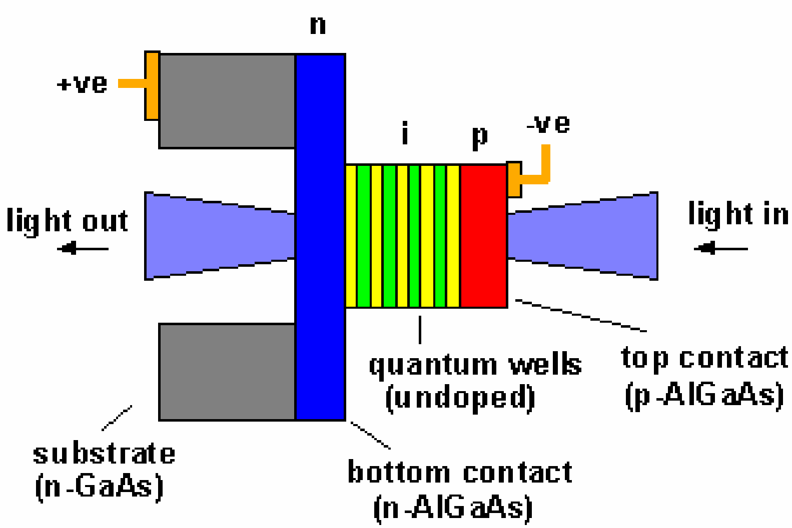


A Quantum Well Structure

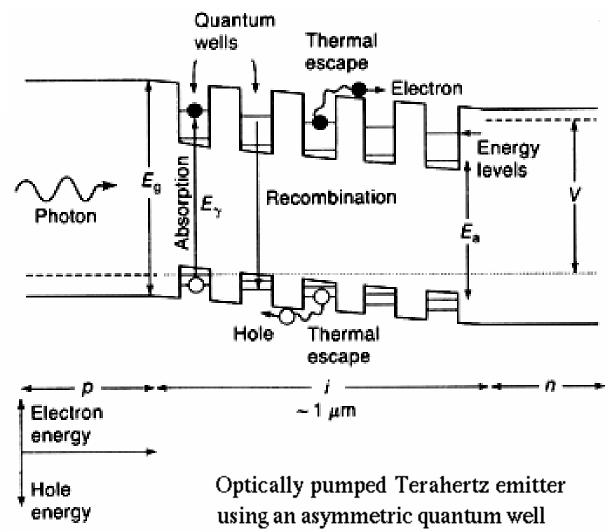


Multiple quantum well lasers

Quantum Well Devices



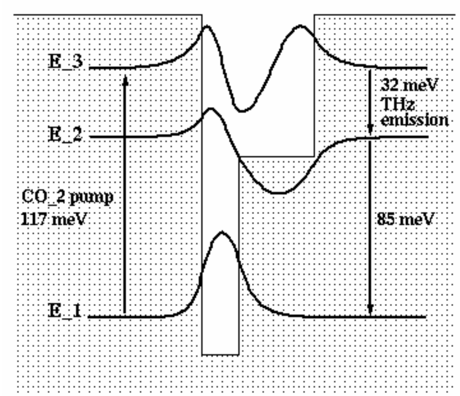
Quantum well modulator



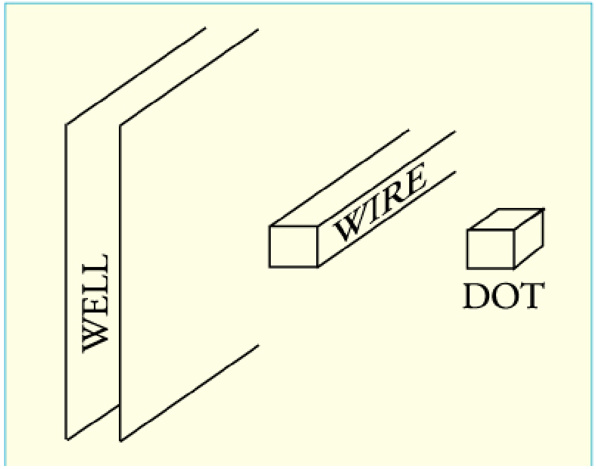
Quantum well solar cells

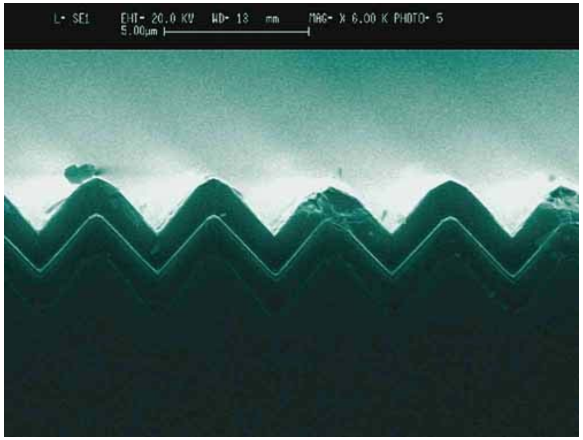
Optically pumped Terahertz emitter using an asymmetric quantum well

This diagram shows the wavefunctions of the electrons at the bottom of each of the three subbands in the well, with the zero amplitude of each wavefunction at the sub-band energy level.



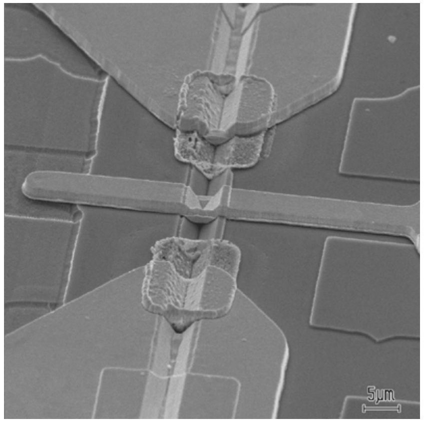
More Quantum – Quantum Wires and Quantum Dots

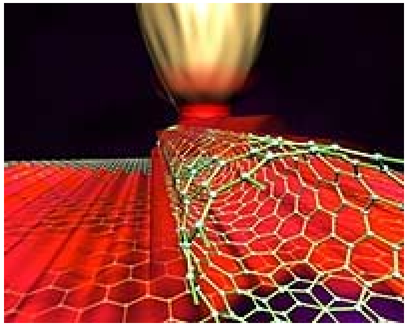




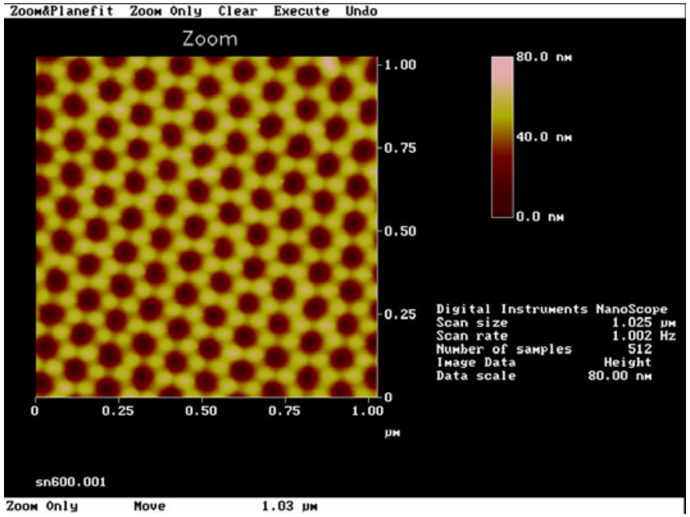
Quantum wire laser operating through the eye of a needle

http://wwwrsphysse.anu.edu.au/ admin/pgbrochure/nano.html





Carbon nanotube



Average pore diameter is 52 nm.

V-groove quantum wire field effect transistor

http://www.shef.ac.uk/eee/research/smd/research/quantum_fet.html

http://www.people.vcu.edu/~sbandy/project1.html