ECE 535: Introduction to Quantum Sensing

Select solutions to Schrodinger equation

Jennifer Choy

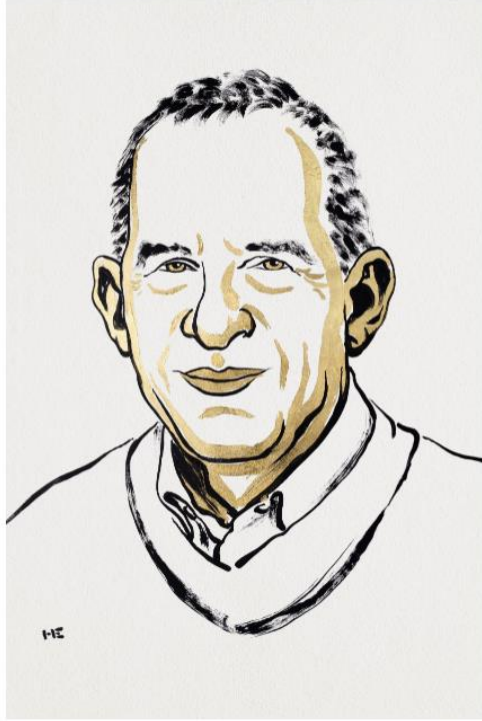Fall 2025

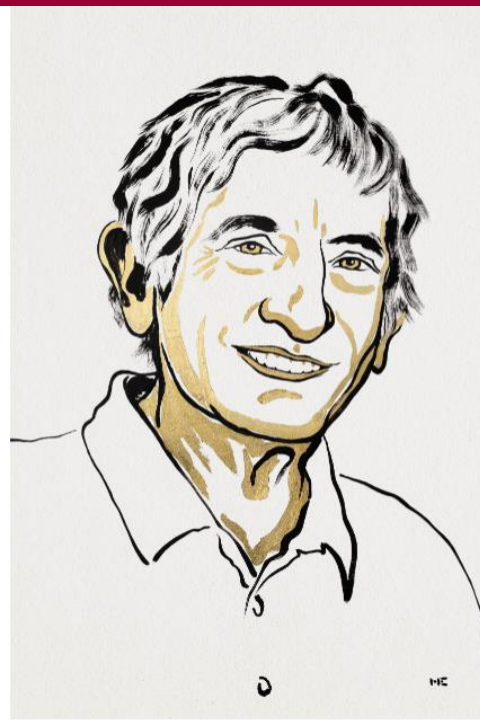# Nobel Prize in Physics 2025

Ill. Niklas Elmehed © Nobel Prize Outreach

John Clarke

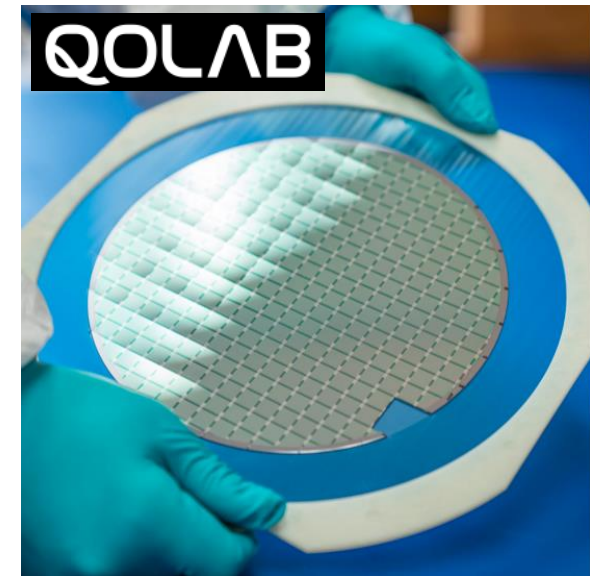Ill. Niklas Elmehed © Nobel Prize Outreach

Michel H. Devoret

Ill. Niklas Elmehed © Nobel Prize Outreach

John M. Martinis

Co-founder and one of the leaders of Qolab, with UW Physics faculty Robert McDermott and Britton Plourde!

Startup on building utility-scale superconducting quantum computers

"for the discovery of macroscopic quantum mechanical tunnelling and energy quantisation in an electric circuit"

2

Recall: Johnson noise thermometry

- Absolute temperature can be determined using

$$T = \frac{V_{rms}^2}{4k_B R B}$$

- Calibration-free: Requires knowledge of Boltzmann constant (k_B) and resistance of a conductor (R)

- Typically uses Superconducting Quantum Interference Devices (SQUIDs)
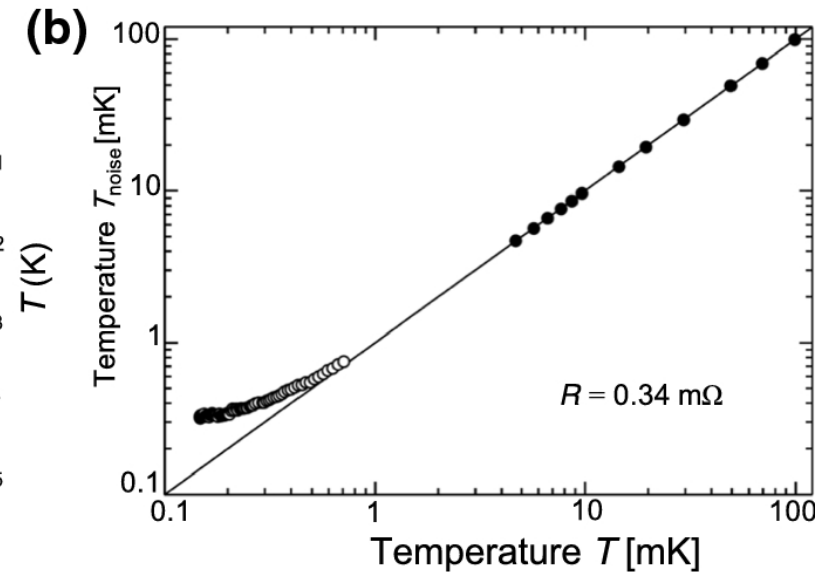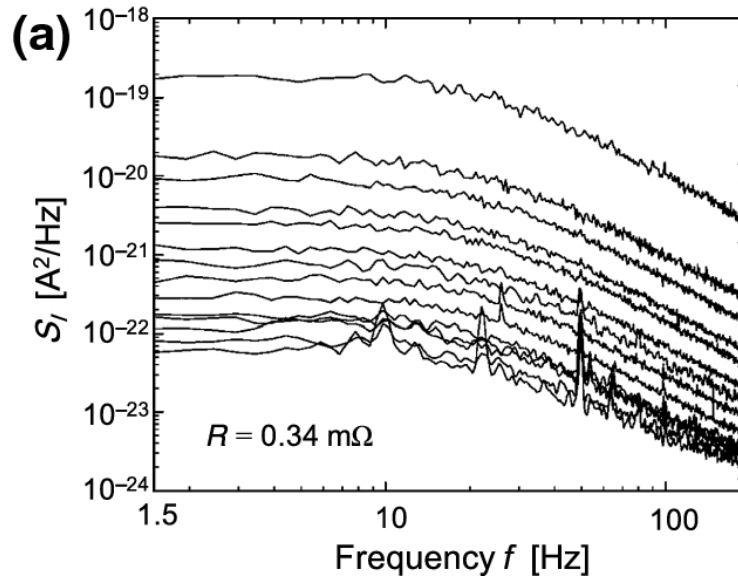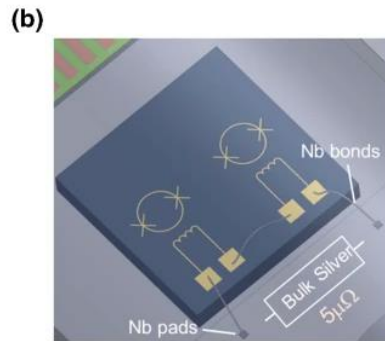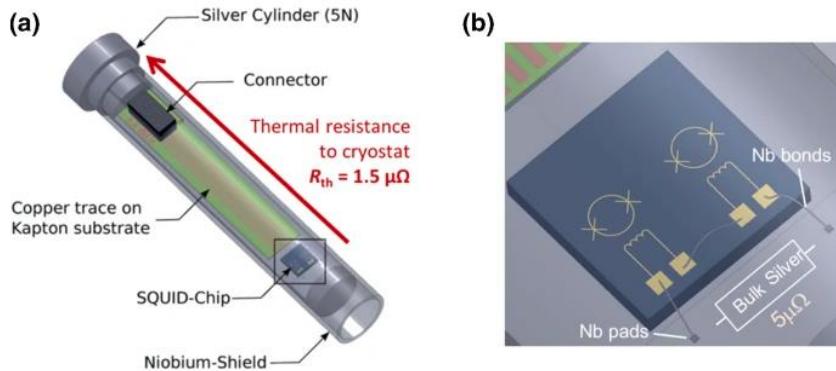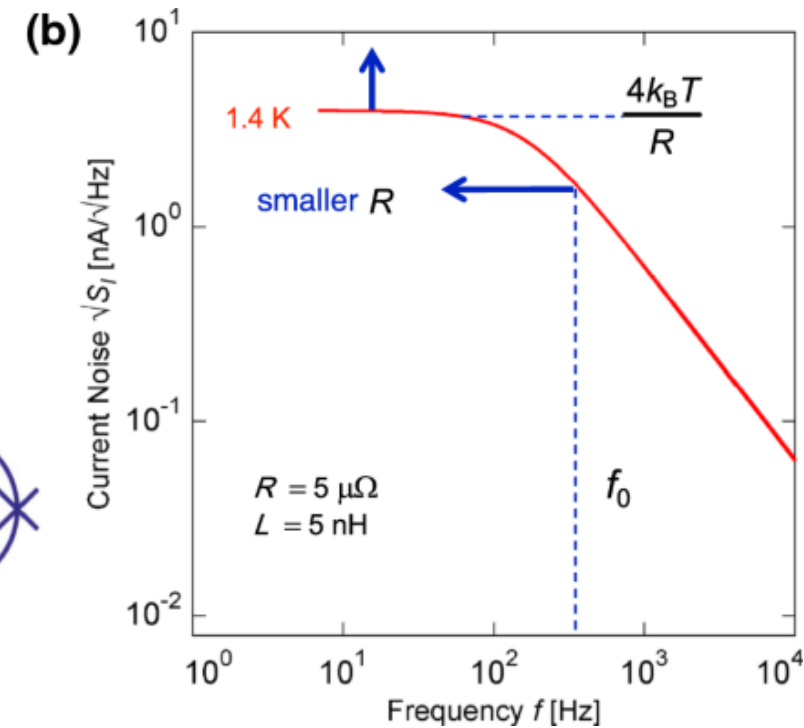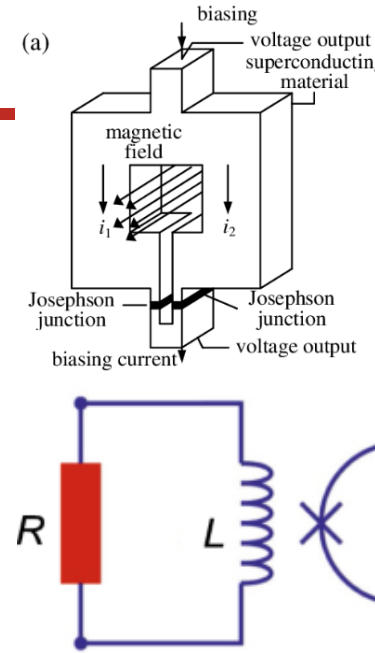
Fleischmann, Andreas, A. Reiser, and C. Enss. "Noise thermometry for ultralow temperatures." *Journal of Low Temperature Physics* 201 (2020): 803-824.

Josephson junction

Top electrode

Base electrode

Nb oxide

Nb

PbIn

I_0 C R I_B $I_{\mu w}\sin\Omega t$ V

a

$\Omega/2\pi = 2$ GHz

$[\Gamma(P) - \Gamma(0)]/\Gamma(0)$

2

0

b

$E_{n,n+1}/h$ (GHz)

2.2

2.0

1.8

$2{\rightarrow}3$ $1{\rightarrow}2$ $0{\rightarrow}1$

30.35   30.46

I (µA)
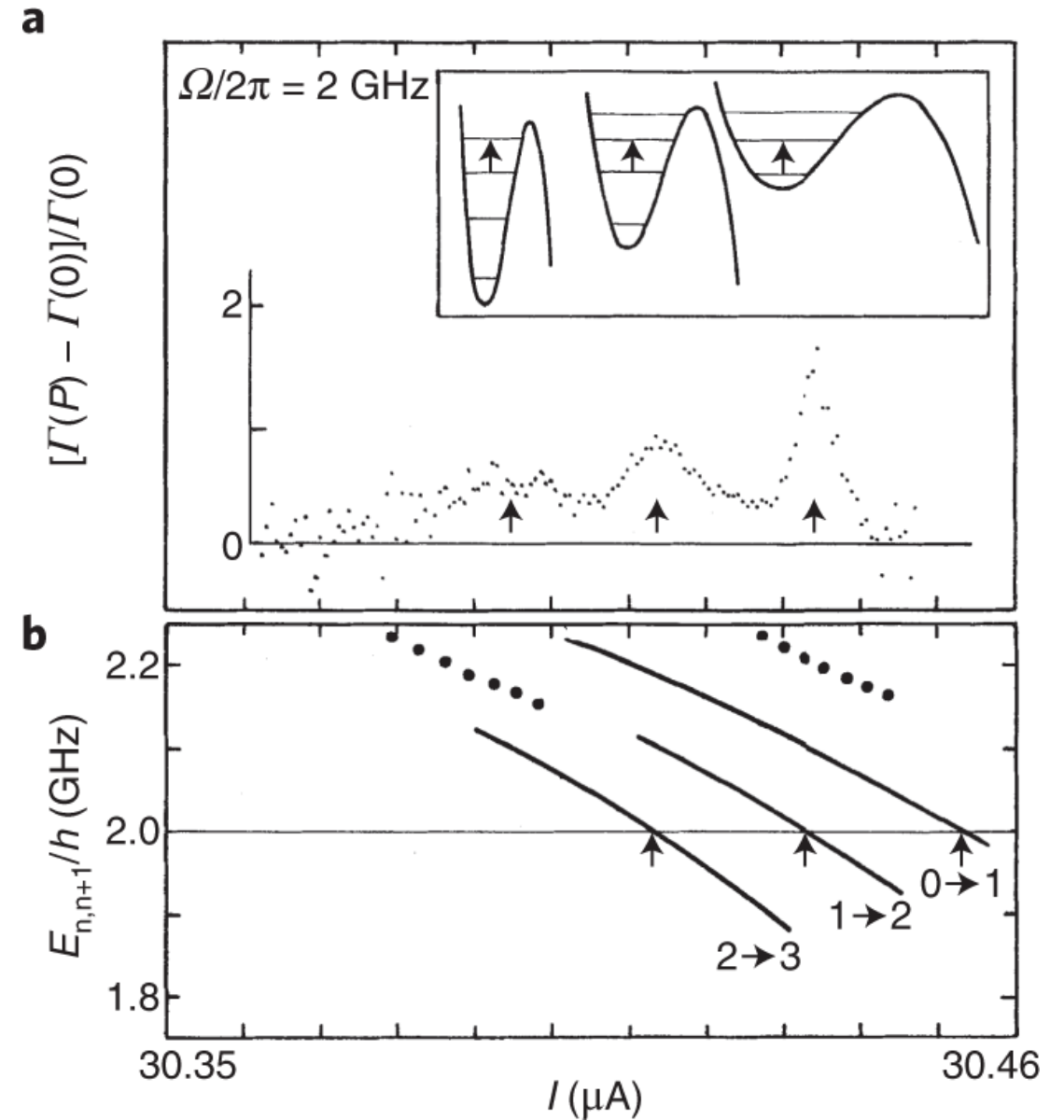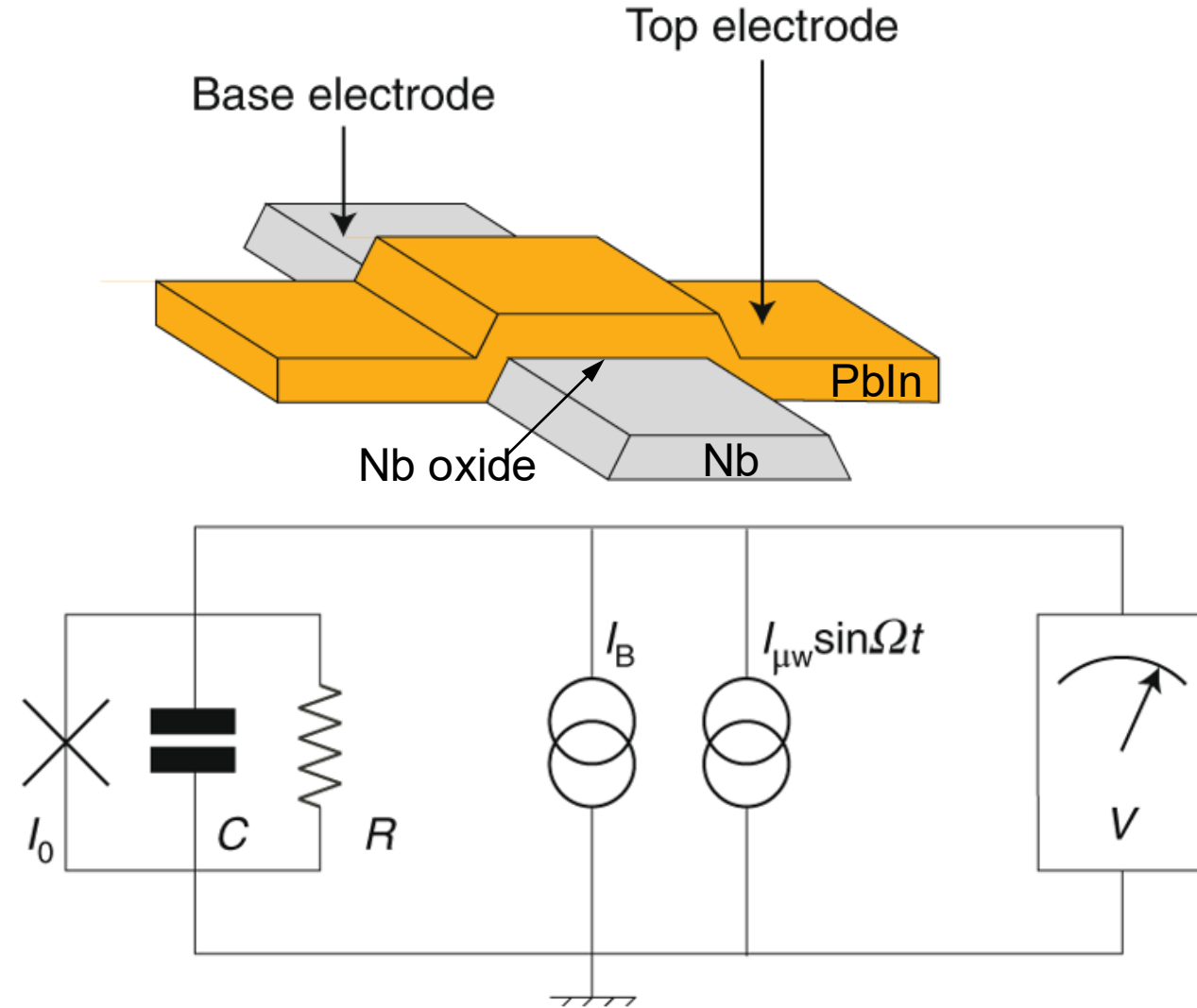
Nice review: Martinis, J.M., Devoret, M.H. & Clarke, J. Nat. Phys. 16, 234–237 (2020).
https://doi.org/10.1038/s41567-020-0829-5

Superconducting qubits
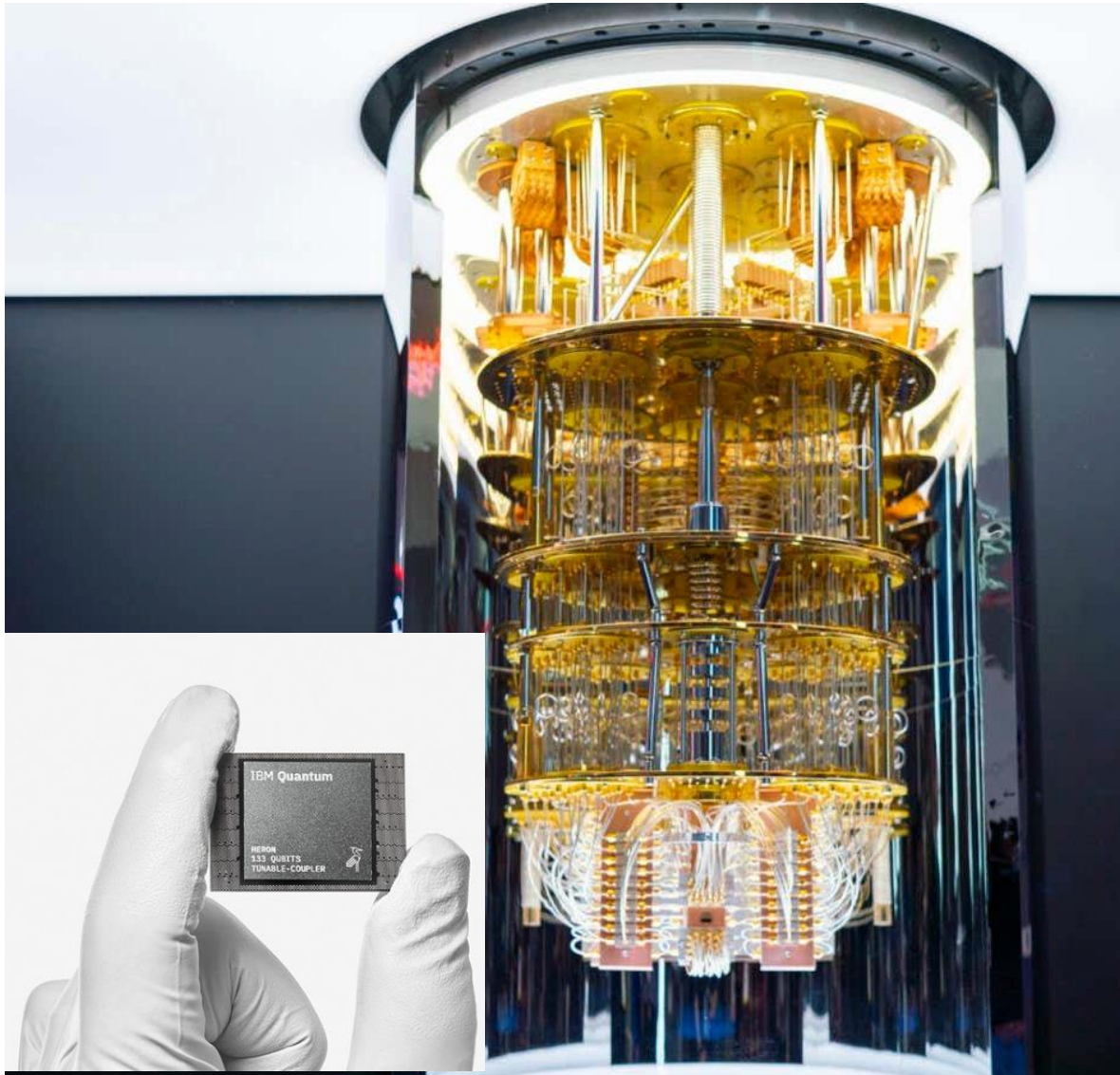
Applications of qubits

- Quantum simulations for new chemicals/materials ($\sim 10^4 - 10^5$ qubits)
- Exponential speedup in cryptography (~20 M qubits)
- Quantum-enhanced sensing (10 – 100 entangled qubits)
- Secure networking (10s – 10^3 qubits)

https://arxiv.org/pdf/2411.10406
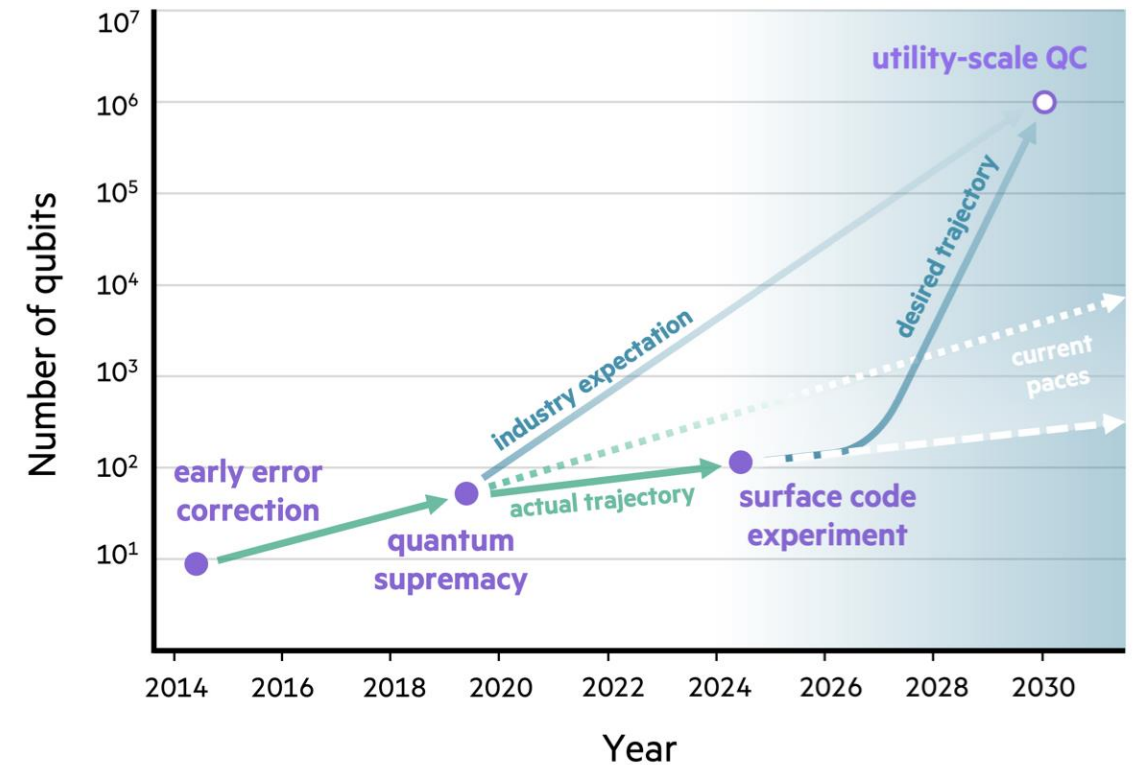
Topics

- The Schrödinger equation

- Select solutions
  - Free particle
  - Particle in infinite well
  - 3D potential wells and particle-in-a-box
  - Particle encountering a barrier
  - Tunneling

The Schrödinger equation and properties of the wave function

- For a particle with mass m_0 moving in a potential with potential energy $V(r)$

$$\left(-\frac{\hbar^2}{2m_0}\nabla^2 + V(\boldsymbol{r}) \right)\psi = E\psi \qquad \text{Time-independent}$$

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m_0}\nabla^2 + V(\boldsymbol{r}) \right)\psi \qquad \text{Time-dependent}$$

- The Schrödinger equation was not derived from first principles
  - It is a postulate that was constructed to fit experimental observations
  - Wave functions can be complex (unlike electromagnetic waves in which complex notations are used to simplify mathematics)
  - Squared modulus $|\psi|^2$ (always positive) describes probability density of finding the electron at some location

- Which one to use and when?
  - Spatial probability distribution does not change with time → time-independent
  - Superposition of quantum states → time-dependent

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The Schrödinger equation and properties of the wave function

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$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m_0}\nabla^2 + V(\boldsymbol{r}) \right)\psi \qquad \text{Time-dependent}$$

- The probability $P(x)\,dx$ of a particle being between x and $x + dx$ at the time t:

$$P(x,t)dx = \psi^*(x,t)\psi(x,t) = |\psi(x,t)|^2 dx$$

- The wave function must also be normalized so that the probability of the particle being somewhere on the x axis is 1:

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

Note, the equations shown here are valid for non-relativistic (velocity $v \ll c$) particles with mass and not for photons. Photon wave functions can be derived from quantization of Maxwell's equations which will be out of the scope of this class.

Free particle

- The potential energy seen by a free particle is constant in space. We will set it to zero here for simplicity ($V = 0$).

- V does not change with time, so it is appropriate to assume that $\psi(x,t) = \psi(x)e^{-i\omega t}$ and use the time-independent form of Schrödinger's equation: $-\dfrac{\hbar^2}{2m}\dfrac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x)$

$$\psi(x,t) = \left(A\, e^{ikx} + B\, e^{-ikx} \right) e^{-i\omega t}$$

$$+\hat{x} \qquad\qquad -\hat{x}$$
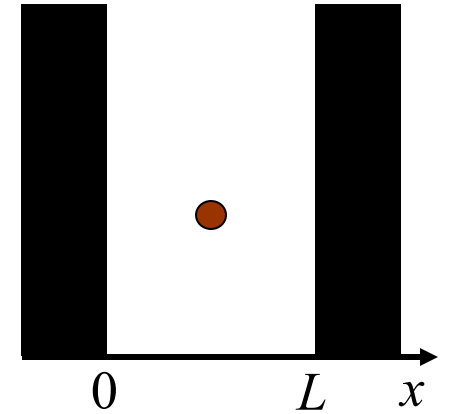
Reference: Demtroder (Chapter 4)

Infinite square-well potential

- Consider a particle trapped in a box with infinitely hard walls that the particle cannot penetrate. This potential is given by:

$$V(x) = \begin{cases} \infty & x \leq 0, x \geq L \\ 0 & 0 < x < L \end{cases}$$

- Outside the box, where the potential is infinite, the wave function must be zero.

- Inside the box, where the potential is zero, the energy is entirely kinetic, so $E > 0 = V_0$:

- So, inside the box, the solution is:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \text{ where } k = \sqrt{2mE/\hbar^2}$$

References: Demtroder, Chapter 4
R. Trebino's lecture notes on Modern Physics

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Infinite square-well potential

- Solution inside the box: $\psi(x) = Ae^{ikx} + Be^{-ikx}$

- Boundary conditions dictate that the wave function must be zero at $x = 0$ and $x = L$.
  - $\psi(x) = A(e^{ikx} + e^{-ikx}) = 2iA \sin kx$
  - $\sin kL = 0 \rightarrow kL = n\pi \rightarrow k_n = n\pi/L$, where n is an integer

- This yields solutions $\psi_n(x) = 2iA \sin(\frac{n\pi x}{L})$

- Normalizing the wave functions:

$$\frac{1}{2} - \frac{1}{2}\cos(2n\pi x/L)$$

$$\int_{-\infty}^{\infty} \psi_n^*(x)\psi_n(x)dx = 1 \implies 4A^2 \int_{-\infty}^{\infty} \sin^2\left(\frac{n\pi x}{L}\right)dx = 1 \implies \frac{4A^2L}{2} = 1 \implies A = \sqrt{1/2L}$$

$$\boxed{\psi_n(x) = i\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)}$$

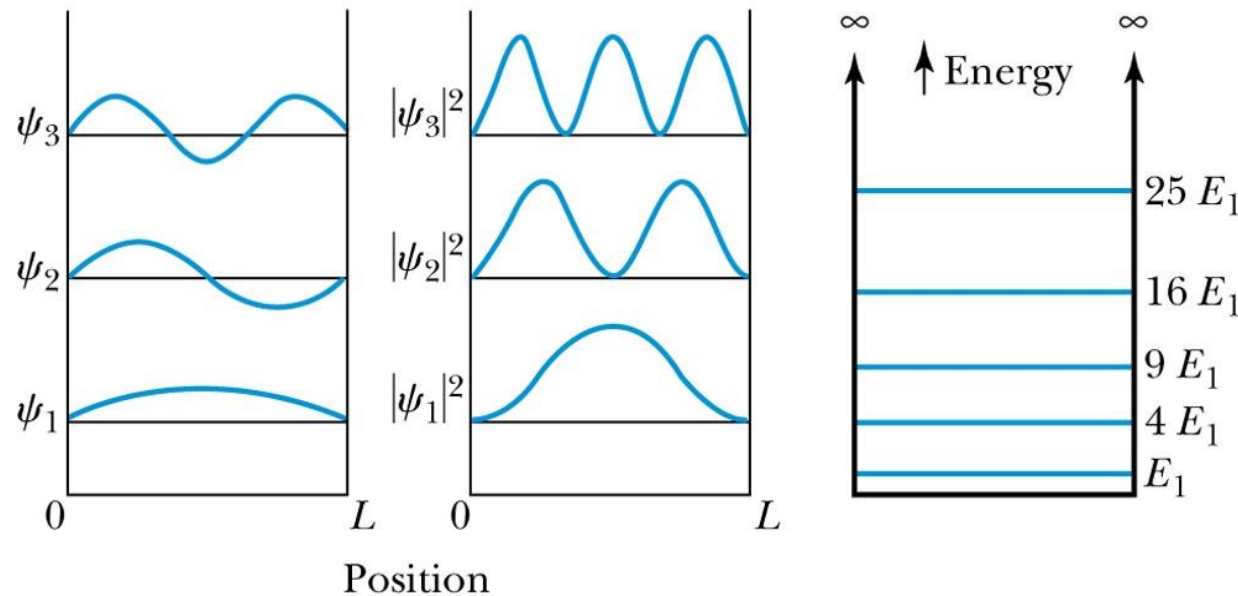the same functions as those for a **vibrating string** with fixed ends

Quantized energy solutions

k is **quantized**: $k_n = \dfrac{n\pi}{L} = \sqrt{\dfrac{2mE_n}{\hbar^2}}$

Using $E = \hbar^2 k^2/(2m)$, and solving for the energy: $E_n = \dfrac{n^2\pi^2\hbar^2}{2mL^2}$
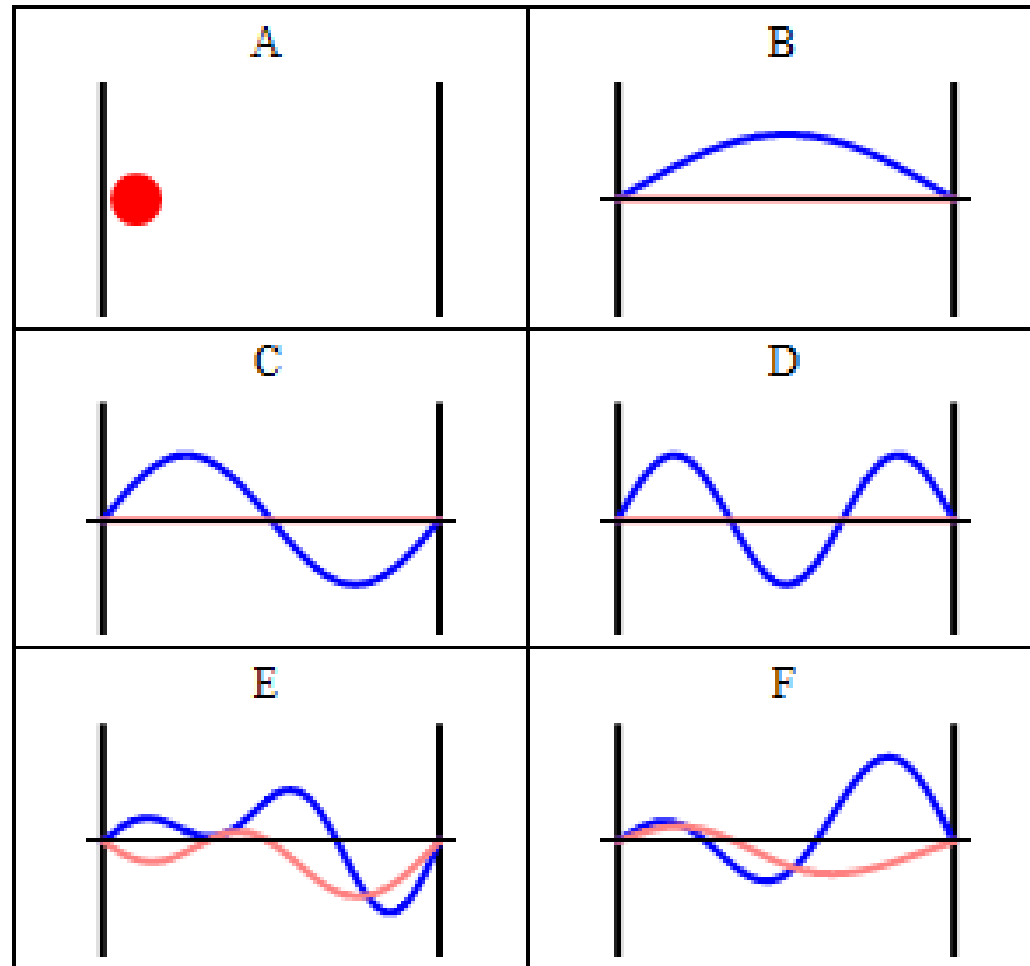
Energy is also **quantized**.

Minimum energy at n = 1 is not zero:

$E_1 = \dfrac{\pi^2\hbar^2}{2mL^2}$ (ground state)

References: Demtroder, Chapter 4
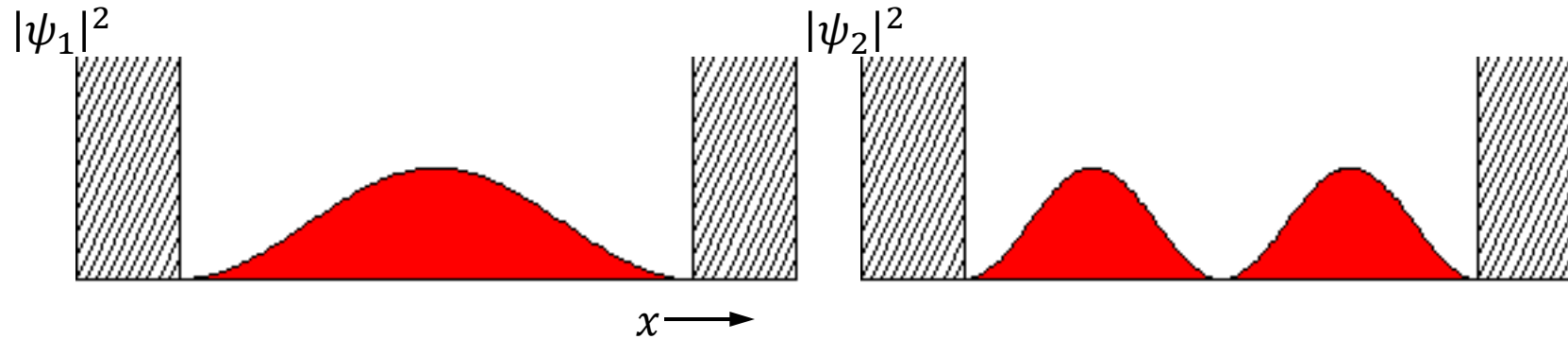R. Trebino's lecture notes on Modern Physics

Time dependence of solutions

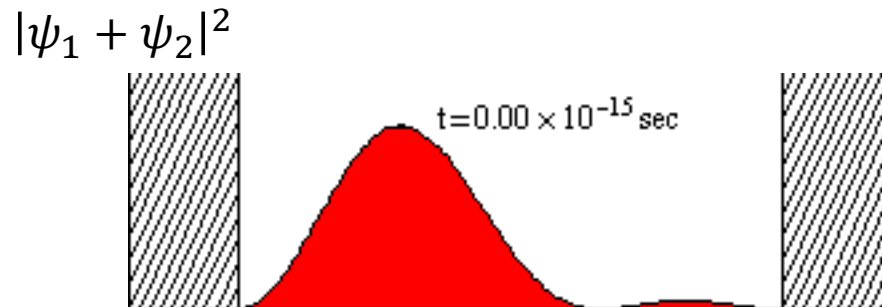Source: S. Byrnes (Sbyrnes321), distributed under CC

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Stationary solutions vs wave packets

Probability density for finding particle for stationary states
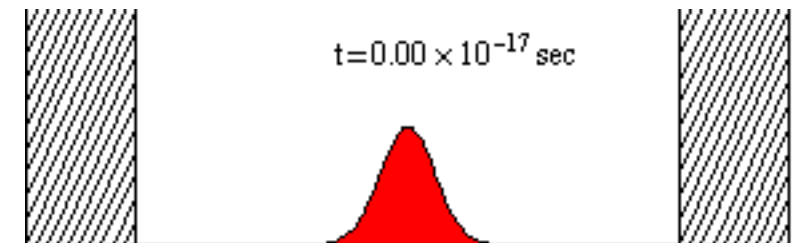
$|\psi_1|^2$

$|\psi_2|^2$

Time-averaged motion of the particle determined with large measurement time Δt so that energy is determined to within $\hbar\omega > \Delta E > h/\Delta t$

$x \longrightarrow$

Superposition of states

$|\psi_1 + \psi_2|^2$

$t = 0.00 \times 10^{-15}\ sec$

Gaussian wave packet

$t = 0.00 \times 10^{-17}\ sec$

Wave packet oscillating back and forth between potential wells

Animations from http://budker.berkeley.edu/physics137a/SquareWellHTML/index.html

Three-dimensional potential well

- The wave function must be a function of all three spatial coordinates.

- The Schrödinger wave equation is generalized to three dimensions the same way that the classical wave equation is:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + V\psi = E\psi$$
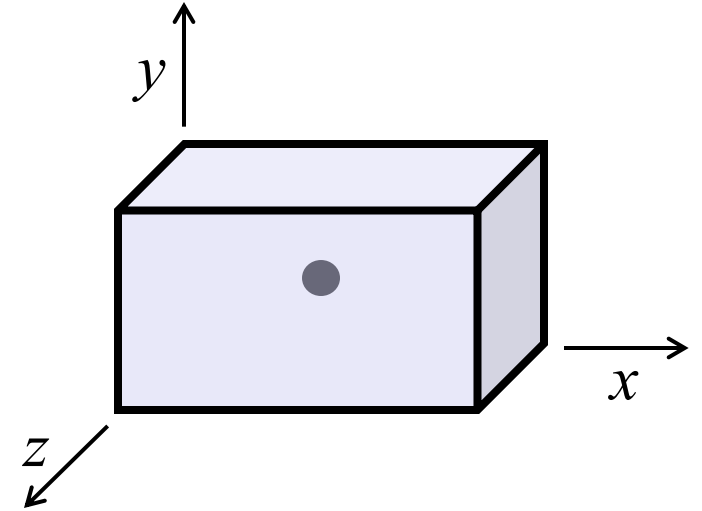
So we'll need to solve for $\psi(x, y, z)$ using separation of variables.

This equation can also be written in terms of spherical coordinates, where we'll need to solve for $\psi(r, \theta, \phi)$.

References: Demtroder, Chapter 4
R. Trebino's lecture notes on Modern Physics

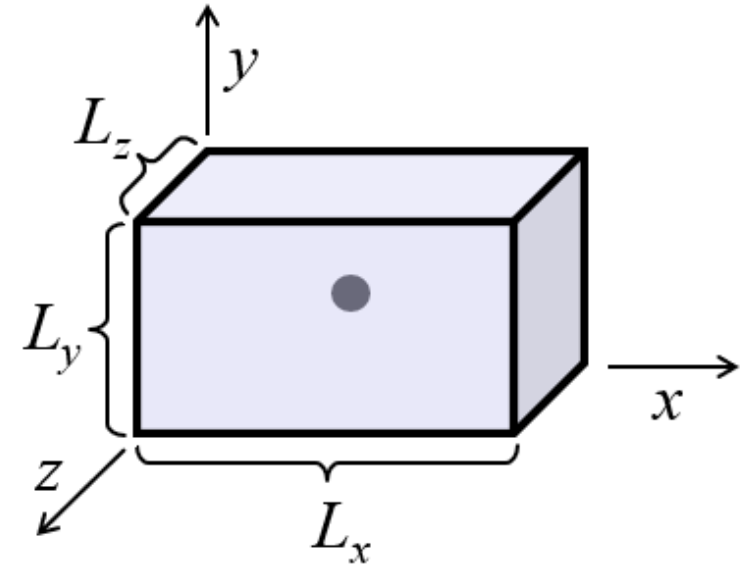# Three-dimensional potential well

Solution:

$$\psi(x, y, z) = A \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

where:
$$k_x = \pi n_x / L_x \qquad k_y = \pi n_y / L_y \qquad k_z = \pi n_z / L_z$$

$$E = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$$

When the box is a cube:

$$E = \frac{\pi^2 \hbar^2}{2mL^2} \left(n_x^2 + n_y^2 + n_z^2 \right)$$

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Degeneracy

Note that more than one wave function can have the same energy.

$$E = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$$

When more than one wave function has the same energy, those quantum states are said to be degenerate.

Try (10, 4, 3) and (8, 6, 5)

- Degeneracy results from <u>symmetries of the potential energy function</u> that describes the system.

- A perturbation of the potential energy can remove the degeneracy.

- Examples of perturbations include external electric or magnetic fields or various internal effects, like the magnetic fields due to the spins of the various particles.
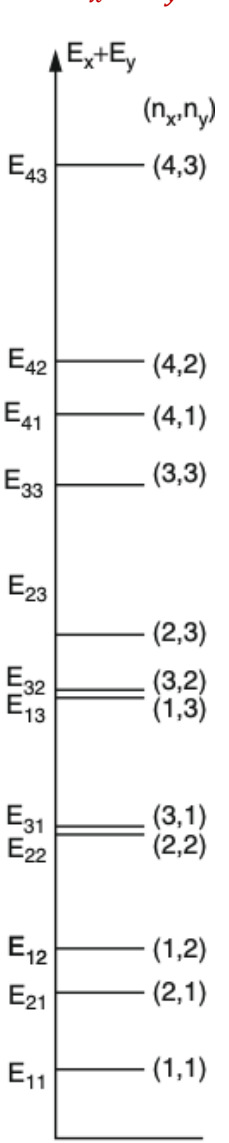
References: Demtroder, Chapter 4
R. Trebino's lecture notes on Modern Physics

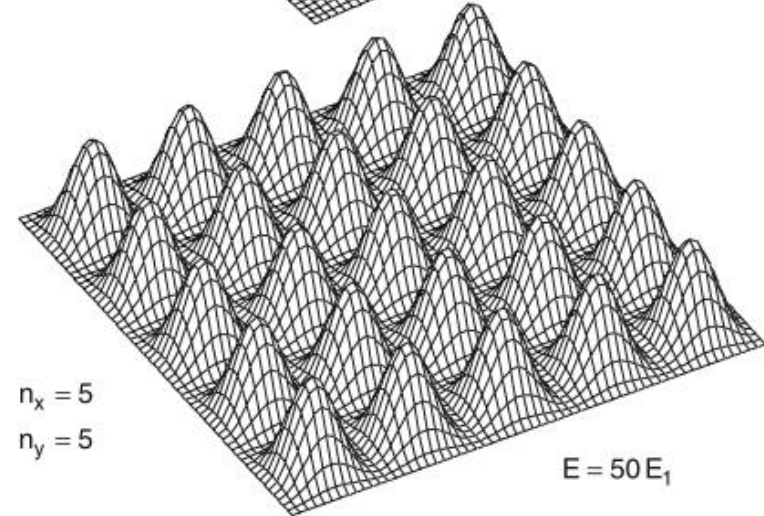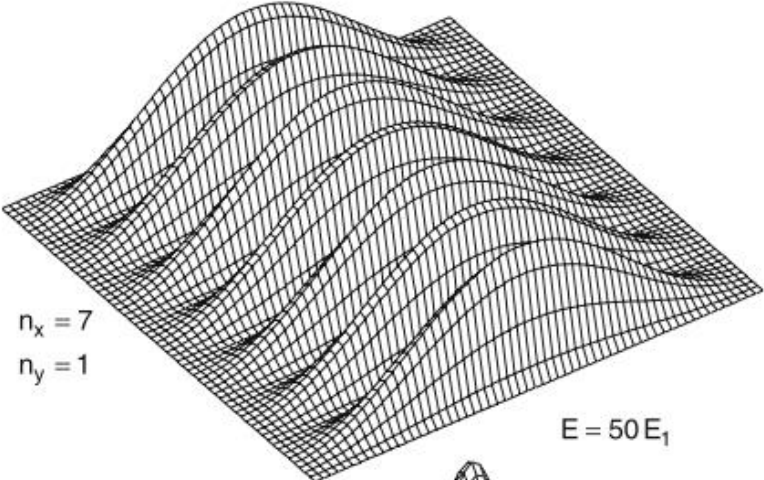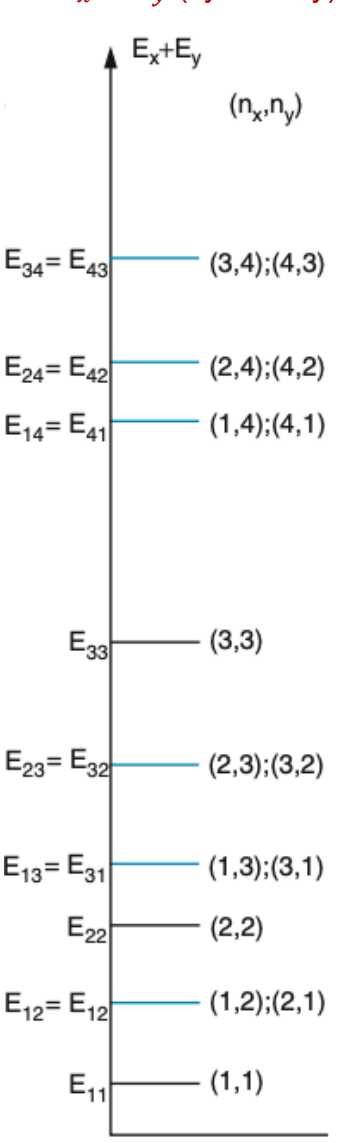# Degenerate states in a two-dimensional potential box
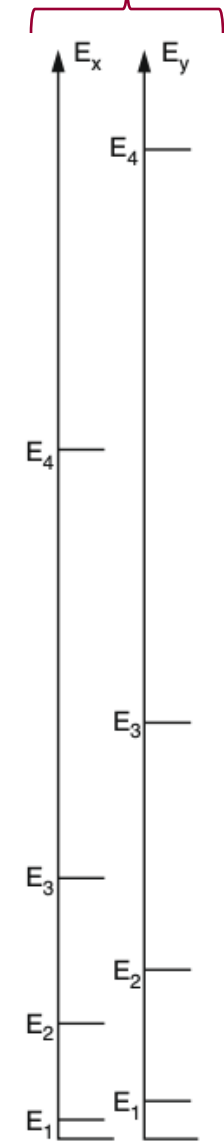
References: Demtroder, Chapter 4

Exam #1 results

- **Mean**: 56.3/70 (80%); **stdev**: 10/70
- **Median**: 56.5/70 (81%)

- Medium score per problem:

Problem	Q1 (10)	Q2 (15)	Q3 (15)	Q4 (15)	Q5 (15)
Score	8.5	11.5	13	14	13.5

- Solutions will be posted right after class. I encourage you to schedule a meeting with me to go through the exam together if you have concerns about your conceptual understanding or grade.

- Course policy:
  - Next exam is 11/24. Each exam is worth 17.5% of the total grade, but there is an optional make-up exam on 12/15. In the case that you take all three exams, grading will be based on the highest two of the three grades.
  - Other course components: attendance and participation (10%), homework (30% - 6 HW total, and final grade will be determined by the 5 highest grade of the 6), and final project (25%)

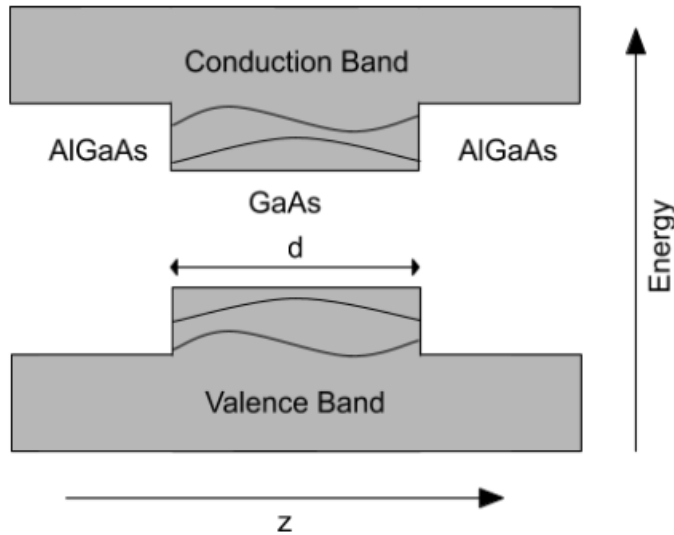# Example particle-in-a-box systems: quantum wells

Semiconductor lasers
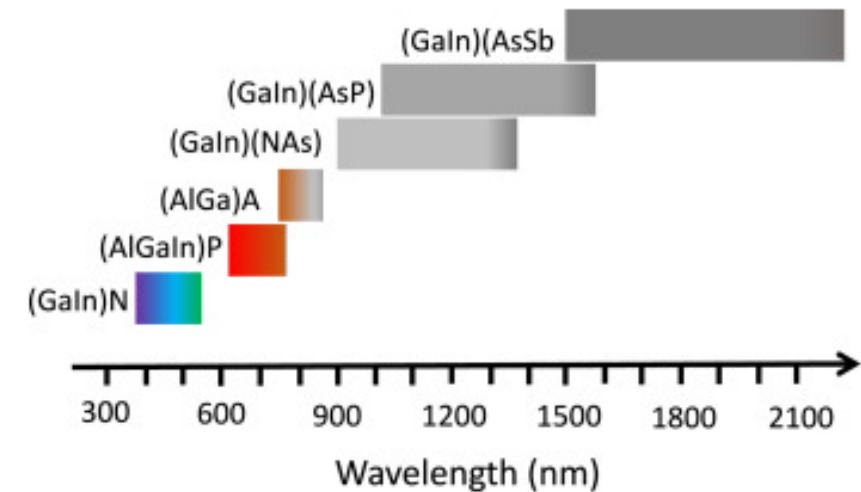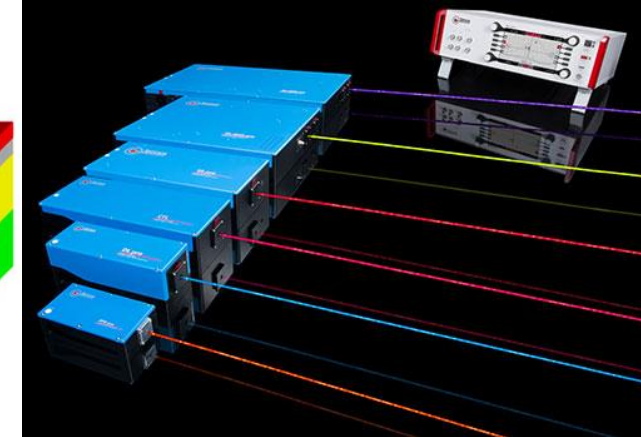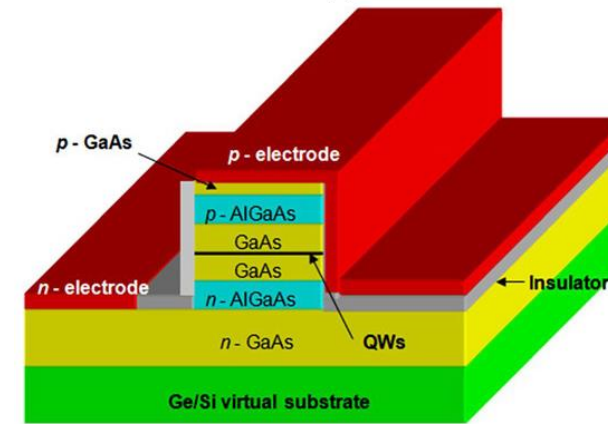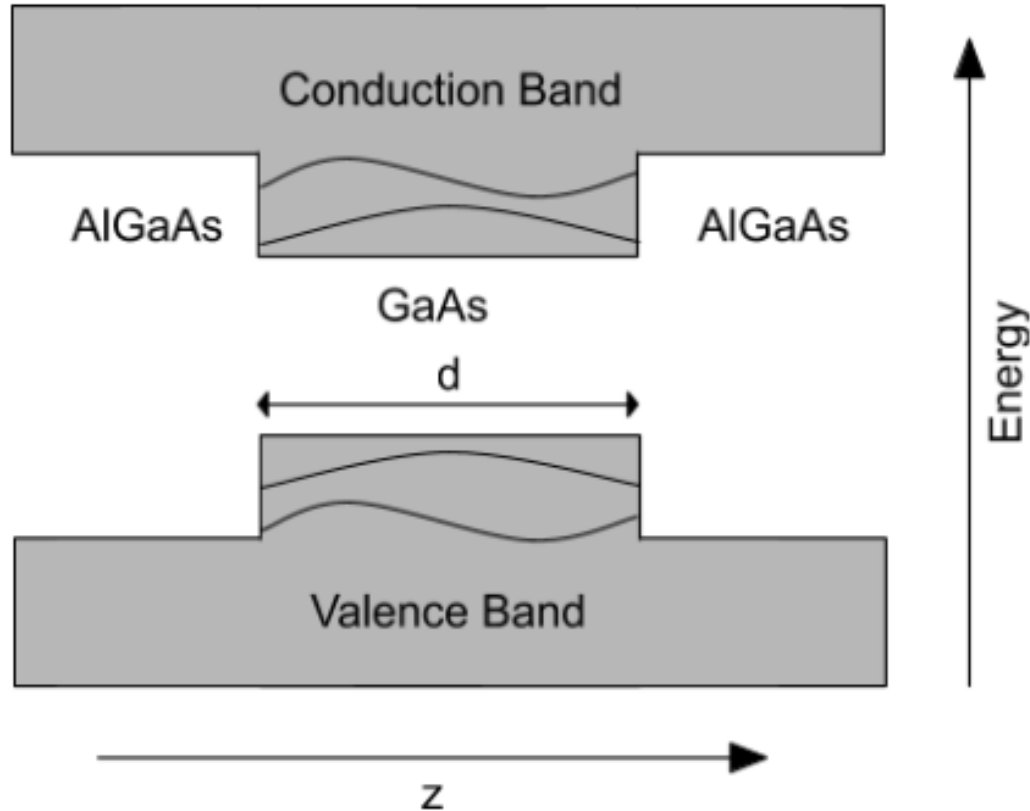
References:
https://en.wikipedia.org/wiki/Quantum_well
http://www.semiconductor-today.com/news_items/2016/sep/ingaas_080916.shtml

GaAs/AlGaAs quantum well laser

Consider a quantum well formed by a thin semiconductor layer (such as GaAs) sandwiched between two layers of materials with higher band gaps (such as AlGaAs), creating a potential well for both electrons and holes. The quantum confinement in one dimension means that electrons and holes can only occupy discrete energy levels within the well.

We can try to calculate the energy difference between the electron and hole energy levels and determine the wavelength of the light emitted when an electron recombines with a hole.

Confinement for electrons and holes in the z direction: $L_z = 10\ nm$

Effective masses for electron and hole:
$$m_e^* = 0.067\ m_0$$
$$m_h^* = 0.45\ m_0$$
$$m_0 = 9.109 \times 10^{-31}\ kg$$

Bandgap of GaAs
$$E_g = 1.42\ eV$$

$$E_{n_e} = \frac{\hbar^2 \pi^2 n_e^2}{2m_e^* L_z^2}$$
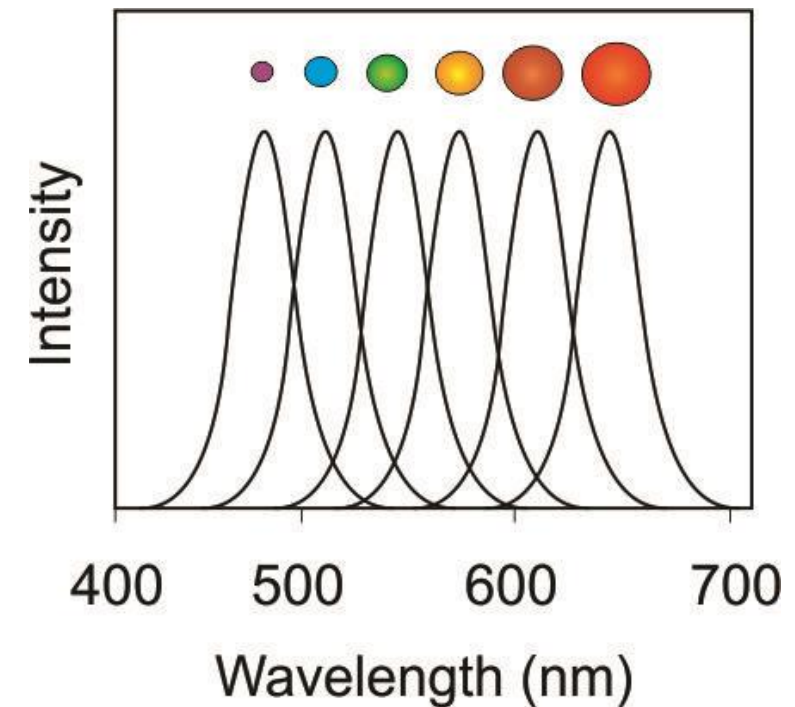
$$E_{n_h} = \frac{\hbar^2 \pi^2 n_h^2}{2m_h^* L_z^2}$$
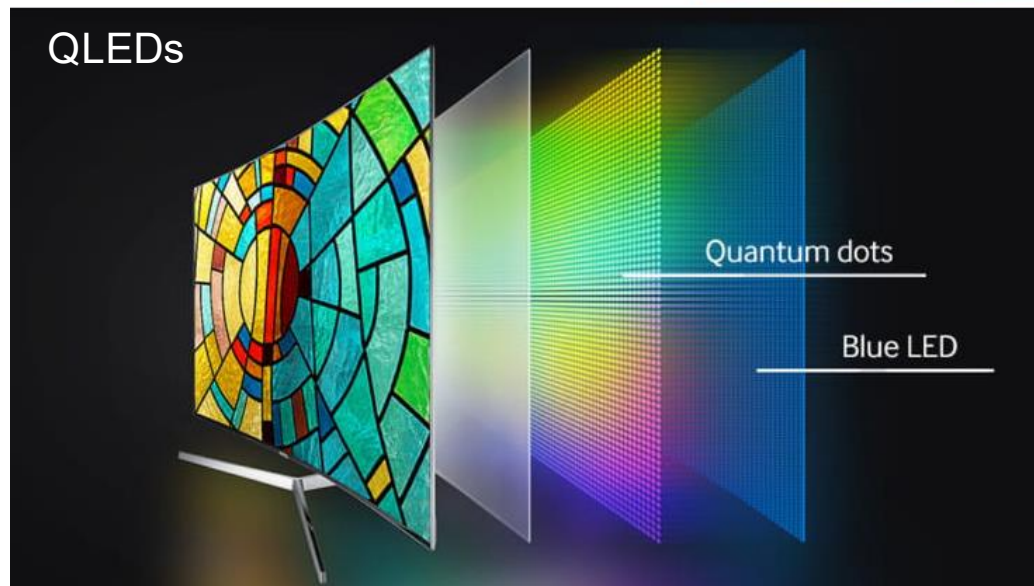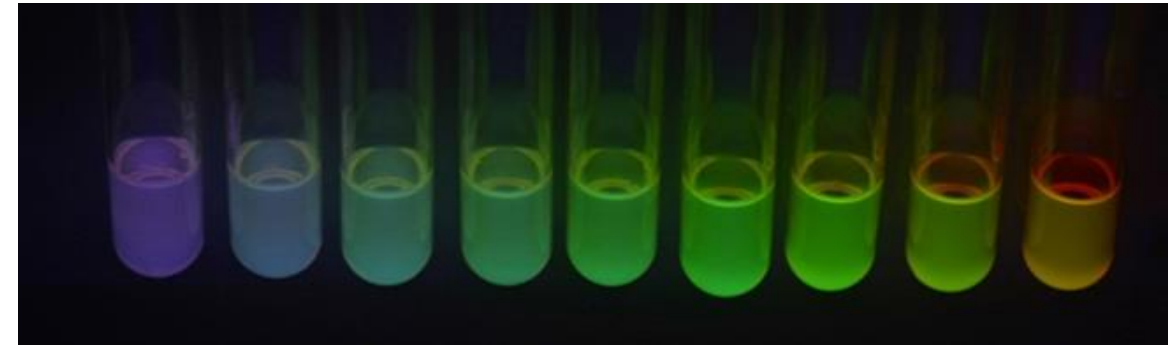
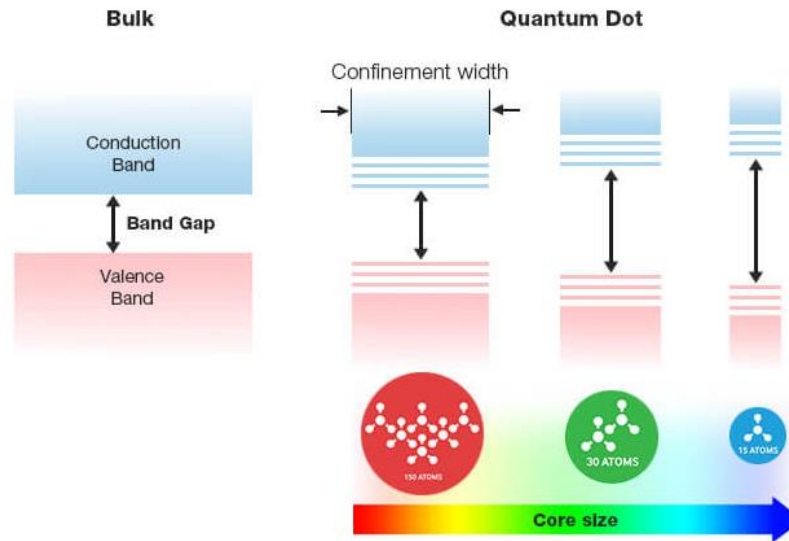$$E_{photon} = E_g + (E_{n_e} - E_{n_h})$$

$$= 1.42 + (0.0057 - 8.4785 \times 10^{-4})\ \text{eV} = 1.4249\ \text{eV}$$

$$E_{photon} = \frac{hc}{\lambda} \rightarrow \lambda = 870.1\ nm$$

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Example particle-in-a-box systems: quantum dots

$$E = \frac{\pi^2 \hbar^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

Bulk

Conduction Band

Band Gap

Valence Band

Quantum Dot

Confinement width

Core size

QLEDs

Quantum dots

Blue LED

Intensity

400 500 600 700

Wavelength (nm)

References: https://education.mrsec.wisc.edu/quantum-dots-and-nanoparticles/
https://www.intechopen.com/books/biomedical-engineering-technical-applications-in-medicine/quantum-dots-in-biomedical-research
https://pid.samsungdisplay.com/en/learning-center/white-papers/guide-to-understanding-quantum-dot-displays

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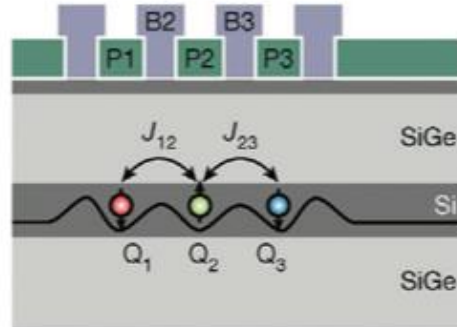
Semiconductor quantum dots as qubits

- Most common are electrostatically defined dots in GaAs/AlGaAs or Si/SiGe, in which gate voltages create tunable confinement potentials
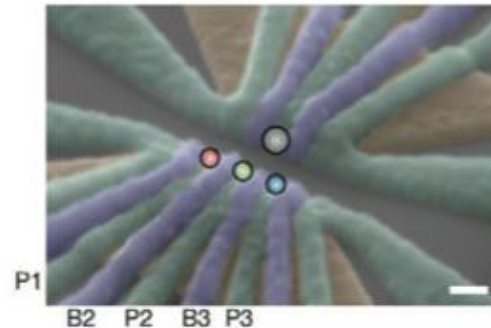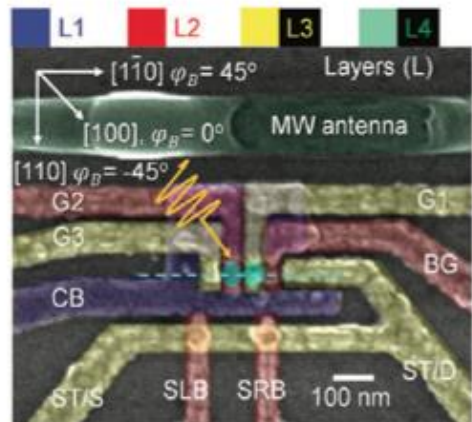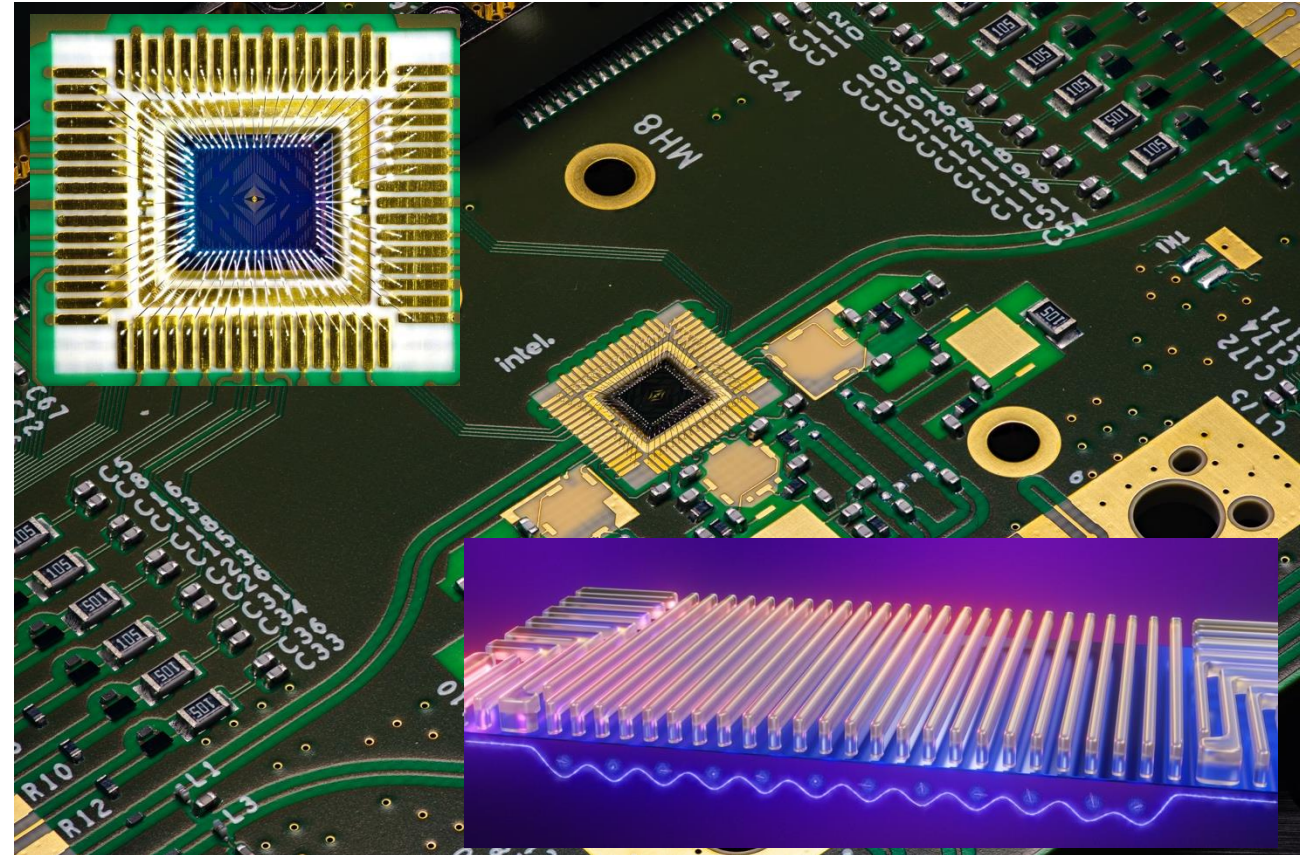

Si Planar MOS

Si/SiGe Heterostructure

Intel's 12-qubit device

Some review papers:
Burkard, Guido, et al. *Reviews of Modern Physics* 95.2 (2023): 025003.
Liu, Yang, et al. Advanced Functional Materials 34.19 (2024): 2304725.

Particle encountering potential barrier

Use time-independent solutions to simplify problem
(valid since potential barrier is constant in time)

$$\left(-\frac{\hbar^2}{2m_0}\nabla^2 + V(\boldsymbol{r})\right)\psi = E\psi$$

$$\psi_I = A e^{ik_1x} + B e^{-ik_1x} \qquad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$E > V_0: \quad \psi_{II} = T e^{ik_2x} + \cancel{D}e^{-ik_2x} \qquad k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

$$E < V_0: \quad \psi_{II} = T e^{-k_2x} + \cancel{D}e^{k_2x}$$

at $x = 0$

$$\psi_I(0) = \psi_{II}(0)$$

$$\frac{d}{dx}\psi_I(0) = \frac{d}{dx}\psi_{II}(0)$$

$$ik_1(A-B) = -k_2 T$$

$$(ik_1 + k_2)A = (ik_1 - k_2)B$$

Incident

$V(x)$

Transmitted

Reflected

E

Particle

V_0

0 L x

Region I   Region II
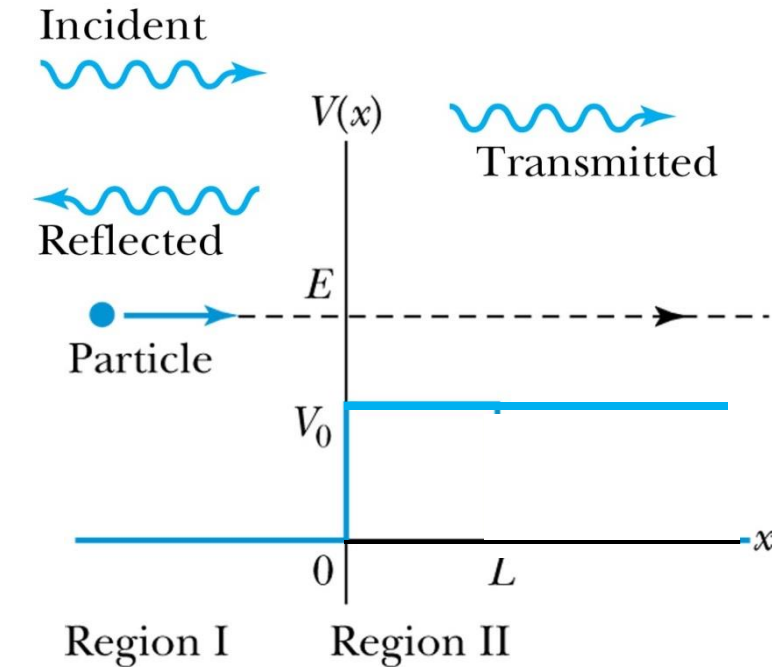
Particle encountering a potential barrier $E < V_o$

$Re(\psi(x))$

$V_0 - E$

e^-

V_0

E

A

B

$|A| = |B|$ 0

- Solution ($\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$):

$$\psi_I(x < 0) = A\left(e^{ikx} + \frac{ik+\alpha}{ik-\alpha}e^{-ikx}\right)$$

$$\psi_{II}(x \geq 0) = D^{-\alpha x} \qquad \text{Evanescent wave}$$

- Reflection coefficient

$$R = \frac{|B|^2}{|A|^2} = \left|\frac{ik+\alpha}{ik-\alpha}\right|^2 = 1$$

- Penetration of wave function into $x \geq 0$

$$P(x \geq 0) = |\psi_{II}(x)|^2 = |De^{-\alpha x}|^2$$

$$P(x \geq 0) = \frac{4k^2}{\alpha^2 + k^2}|A|^2 e^{-2\alpha x}$$

- Interpretation: Particle can penetrate into the barrier and is not reflected at x = 0.
  - Exponentially decaying, but nonzero probability distribution inside barrier
  - Note this does not mean that the particle is "stopped" inside the barrier, but rather it can penetrate into the barrier before returning to the –x direction

Reference: Demtroder, Chapter 3
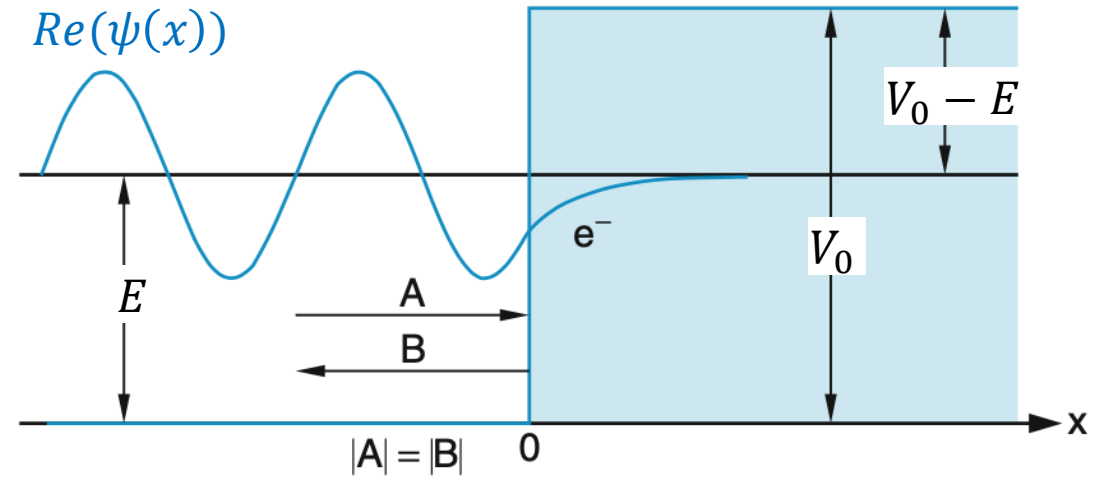
Tunneling

- Consider a particle of energy E approaching a potential barrier of height V_0, and the potential everywhere else is zero. Also $E < V_0$.

- Solutions:

$$\psi_I(x < 0) = Ae^{ikx} + Be^{-ikx}$$

$$\psi_{II}(0 \le x \le L) = Ce^{\alpha x} + De^{-\alpha x}$$

$$\psi_{III}(x > L) = A'e^{ikx} + B'e^{-ikx}$$

- Boundary conditions: $\quad \psi_I(0) = \psi_{II}(0); \; \psi_{II}(L) = \psi_{III}(L)$
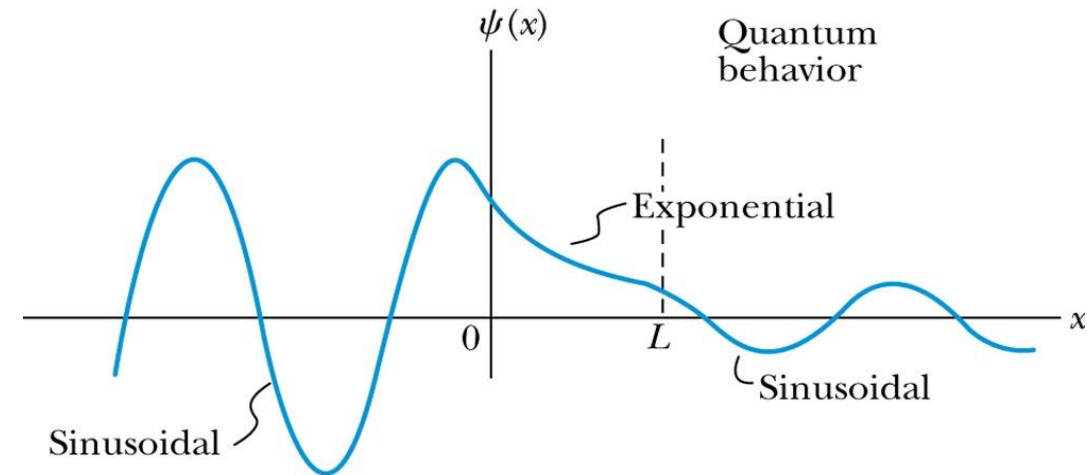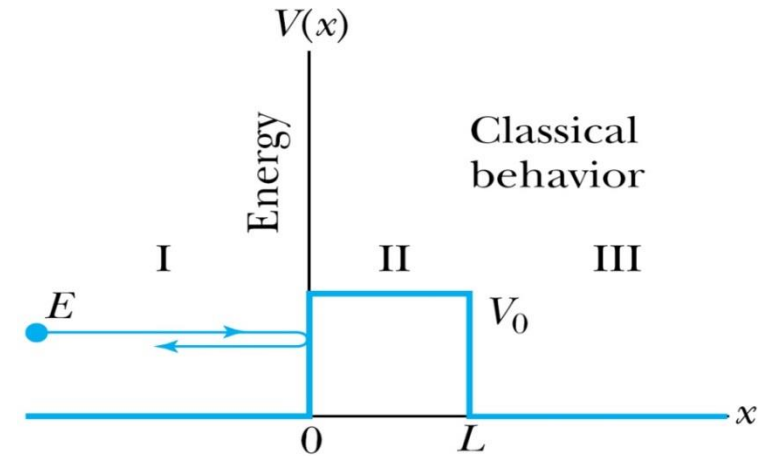
$$\frac{d\psi_I}{dx}(x = 0) = \frac{d\psi_{II}}{dx}(x = 0)$$

$$\frac{d\psi_{II}}{dx}(x = L) = \frac{d\psi_{III}}{dx}(x = L)$$

- Transmission coefficient

$$T = \frac{1 - E/V_0}{\left(1 - \frac{E}{V_0}\right) + \left(\frac{V_0}{4E}\right)\sinh^2 L\alpha}$$

$$T \approx \frac{16E}{V_0^2}(V_0 - E)e^{-2L\alpha} \qquad \text{for large barrier widths}$$

$V(x)$

Classical behavior

I, II, III

E

V_0

x

0, L

$\psi(x)$

Quantum behavior
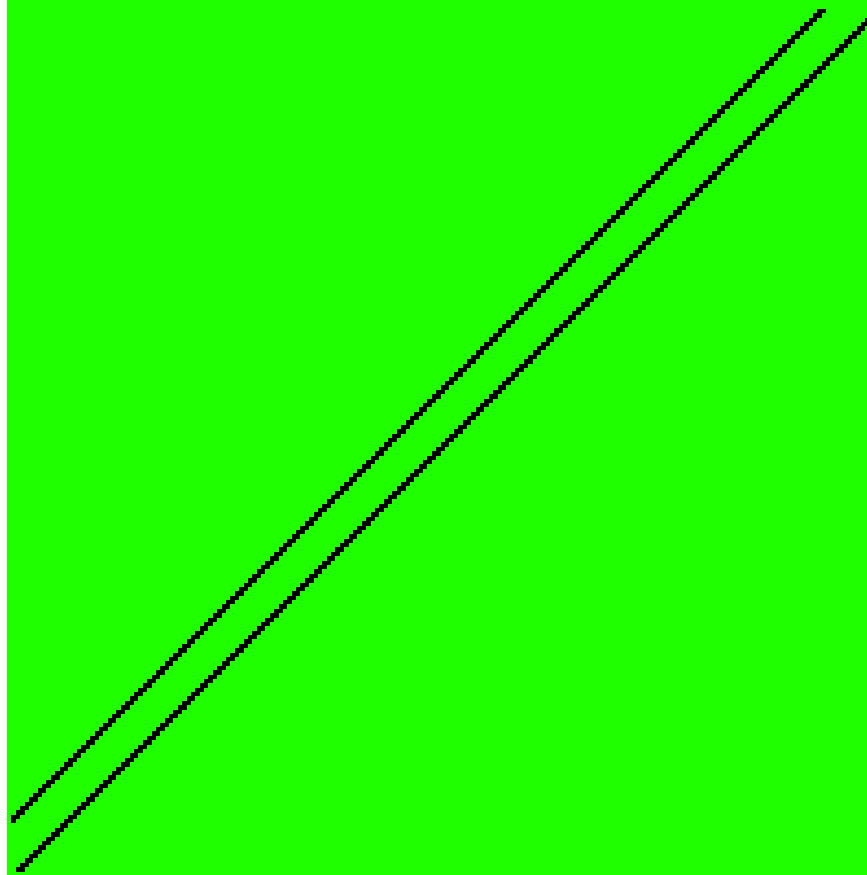
Exponential

Sinusoidal

Sinusoidal

0, L

x

References: Demtroder, Chapter 3
R. Trebino's lecture notes on Modern Physics

Quantum tunneling is analogous to frustrated total internal reflection in optics

Dielectric constant distribution
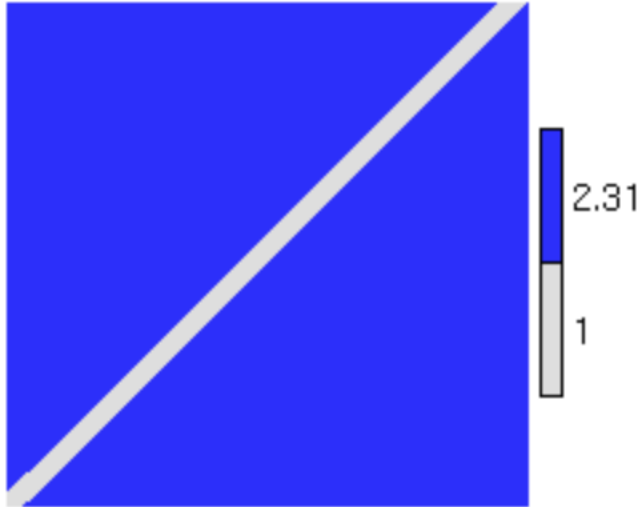
Electric field (out of plane)

Time-averaged Pointing vector
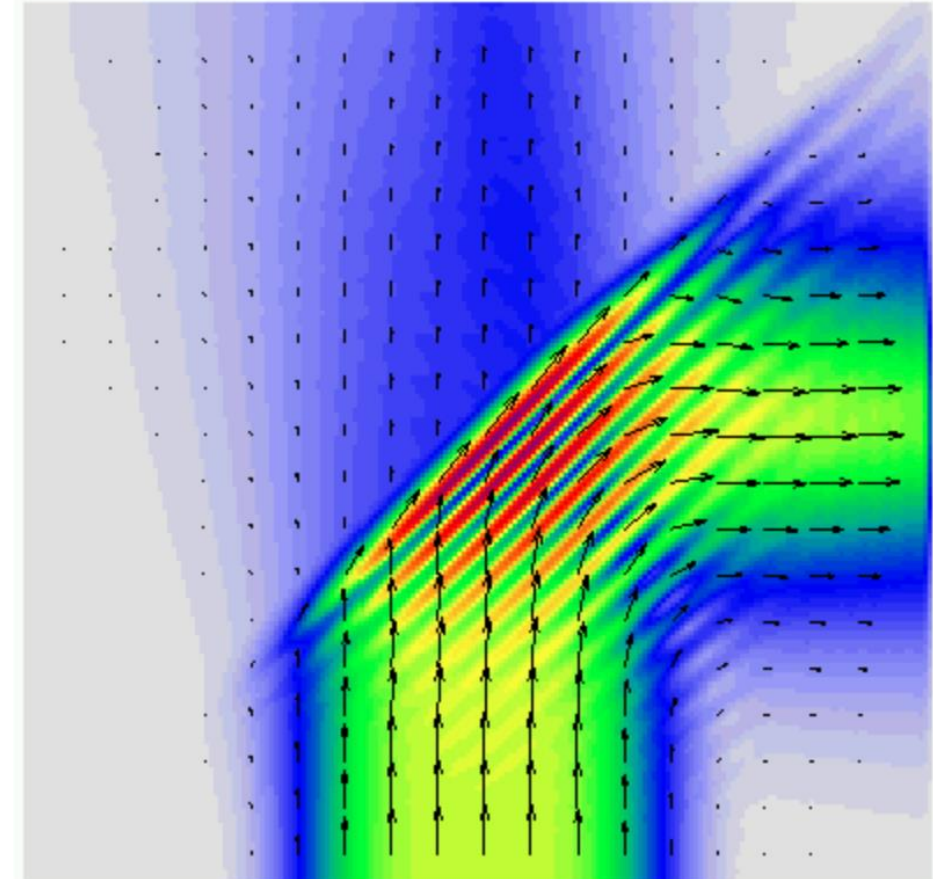
Create your own animations at https://www.falstad.com/ripple/

Source: http://www.met.reading.ac.uk/clouds/maxwell/frustrated_total_internal_reflection.html

Frustrated total internal reflection demonstration

ECE 535 – Introduction to Quantum Sensing – Fall 2025   Select solutions to the Schrodinger equation (complete)
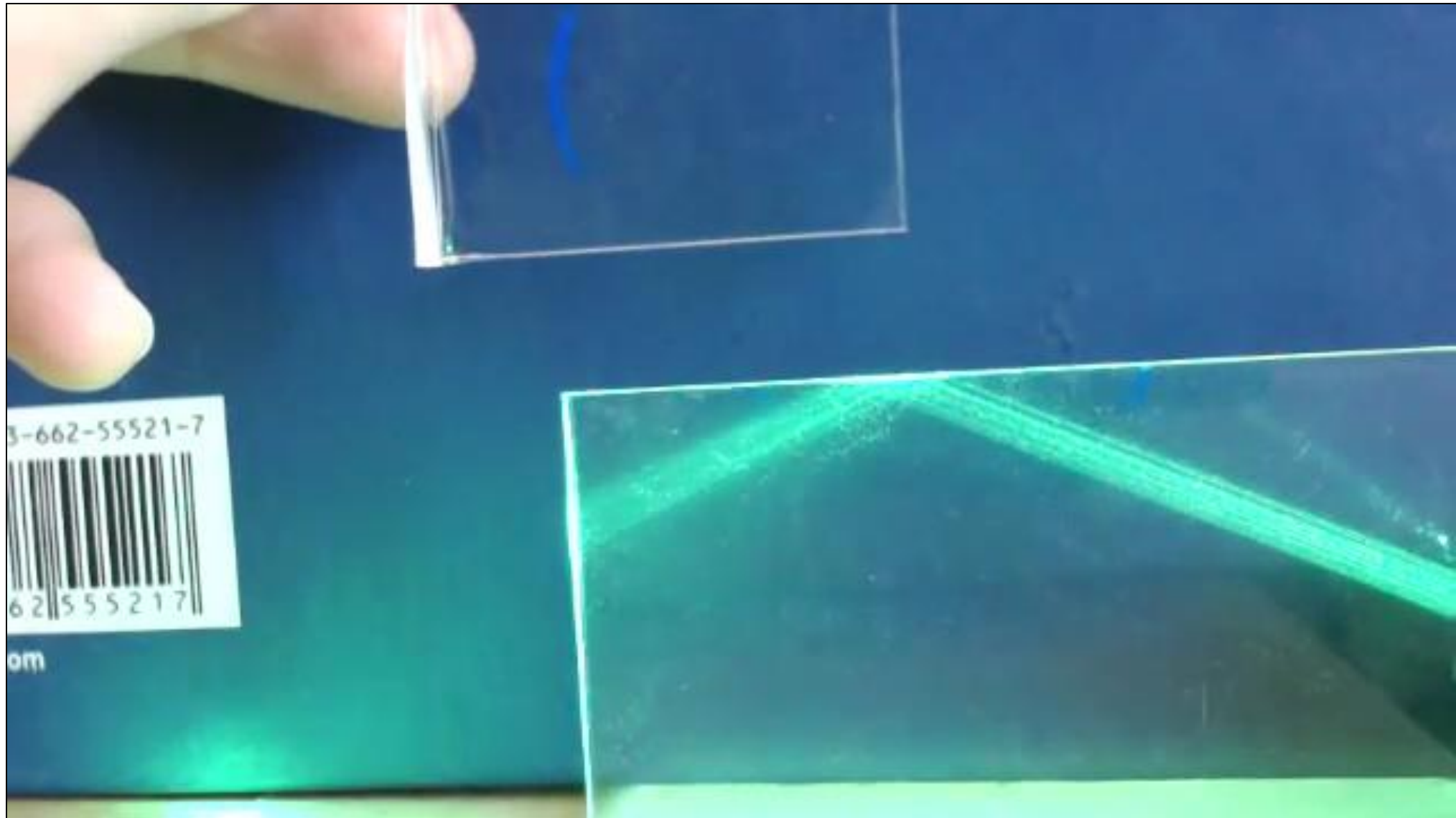
Other examples of frustrated total internal reflection

Credit: Olli Niemitalo

Acrylic (Plexiglass) Surface
Total Internal Reflection
Frustrated Total Internal Reflection
Projection Material
Infra Red Lighting
Infra Red Camera

https://sethsandler.com/multitouch/ftir/
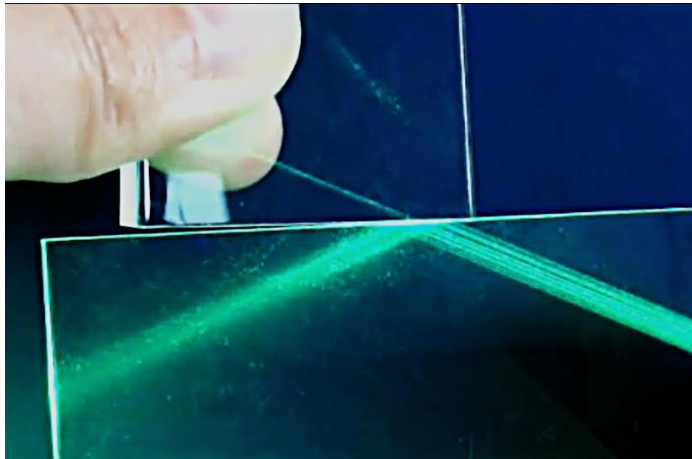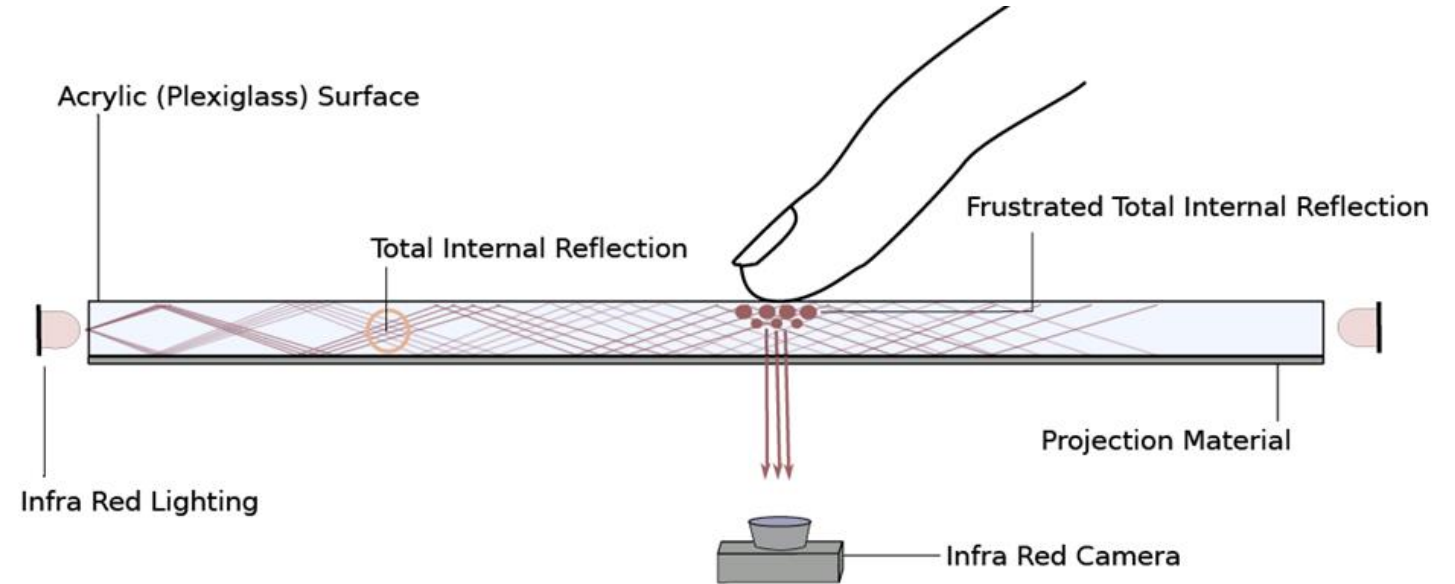
Scanning-tunneling microscope (STM)

- Tip is brought close to surface and is scanned laterally

- Electrons that tunnel through the vacuum barrier are measured as electrical current

- Tunneling probability varies exponentially with the distance between the tip and surface and is highest when the tip is right on top of an atom → atomic scale resolution

M. Schmid and G. Pietrzak, distributed under CC BY-SA 2.0
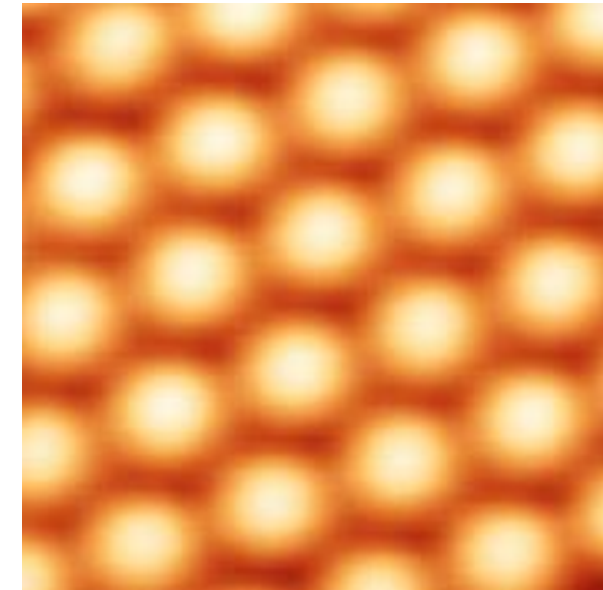
G. Baffou, distributed under CC BY-SA 3.0

https://en.wikipedia.org/wiki/Scanning_tunneling_microscope

Calculation of tunneling current

(Based on the solutions to the Schrodinger equation for an electron tunneling through a barrier, write a valid expression for the tunneling current I, as a function of $\Delta\phi$, d, m_e, I_0, where
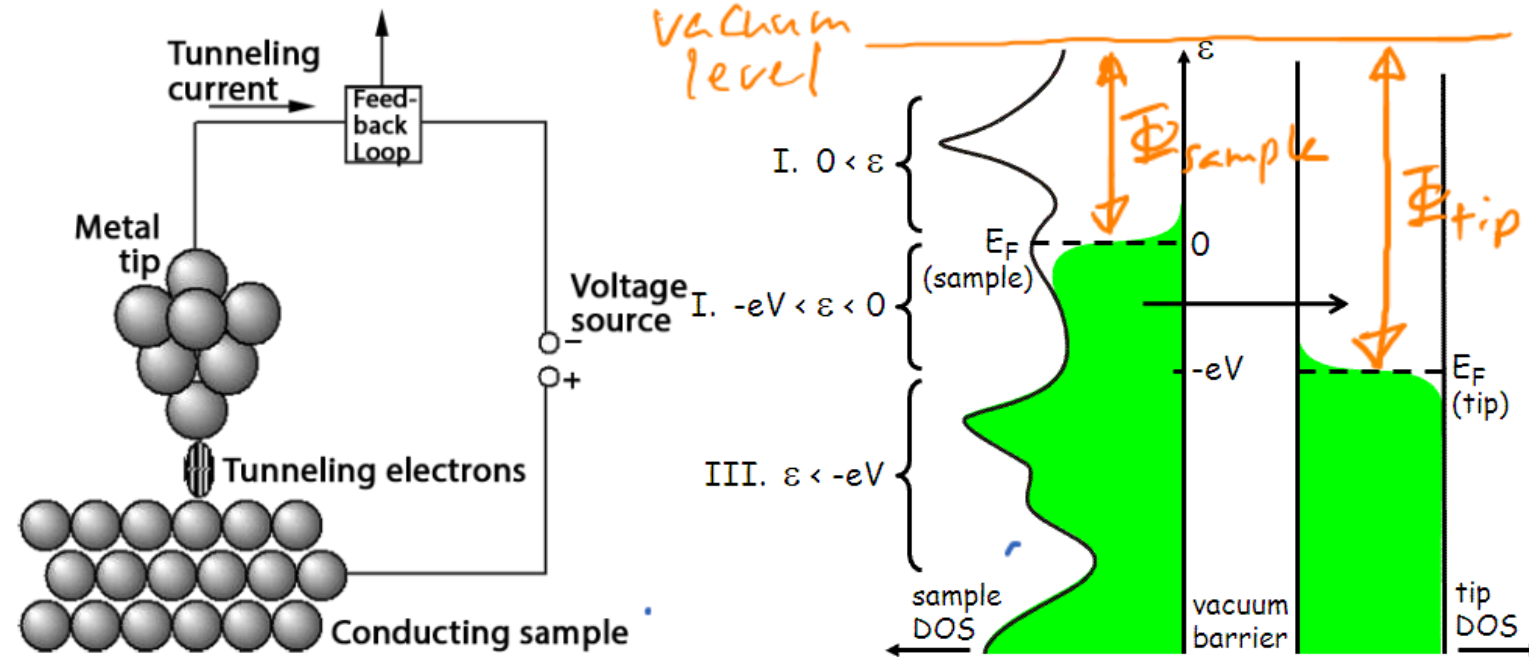
    $\Delta\phi$ = the barrier height

    d = tip-sample distance

    I_0 = some scaling factor for I

$$I(d) = I_0 \exp\left(-\frac{2d\sqrt{2m_e\Delta\phi}}{\hbar}\right)$$

Metal tip

Tunneling electrons

Conducting sample

Tunneling current — Feed-back Loop

Voltage source

I. $0 < \varepsilon$
I. $-eV < \varepsilon < 0$
III. $\varepsilon < -eV$

E_F (sample)

sample DOS — vacuum barrier — tip DOS

- Constant current mode → height = surface profile
- Constant height mode → current variation = local density of states

Now let's suppose $\Delta\phi = 1$ eV, $I_0 = 1$ A, $d_0 = 1\ nm$. What is the fraction of tunneling current change if d changes on the order of the size of an atom, 0.1 nm.

$$\frac{I_1(d_0+\delta d)}{I_2(d_0)} = \exp\left(-\frac{2\delta d\sqrt{2m_e\Delta\phi}}{\hbar}\right) = 0.36$$

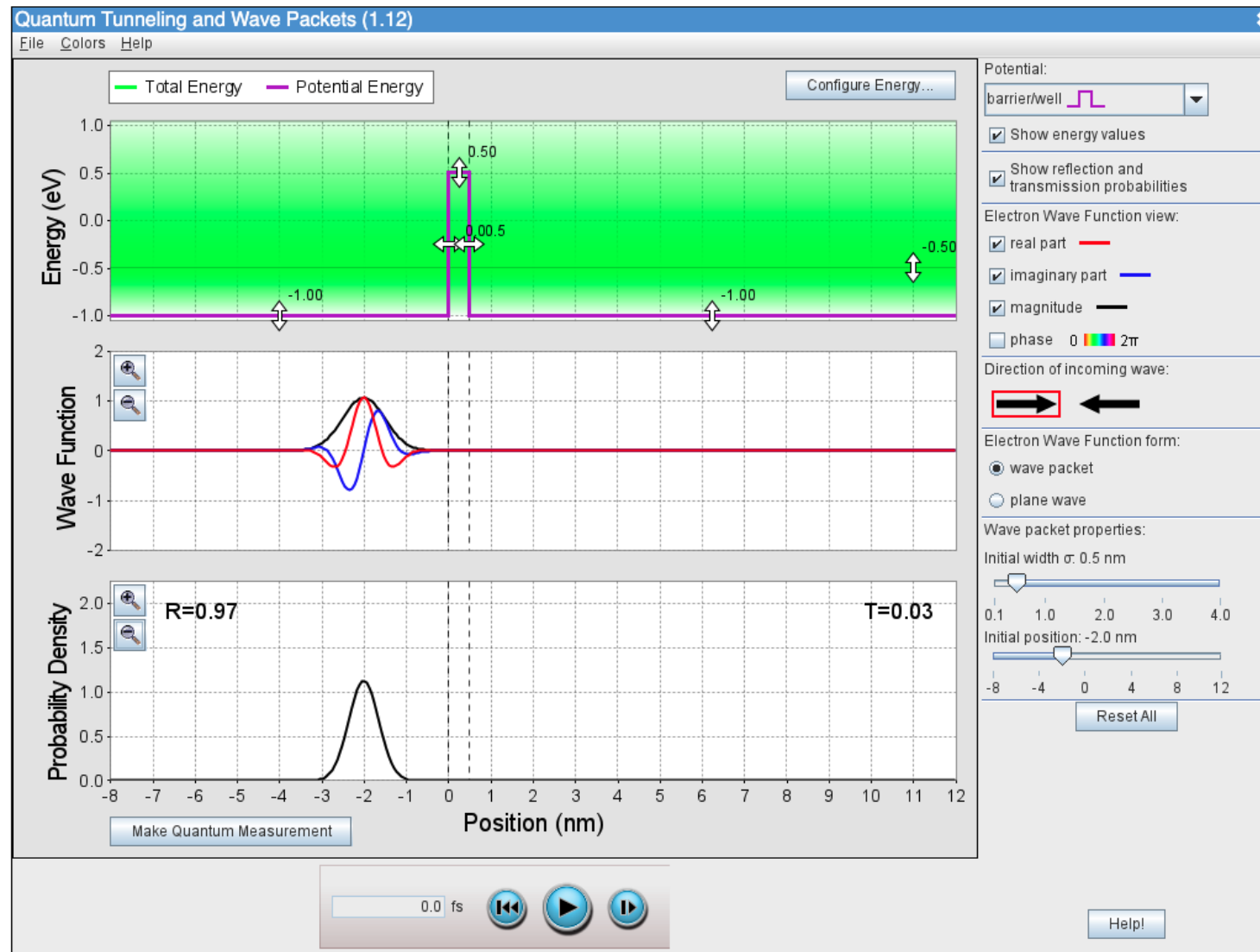$$\alpha = 5.12\times10^9\ m^{-1}$$

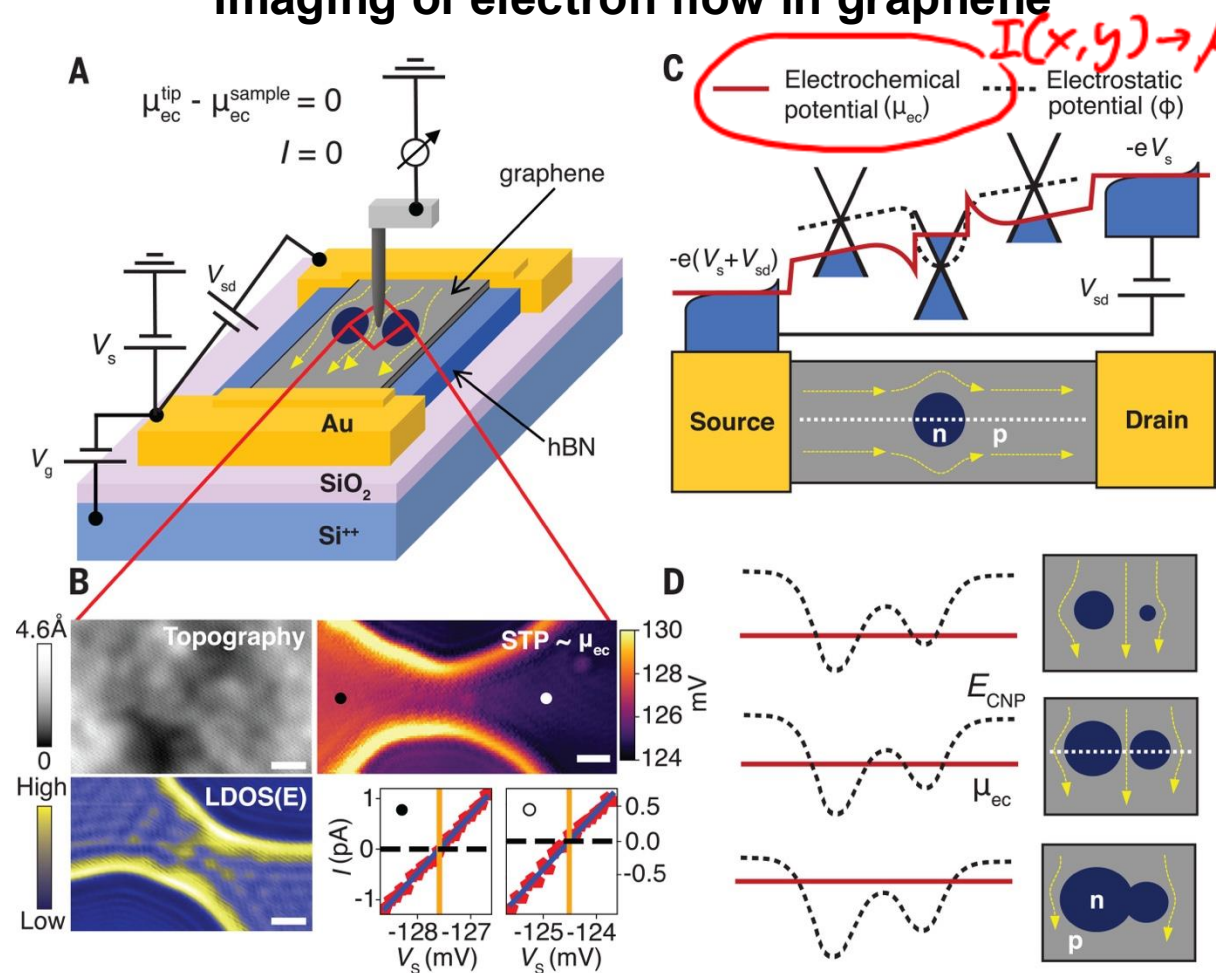Sample $\uparrow V(x)$ tip

$(\Phi_{sample} + \Phi_{tip})/2$

Vacuum

Visualize your results

https://phet.colorado.edu/sims/cheerpj/quantum-tunneling/latest/quantum-tunneling.html?simulation=quantum-tunneling

Imaging of electron flow in graphene

Atomic-scale measurements of E and B fields
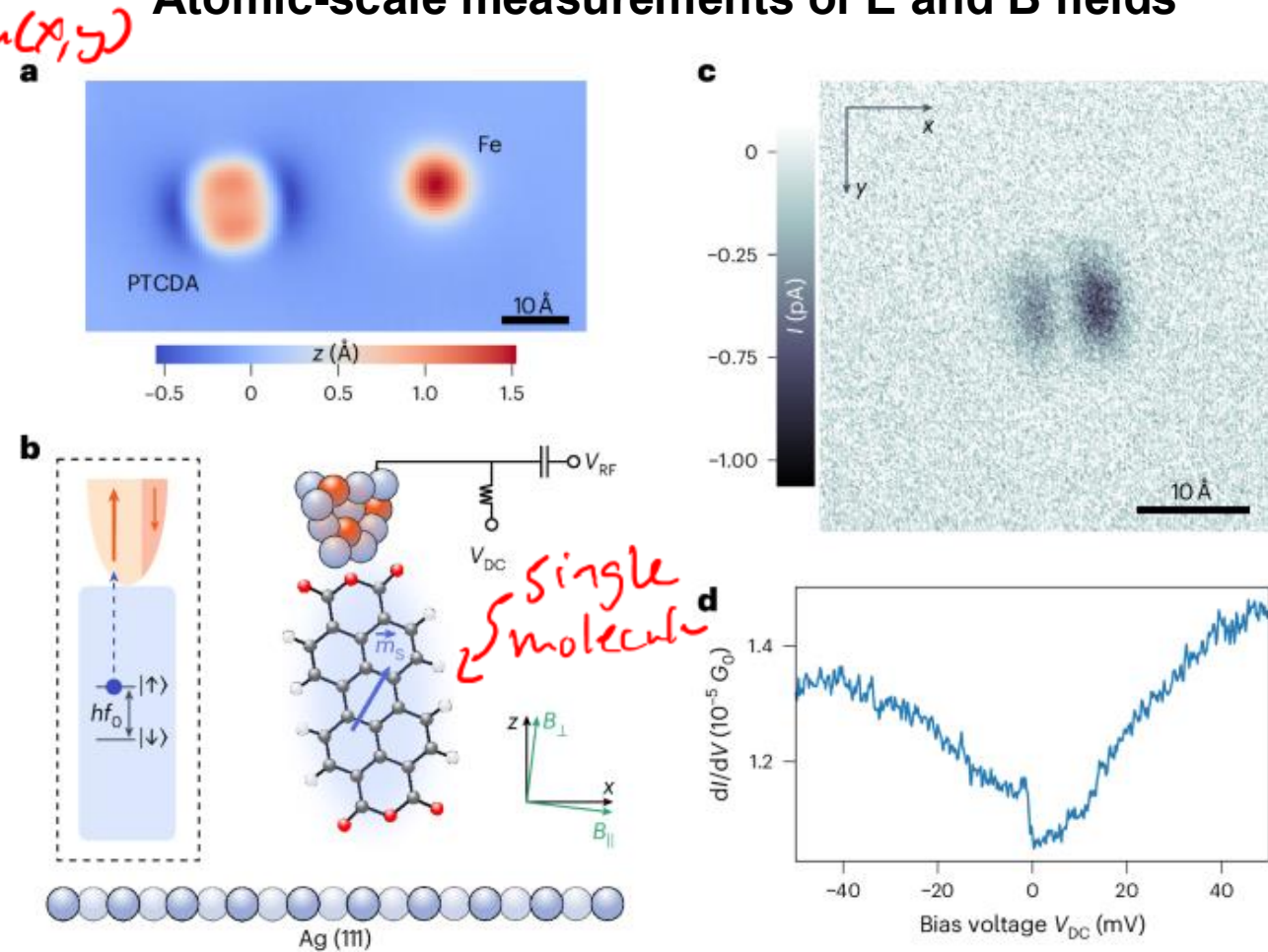
Krebs, Z. J., Behn, W. A., Li, S., Smith, K. J., Watanabe, K., Taniguchi, T., ... & Brar, V. W. (2023). Imaging the breaking of electrostatic dams in graphene for ballistic and viscous fluids. *Science, 379*(6633), 671-676

Esat, T., Borodin, D., Oh, J., Heinrich, A. J., Tautz, F. S., Bae, Y., & Temirov, R. (2024). A quantum sensor for atomic-scale electric and magnetic fields. *Nature Nanotechnology*, 1-6.

Alpha decay

- Alpha particle (^4_2He) sees strong nuclear force (attractive) as well as Coulomb force between alpha particle and positive nucleus (repulsive)

- If alpha particle energy is above total potential energy at any point in $r > r_0$, alpha can tunnel through barrier and leave nucleus

- Decay rate

$m = mass\ of\ alpha\ particle$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi = E\psi$$

$$V(r) = \begin{cases} -\infty & r \le r_0 \\ \dfrac{2Ze^2}{4\pi\varepsilon_0 r} & r > r_0 \end{cases}$$

challenging to solve

$Half\ time\quad T_{1/2} \propto (rate)^{-1}$

tunneling

$rate = T^{\sqrt{\alpha}}/(2r_0)$

tunneling probability v_α *is velocity of the α particle*

Repulsive Coulomb potential

$$E_p(r) = \frac{Z \cdot 2e^2}{4\pi\varepsilon_0 r}$$

Tunnelling

E_k

0   r_0

← Nuclear radius

Attractive nuclear potential

Alpha decay

- Alpha particle ($^4_2 He$) sees strong nuclear force (attractive) as well as Coulomb force between alpha particle and positive nucleus (repulsive)

- If alpha particle energy is above total potential energy at any point in $r > r_0$, alpha can tunnel through barrier and leave nucleus

- Decay rate is proportional to transmission coefficient times the frequency of alpha particle hitting the wall: $P \cdot v/2r_0$, where v is the mean velocity of the alpha particle and P is the tunneling probability (equivalently the transmission coefficient)

  - Lifetime $\propto \dfrac{1}{v} \propto \dfrac{1}{\sqrt{E}}$
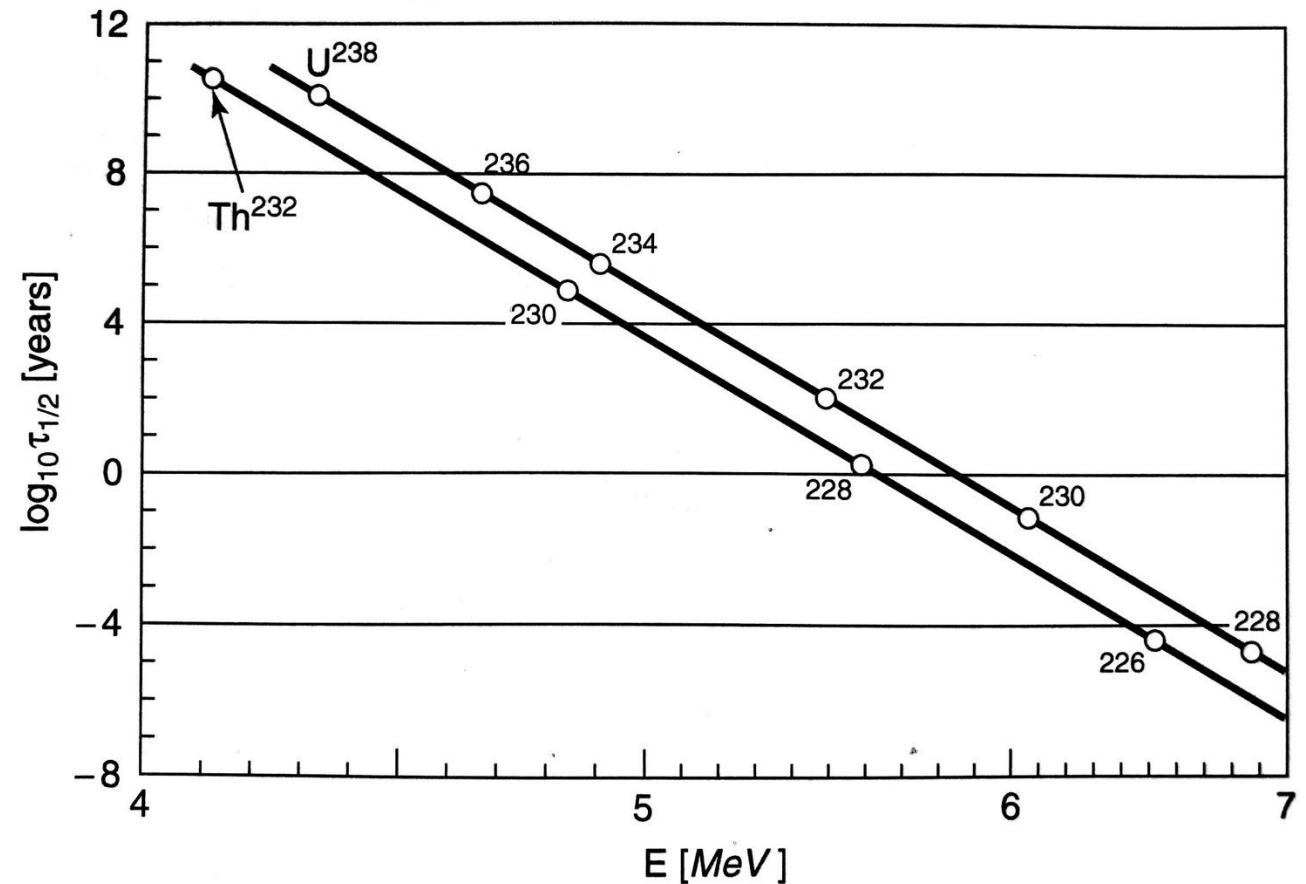
Source: Demtroder, Chapter 3
Griffiths, Chapter 8

Modeling alpha decay (related to HW 3 problem)

Let's consider the alpha particle decay of uranium-238 ($^{238}_{92}U$, where the atomic mass number is 238 and the number of protons is 92) into thorium-234 ($^{234}_{90}Th$). For $^{238}_{92}U$, alpha particles are produced with mean energy 4.267 MeV and mean lifetime (half-life) of 1.41×10^{17} s, or 4.468 billion years.

- What is the charge of the nucleus contributing to the Coulomb potential? (Answer on Top Hat)

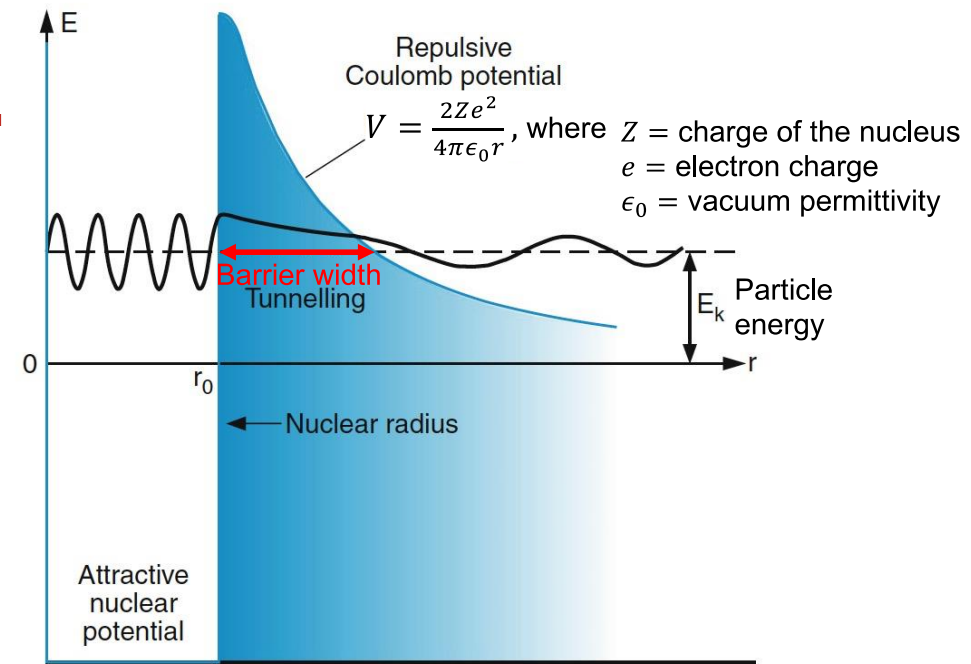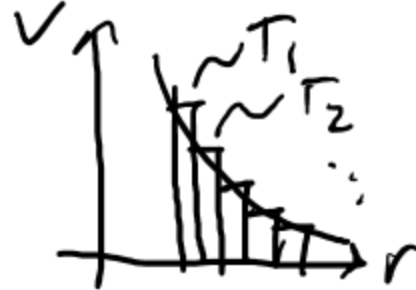$$V = \frac{2Ze^2}{4\pi\epsilon_0 r} \qquad Z = 90$$

- What is the barrier width of the potential?
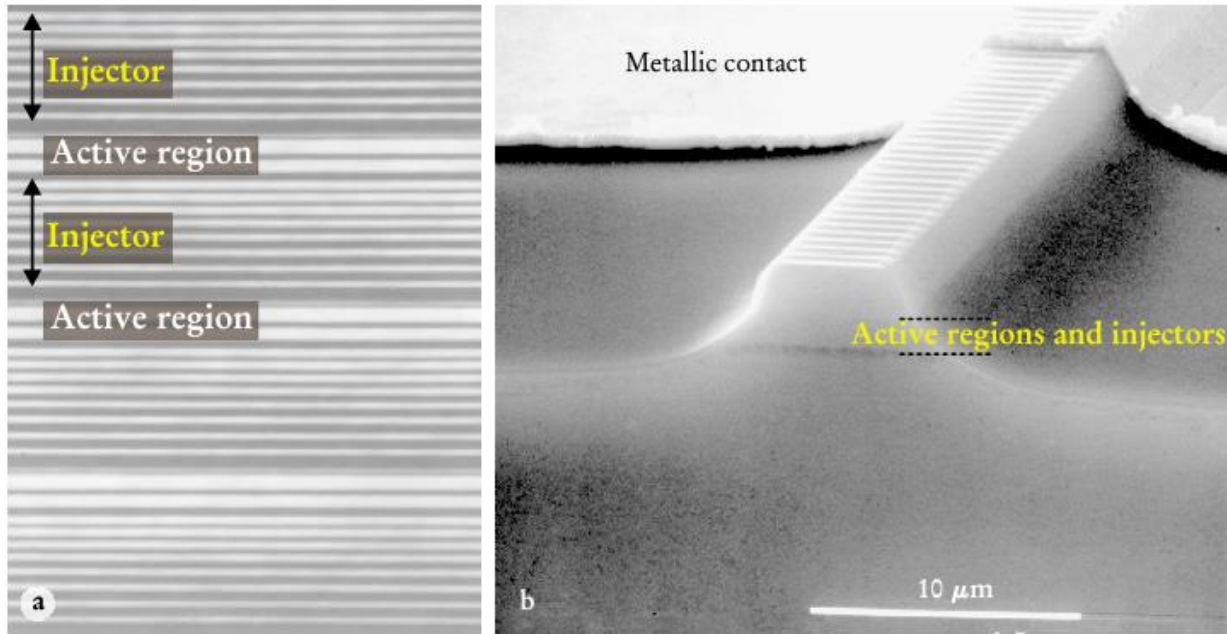
$$4.3 \, MeV = \frac{2(90)e^2}{4\pi\epsilon_0(w+r_0)} \qquad \text{Solve for } w$$

- How can we numerically model the Coulomb potential so that we can easily solve the Schrodinger equation?

$$T_{tot} = T_1, T_2 \ldots T_N$$

The figure in the upper right shows:

$$V = \frac{2Ze^2}{4\pi\epsilon_0 r}, \text{ where } Z = \text{charge of the nucleus}$$
$e = $ electron charge
$\epsilon_0 = $ vacuum permittivity

Repulsive Coulomb potential

Barrier width — Tunnelling

E_k Particle energy

Nuclear radius — r_0

Attractive nuclear potential

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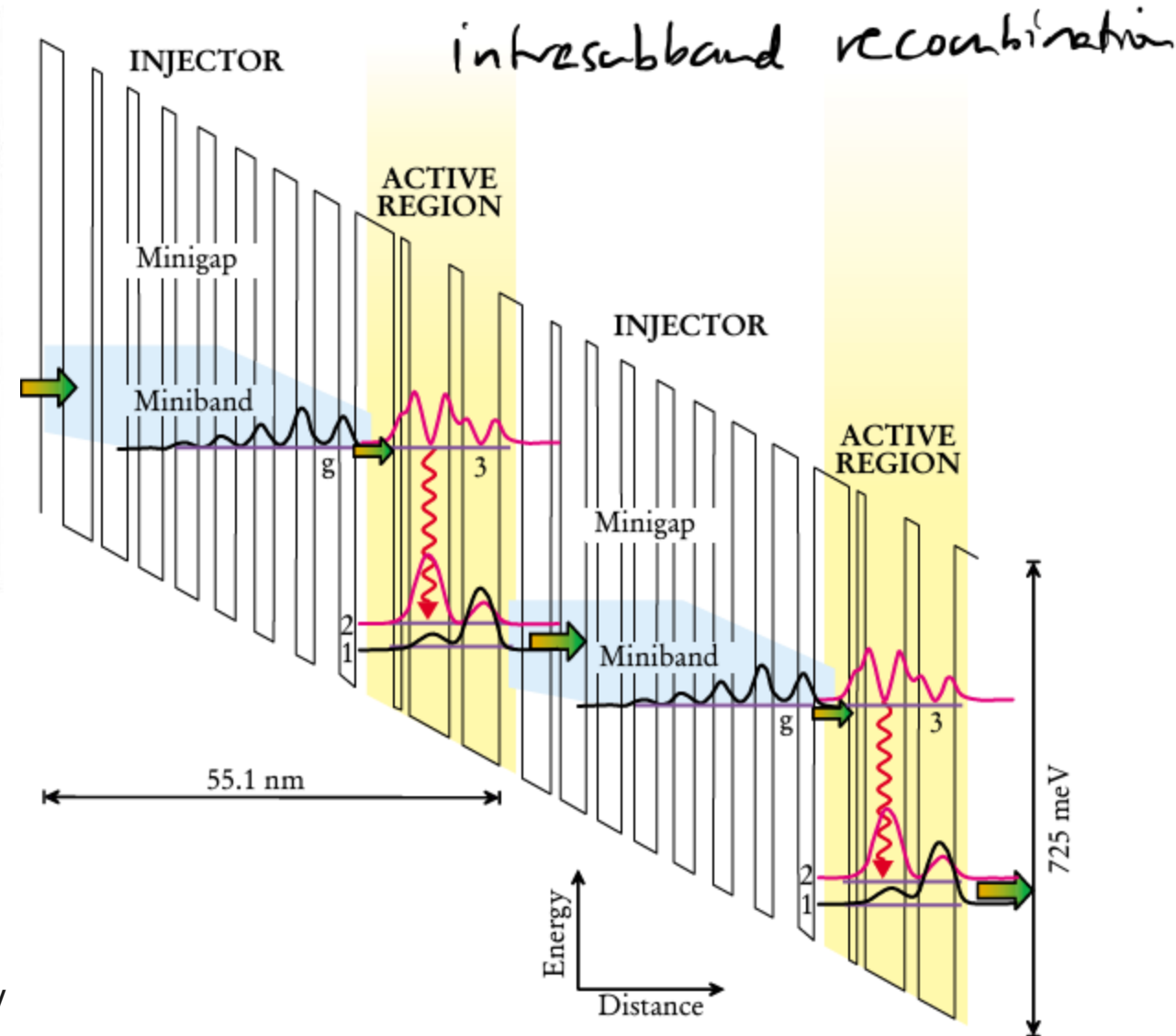
Tunneling is also key to the operation of Quantum cascade lasers (QCLs)

- Combines concepts in quantum well lasers (involving heterostructures) and quantum tunneling

- Enables mid-infrared (> 2 μm) lasers

Good review article: Federico Capasso, Claire Gmachl, Deborah L. Sivco, Alfred Y. Cho; Quantum Cascade Lasers. *Physics Today* 1 May 2002; 55 (5): 34–40. https://doi.org/10.1063/1.1485582

References on solutions to Schrodinger equation

- Please review Chapter 4 from "Atoms, Molecules, and Photons" by W. Demtroder (Springer, available for free online with UW NetID)

- Posted on Canvas select chapters from "Quantum Mechanics for Scientists and Engineers" by D. A. B. Miller (Cambridge)
  - Chapter 2.6 Particle in an infinitely deep potential well
  - Chapter 2.8 Particles and barriers of finite heights
  - Chapter 2.9 Particle in a finite potential well
  - Chapter 11.1 Tunneling probabilities