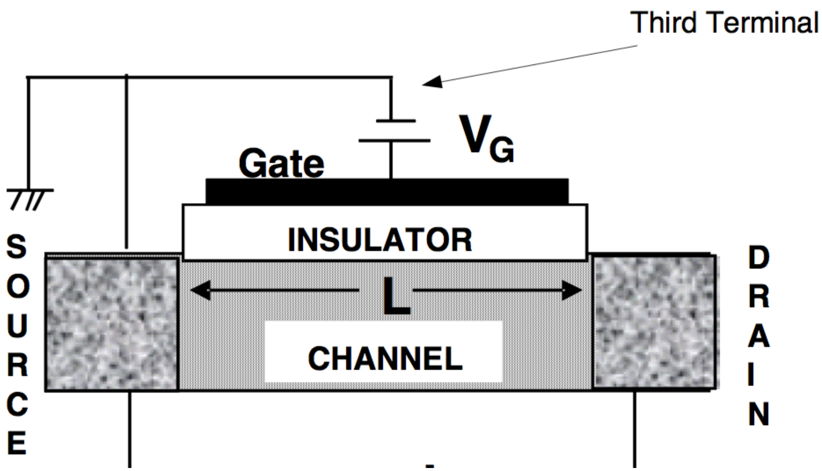
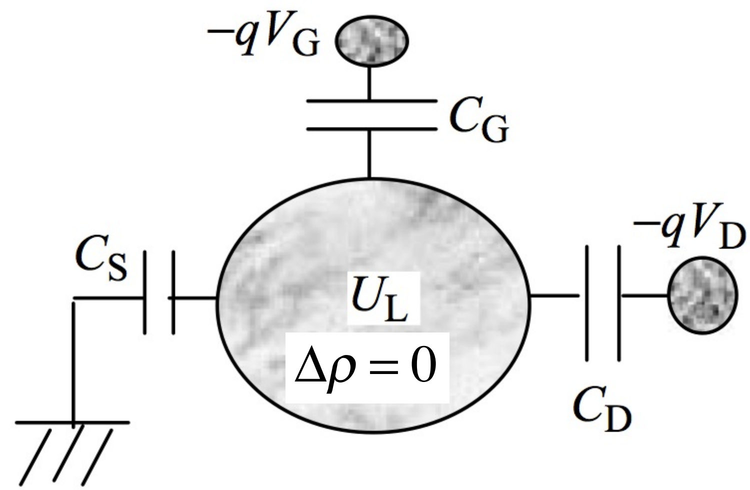
Fundamentals of NanoElectronics

Lecture – III Review

ELECTROSTATIC MODEL

Capacitor Network (Laplace Potential)





$$\vec{\nabla} \cdot \left(\varepsilon_r \vec{\nabla} V \right) = 0$$

Laplace Potential

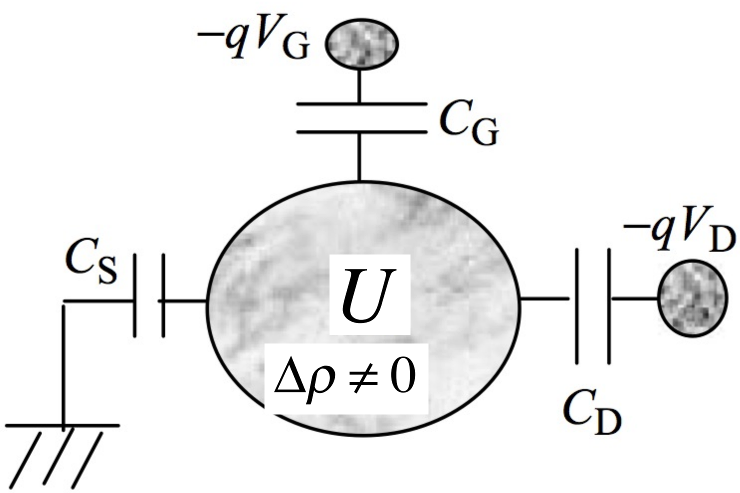
$$U_L = \frac{C_S}{C_E}\left(-qV_S\right) + \frac{C_G}{C_E}\left(-qV_G\right) + \frac{C_D}{C_E}\left(-qV_D\right)$$

where $C_E = C_S + C_G + C_D$

$$U_L = \frac{C_G}{C_E}\left(-qV_G\right) + \frac{C_D}{C_E}\left(-qV_D\right)$$

since $V_S = 0$

Charge Transfer & Charging Potential



Total Charge

$$-q\Delta N = C_S V + C_G\left(V - V_G\right) + C_D\left(V - V_D\right)$$

where $-qV = U$

$$U_L = \frac{C_G}{C_E}\left(-qV_G\right) + \frac{C_D}{C_E}\left(-qV_D\right)$$

$$U = U_L + \frac{q^2}{C_E}\Delta N$$

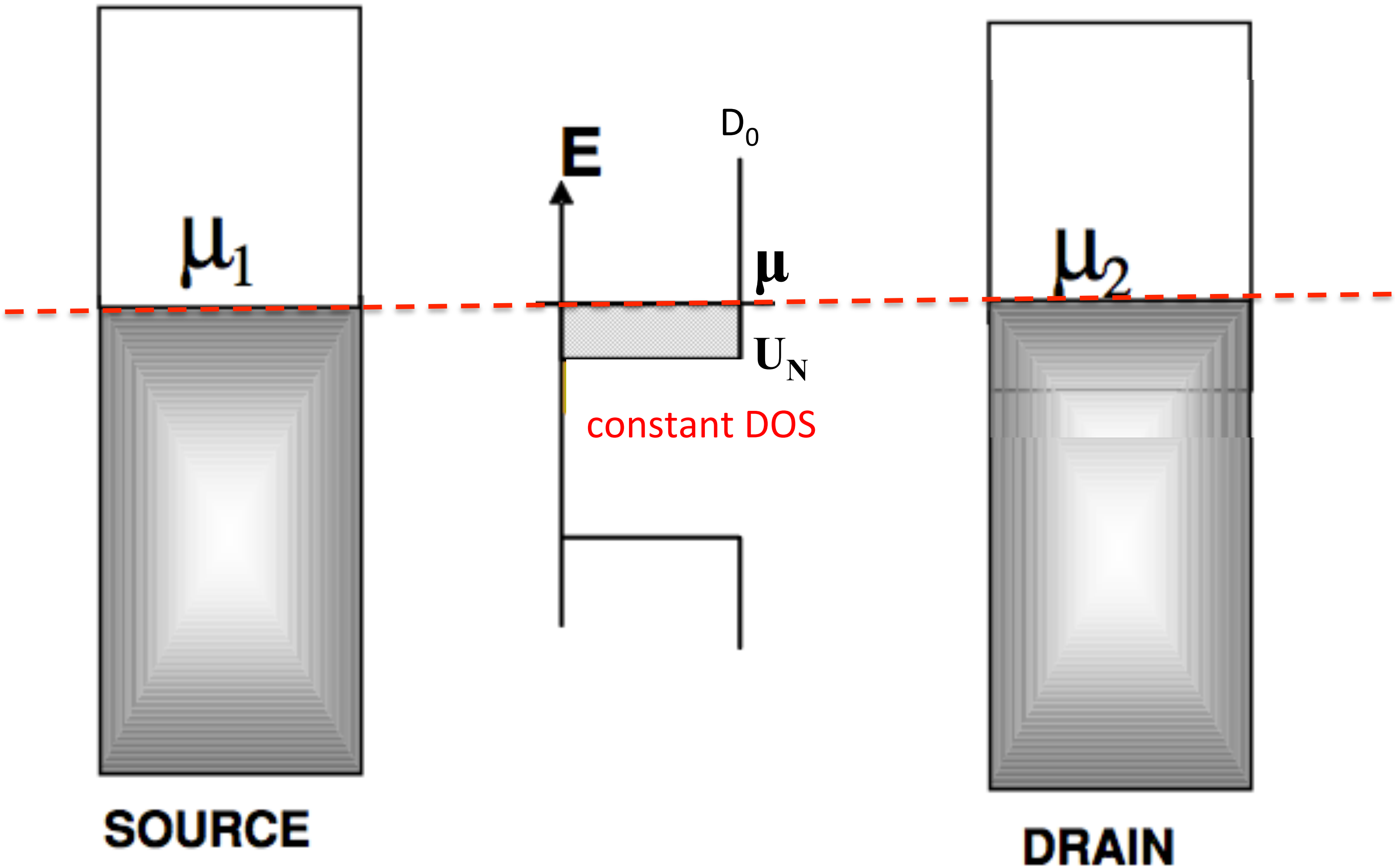
$$U_0 = \frac{q^2}{C_E}$$

single electron charging energy

$$U = U_L + U_0\left(N - N_0\right)$$

QUANTUM MODEL

Number of Electrons (Equilibrium)



$$N_0 = \int_{-\infty}^{\infty} dE \cdot D(E - U_N) \cdot f(E)$$

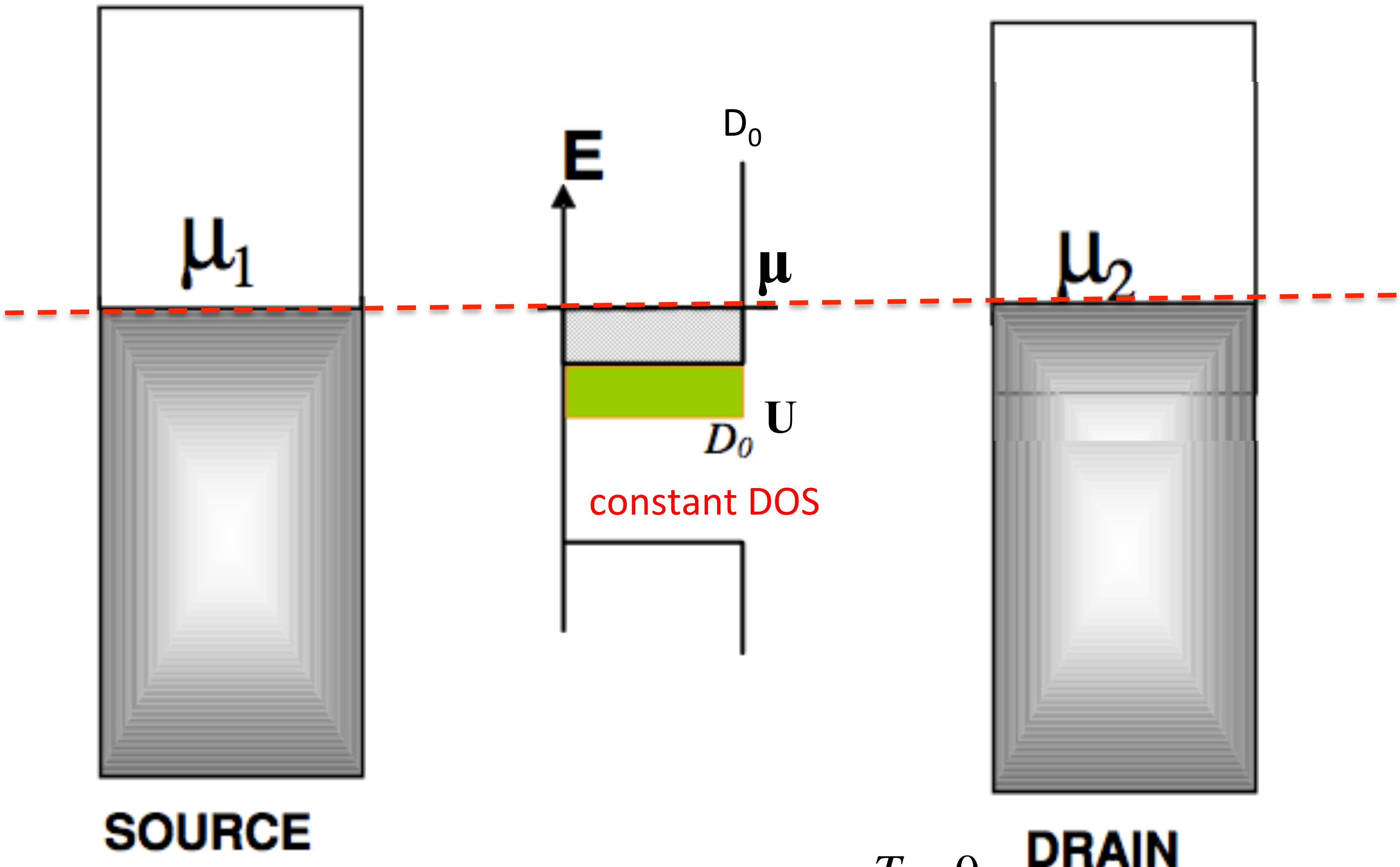
2 is for spin

$U_N = 0$

$T \sim 0$

$$N_0 = D_0(\mu - U_N)$$

Number of Electrons (Non-Equilibrium)



$$N = \int dE \cdot D(E-U)\left[\frac{\gamma_1 f_1(E)+\gamma_2 f_2(E)}{\gamma_1+\gamma_2}\right]$$

$T \sim 0$

$$N = D_0(\mu - U)$$

Quantum Capacitance

$$N = D_0(\mu - U)$$

$$N_0 = D_0(\mu - U_N)$$

$$\Delta N = N - N_0 = -D_0(U - U_N)$$

$$\Delta Q = -q\Delta N = qD_0(U - U_N)$$

$$\Delta Q = \underbrace{q^2 D_0}(\Delta V)$$

C_Q quantum conductance

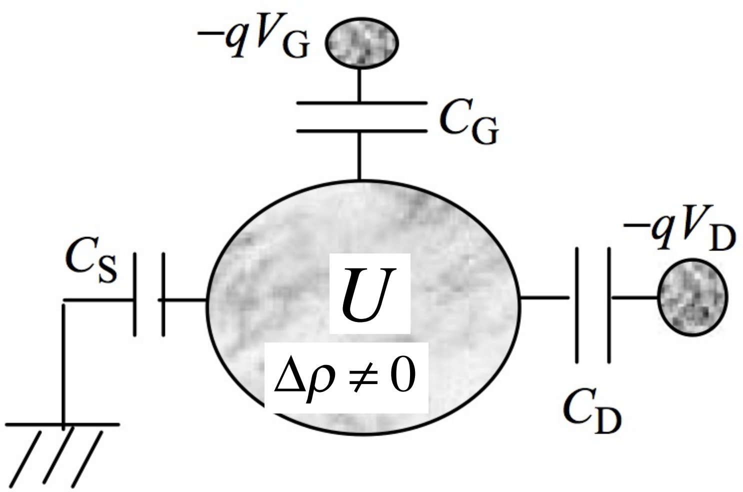
Quantum Capacitance C_Q

Extra Electrons

$$\frac{\Delta Q}{\Delta V} = C_Q = q^2 D_0$$

WHERE TO PUT
QUANTUM CAPACITANCE

Charge Transfer & Charging Potential



$$U = U_L + U_0 \left(N - N_0 \right) \qquad U_0 = \frac{q^2}{C_E}$$

$$\Delta N = N - N_0 = -D_0 \left(U - U_N \right)$$

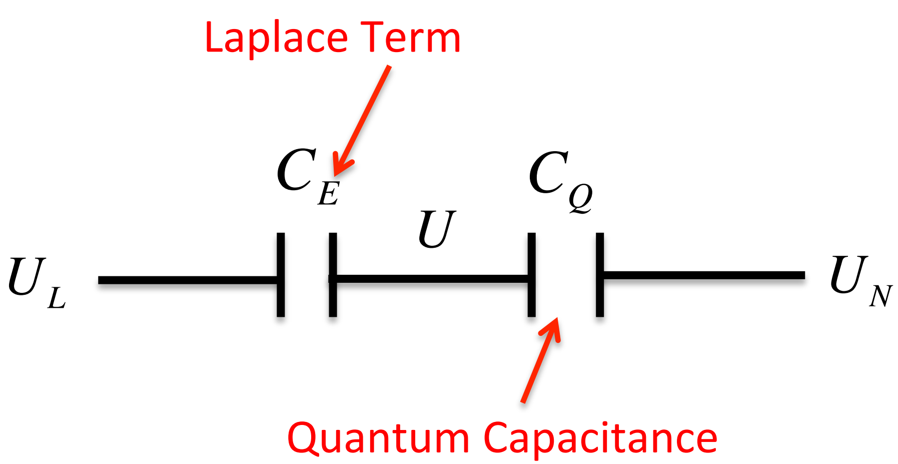
$$C_Q = q^2 D_0$$

quantum capacitance

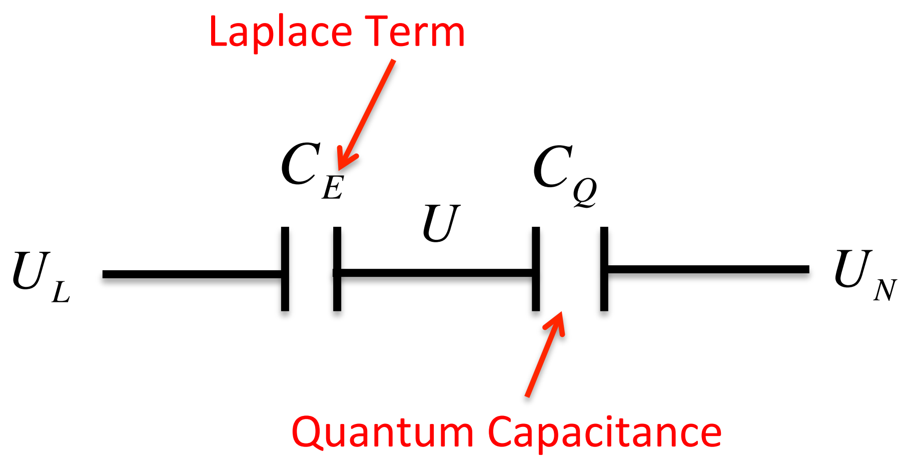
$$N - N_0 = -C_Q \left(U - U_N \right) / q^2$$

$$U = U_L + \frac{C_Q}{C_E} \left(U_N - U \right)$$

$$U = \frac{C_E U_L + C_Q U_N}{C_E + C_Q}$$

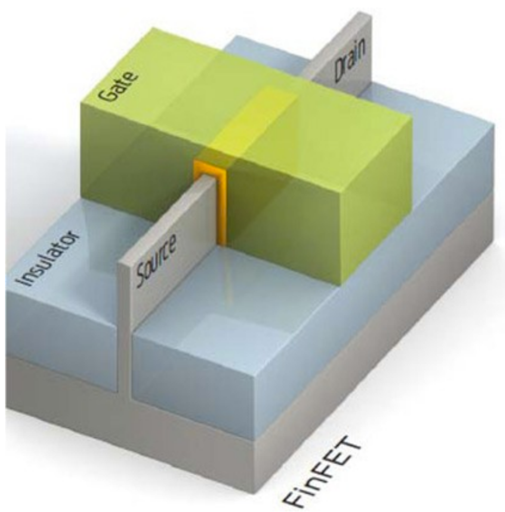


Charge Transfer & Charging Potential



Smaller Capacitor Dominates

$$C = \frac{C_E C_Q}{C_E + C_Q}$$



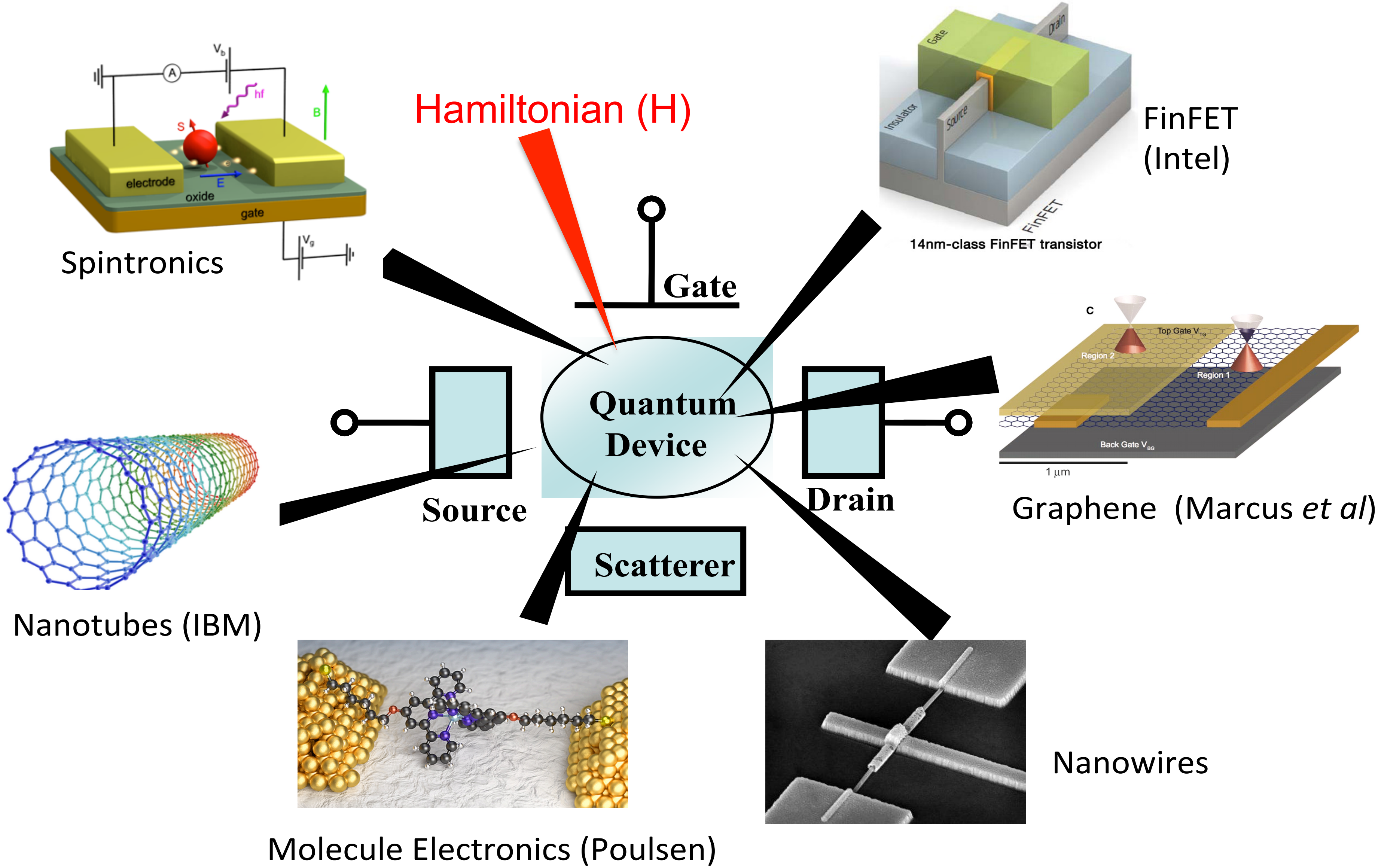
$$C_G = \frac{\varepsilon A}{d}$$

$$C_E = C_G + C_S + C_D$$

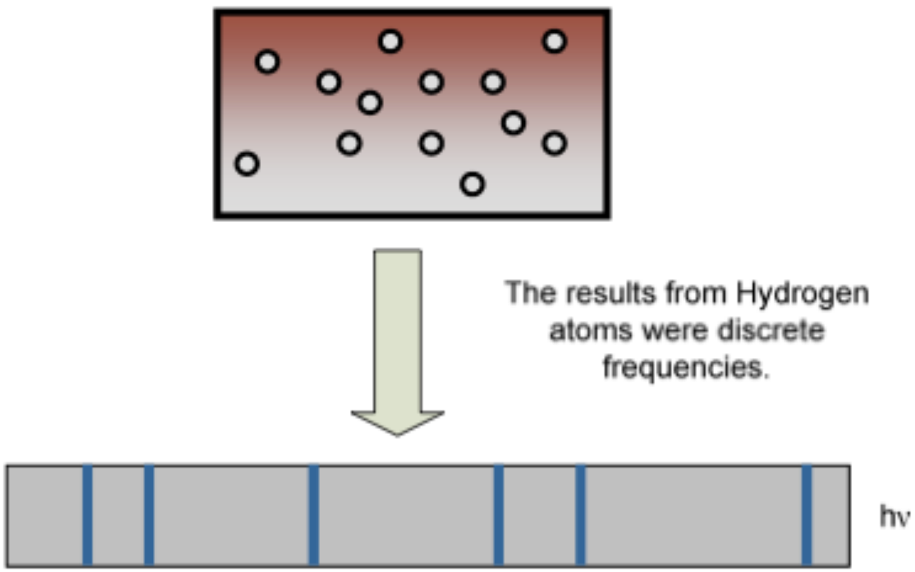
Quantum Capacitance

$$C_Q = q^2 D_0$$

UNIFIED FORMALISM



Discrete Energy Levels in Atoms

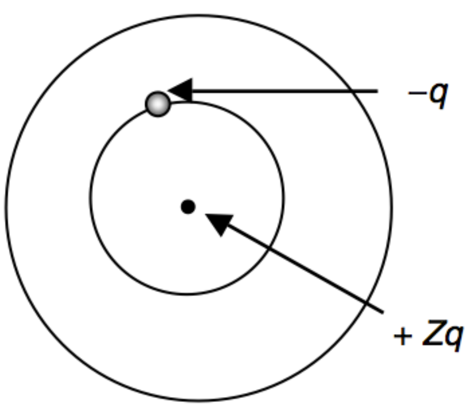


Emitted Photon Energies

$$h\nu = E_m - E_n = E_0 Z^2 \left(\frac{1}{n^2} - \frac{1}{m^2}\right)$$

$$E_0 = \frac{q^2}{8\pi\varepsilon_o a_0} = 13.6\ eV$$

Bohr Model



$$E = -\frac{Zq^2}{4\pi\varepsilon_o r} + \frac{mv^2}{2} = -\left(Z^2/n^2\right)E_0$$

$$\lambda = h/mv$$

de Broglie wavelength

$$2\pi r = n\lambda$$

quantized angular momentum

$$n = 1,2,3\ldots$$

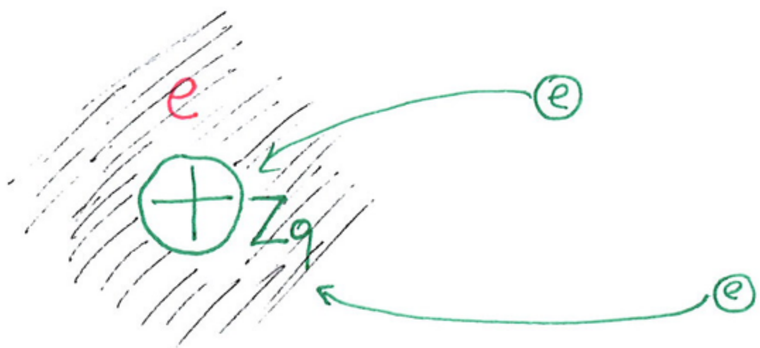
Schrödinger Equation

$$i\hbar\frac{\partial\Psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})\right)\Psi$$

(heuristic insight on a formal quantitative basis)

Potential Energy

Electron Cloud



Potential Energy

$$U(r)=-\frac{Zq^2}{4\pi\varepsilon_o r}$$

negative sign!

Match experimental observation!!

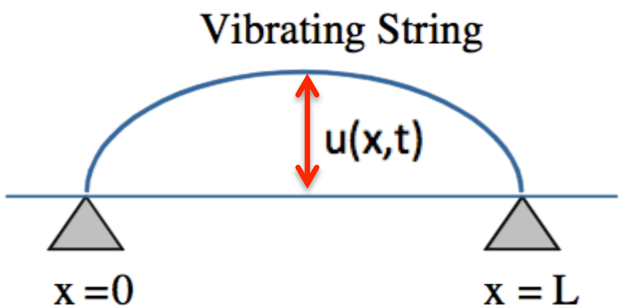
Meaning of the wavefunction was not known!!

You cannot solve analytically other than “Hydrogen” atom (e-e interactions)

You need numerical methods. Use computers !!

Acoustic Waves

An Analogy: Acoustic Waves



$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$

v is speed and u is displacement

$u(x,t) = \tilde{u}(x)e^{-i\omega t}$

$$-\omega^2 \tilde{u}(x) = v^2 \frac{\partial^2}{\partial u^2} \tilde{u}(x)$$

e^{ikx}, e^{-ikx}

Dispersion Relation

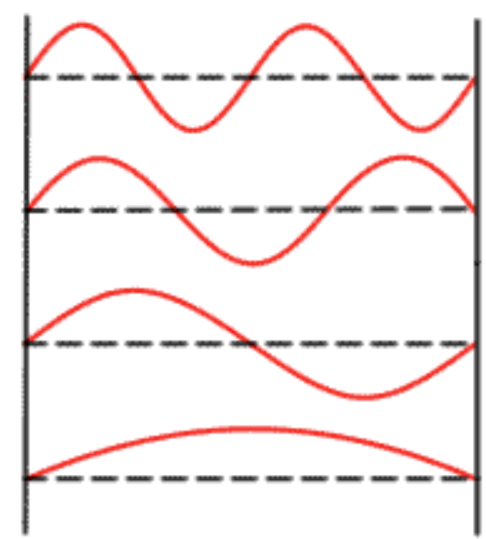
$$-\omega^2 = v^2 (ik)^2 \Rightarrow \omega^2 = v^2 k^2$$

$$\tilde{u}(x) = Ae^{ikx} + Be^{-ikx}$$

$x = 0$ $\tilde{u}(x) = 0$

$$A = -B$$

where



Standing waves on a string

Schrödinger Equation in 1-D

$$i\hbar\frac{\partial\Psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})\right)\Psi$$

(Schrödinger Equation)

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial^2 x}$$

(constant potential & 1-D)

$$\Psi=Ae^{-iEt/\hbar}e^{ikx}$$

(solution of PDE for constant coefficients in space and/or time)

$$i\hbar\cdot\frac{-iE}{\hbar}\cdot\Psi=-\frac{\hbar^2}{2m}(ik)^2\cdot\Psi$$

Dispersion Relation

$$E=\frac{\hbar^2k^2}{2m}$$

Schrödinger Equation in 2-D

$$i\hbar\frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\Psi$$

(Schrödinger Equation)

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial^2 x} - \frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial^2 y}$$

(constant potential & 2-D)

$$\Psi = Ae^{-iEt/\hbar}e^{ikx}e^{iky}$$

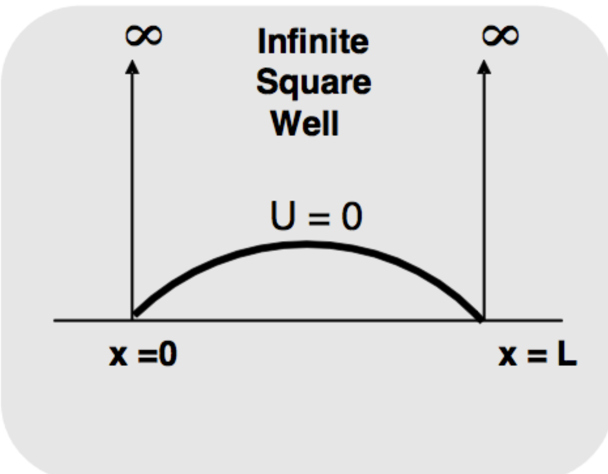
(constant coefficients space and/or time)

$$E\Psi = \frac{\hbar^2 k_x^2}{2m}\Psi + \frac{\hbar^2 k_y^2}{2m}\Psi$$

Dispersion Relation

$$E = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m}$$

Particle in a Box



$$i\hbar\frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\Psi$$

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial^2 x}$$

Time Independent Problem

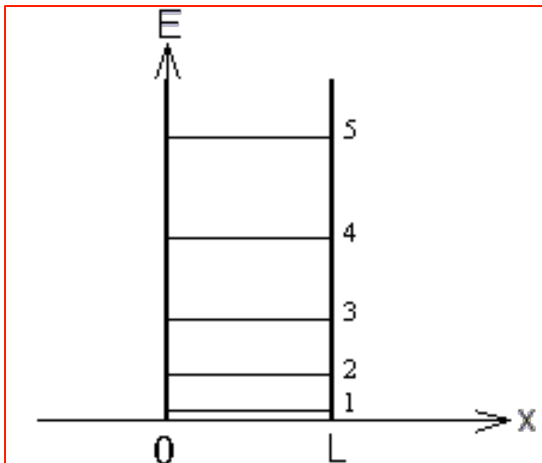
$$\Psi = Ae^{-iEt/\hbar}e^{ikx}$$

$$E = \frac{\hbar^2 k^2}{2m}$$

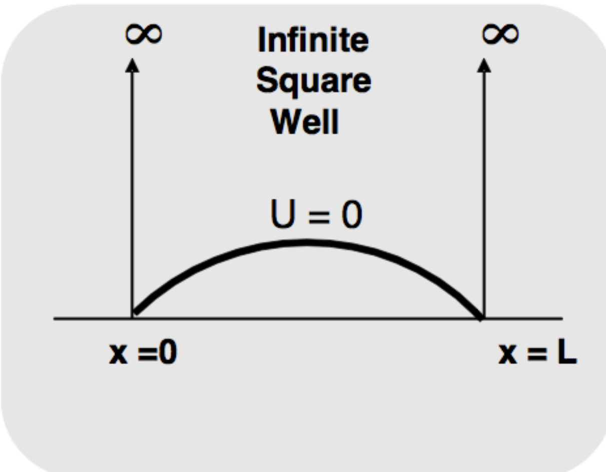
$$kL = \pi n$$

$$E = \frac{\hbar^2}{2m}\frac{\pi^2}{L^2}n^2$$

(Discrete Energy Levels)



Particle in a Box



$$i\hbar\frac{\partial\Psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})\right)\Psi$$

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial^2 x}$$

Time Independent Problem

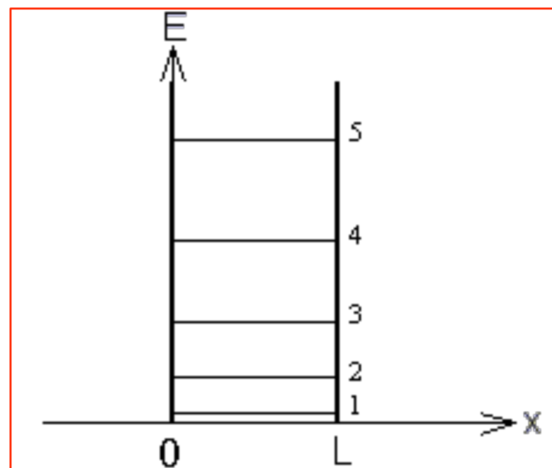
$$\Psi=Ae^{-iEt/\hbar}e^{ikx}$$

$$E=\frac{\hbar^2k^2}{2m}$$

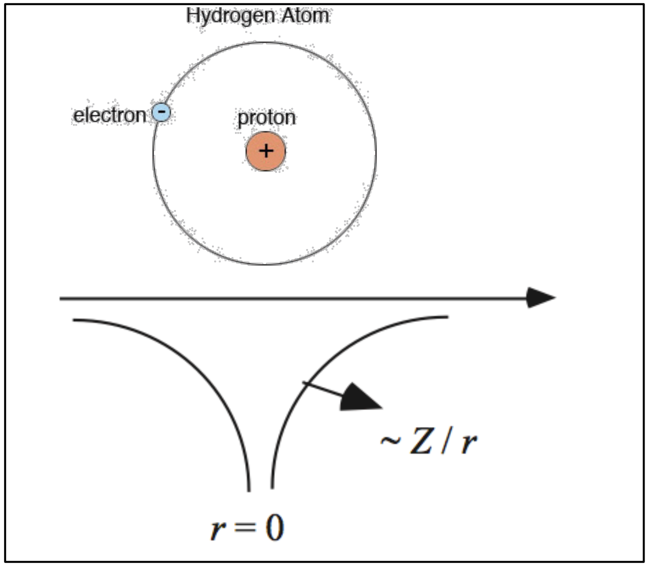
$$kL=\pi n$$

$$E=\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}n^2$$

(Discrete Energy Levels)



Hydrogen Atom: Particle in a Box



$$i\hbar\frac{\partial\Psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})\right)\Psi$$

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial^2 x}$$

Time Independent Problem

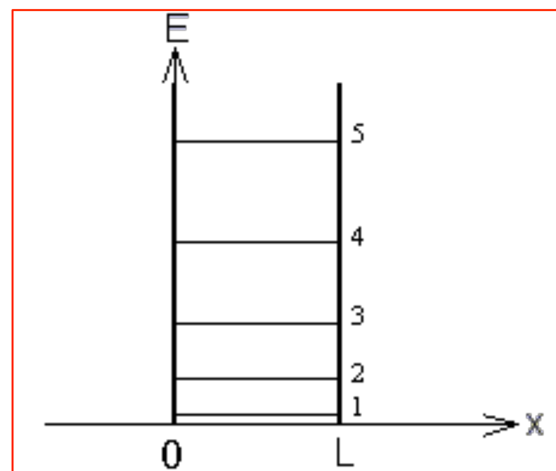
$$\Psi=Ae^{-iEt/\hbar}e^{ikx}$$

$$E=\frac{\hbar^2k^2}{2m}$$

$$kL=\pi n$$

$$E=\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}n^2$$

(Discrete Energy Levels)



Time-Independent Schrödinger Equation

$$i\hbar\frac{\partial\Psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})\right)\Psi$$

(Time Dependent Schrödinger Equation)

(coefficients depend on SPACE but NOT on TIME)

$$\Psi(r,t)=\Phi(r)e^{-iEt/\hbar}$$

(Amplitude is not constant)

$$E\Phi(r)=-\frac{\hbar^2}{2m}\nabla^2\Phi(r)+U(r)\Phi(r)$$

(Time Independent Schrödinger Equation)

$$U(r)=-\frac{Zq^2}{4\pi\varepsilon_o r}$$

$$E=-\frac{E_0}{n^2}$$