Electrostatics

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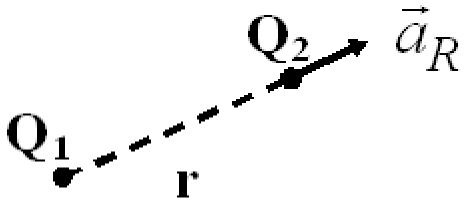
Course Overview

1. Charge and Electrostatic Field
2. Electric Displacement and Polarization Density
3. Potential and Gauss Law
4. Poisson's Equation
5. Debye (Screening) Length
6. Electrostatic Energy and Capacitance
7. Boundary Conditions

1. Charge and Electrostatic Field (1)

Two point charges repel each other with a force (experimental results)



$$\mathbf{F} = \frac{Q_1 Q_2}{4\pi\varepsilon r^2}\mathbf{a_R}$$

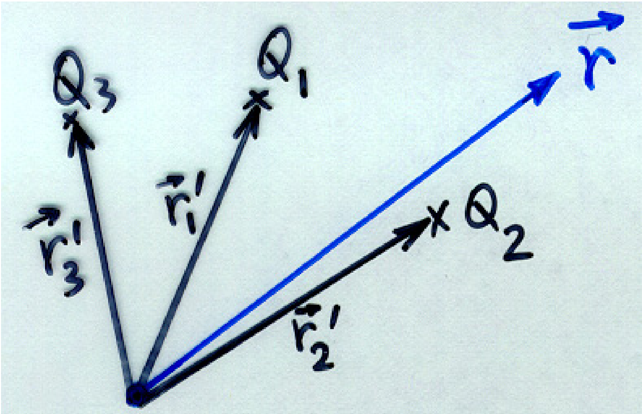
ε permittivity

Electric field $\mathbf{E}$ → force on a unit charge

$$\mathbf{F} = \frac{Qq}{4\pi\varepsilon r^2}\mathbf{a_R} \qquad \mathbf{E} = \frac{\mathbf{F}}{q} = \frac{Q}{4\pi\varepsilon r^2}\mathbf{a_R}$$

 Ref: Xie, Section 2.1 & 2.2

1. Charge and Electrostatic Field (2)



$\mathbf{r}$ observation point

$\mathbf{r}_\mathbf{i}'$ positon of Q_i (source point)

$$\mathbf{a}_\mathbf{R}^\mathbf{i} = \frac{\mathbf{r} - \mathbf{r}_i'}{|\mathbf{r} - \mathbf{r}_i'|}$$

A unit normal vector pointed from source point to observation point

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi\varepsilon}\sum_{i=1}^{N}\frac{Q_i}{|\mathbf{r} - \mathbf{r}_\mathbf{i}'|^2}\mathbf{a}_\mathbf{R}^\mathbf{i}$$

$$\rho_i \to Q_i\delta(\mathbf{r} - \mathbf{r}_\mathbf{i}')$$

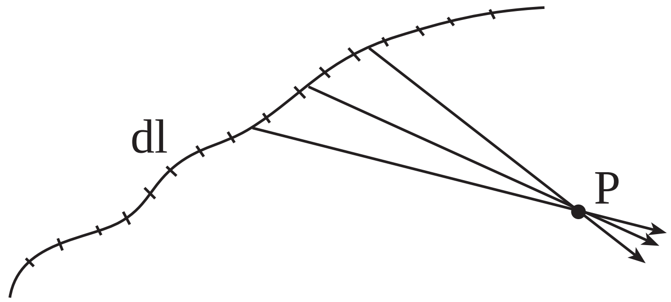
charge density for point charge

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi\varepsilon}\iiint_{v'}\frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^2}\mathbf{a}_\mathbf{R}\,dv'$$

$$= \frac{1}{4\pi\varepsilon}\iiint_{v'}\frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3}(\mathbf{r} - \mathbf{r}')\,dv'$$

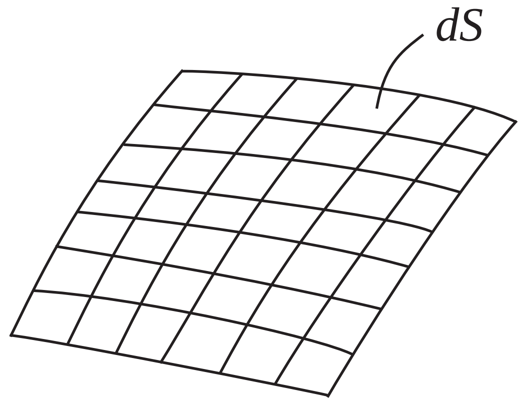
(a) <u>Line Charges</u>

Line charge density, ρ_L (C/m)



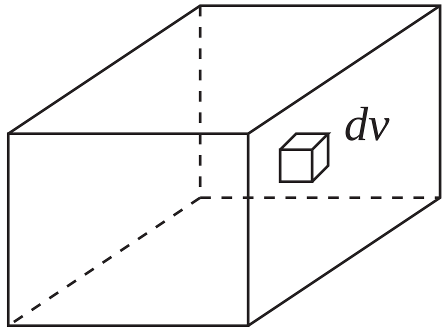
(b) <u>Surface Charges</u>

Surface charge density, ρ_S (C/m^2)



(c) <u>Volume Charges</u>

Volume charge density, ρ_V (C/m^3)



1. Charge and Electrostatic Field (4)

What are charges in optoelectronic devices?

Electrons, Holes,
Excitons (bound e-h pair),
Positive and Negative Ions ….

2. Electric Displacement and Polarization Density

In a dielectric material, the presence of an electrostatic field **E** causes the bound charges in the material (atomic nuclei and their electrons) to slightly separate, inducing a local electric dipole moment.

In a linear, homogeneous, isotropic dielectric

$$\mathbf{D} = \varepsilon \mathbf{E} = \varepsilon_0 \mathbf{E} + \mathbf{P} = \varepsilon_0 \mathbf{E} + \varepsilon_0 \chi \mathbf{E}$$

ε_0 vacuum permittivity (permittivity of free space)

$\mathbf{P}$ the density of the permanent and induced electric dipole moments in the material, called the polarization density

χ susceptibility

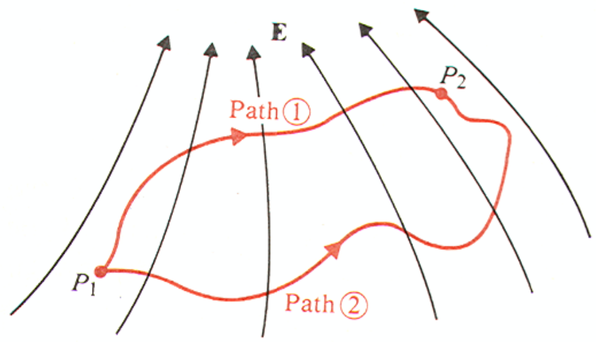
$\varepsilon_r = 1 + \chi$ relative permittivity (dielectric constant)

 Ref: Xie, Section 2.4

3. Potential and Gauss Law (1)

The work done to move a point charge from one point to another is independent of the path taken!

$$W = \oint_{\Gamma} \mathbf{F} \cdot d\mathbf{l} = q\oint_{\Gamma} \mathbf{E} \cdot d\mathbf{l} = 0$$



Electrostatic Field is conservative. Is there other field is conservative?

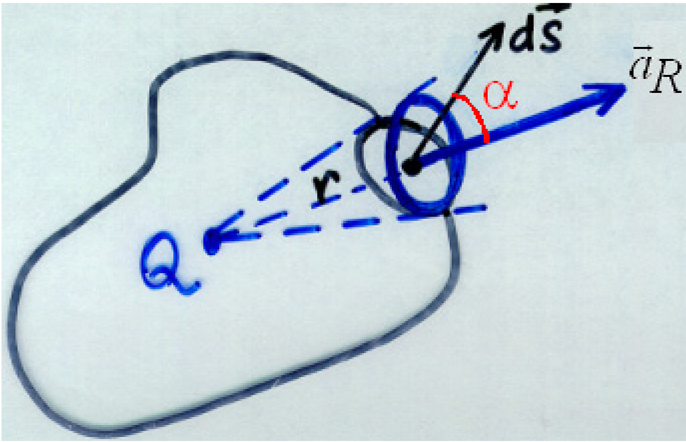
$$\oint_{\Gamma} \mathbf{E} \cdot d\mathbf{l} = \iint_{S} \nabla \times \mathbf{E} \cdot d\mathbf{S} = -\iint_{S} (\nabla \times \nabla\Phi) \cdot d\mathbf{S} = 0$$

$\mathbf{E} = -\nabla \Phi$ **Φ is a scalar quantity called electrostatic potential**

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi\varepsilon} \iiint_{v'} \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^2} \mathbf{a}_{\mathbf{R}} dv' \longrightarrow \Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon} \iiint_{v'} \frac{\rho(\mathbf{r}')dv'}{|\mathbf{r} - \mathbf{r}'|}$$

Ref: Xie, Section 3.1

3. Potential and Gauss Law (2)



<u>Gauss Law</u>

$$\oiint_S \mathbf{D}\cdot d\mathbf{S} = Q \longrightarrow \nabla\cdot\mathbf{D} = \rho$$

$d\mathbf{S}$ **: area element normal to an arbitrary surface**

$\mathbf{a_R}$ **: a unit normal vector to the spherical surface**

$$\mathbf{E}\cdot d\mathbf{S} = \frac{Q}{4\pi\varepsilon}\frac{\mathbf{a_R}\cdot d\mathbf{S}}{r^2} = \frac{Q}{4\pi\varepsilon r^2}(\cos\alpha dS) = \frac{Q}{4\pi\varepsilon r^2}(r^2\sin\theta d\theta d\varphi)$$

$\cos\alpha\, d\mathbf{S}$ is an elemental area on a spherical surface of radius r

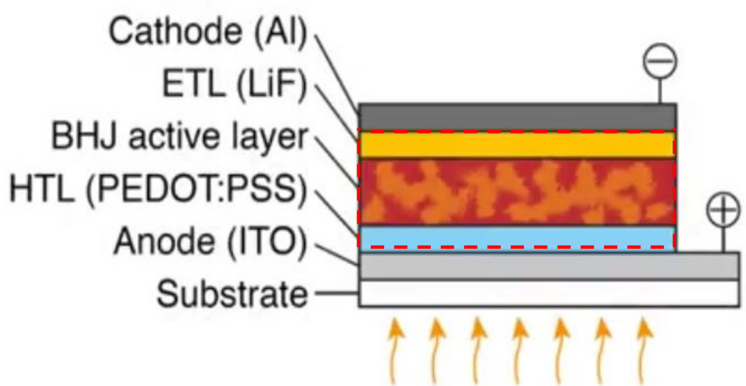
4. Poisson's Equation (1)

$$\mathbf{D} = \varepsilon(\mathbf{r})\mathbf{E} \qquad \mathbf{E} = -\nabla\Phi \qquad \nabla \cdot \mathbf{D} = \rho$$ → free charge

Poisson equation: governing equation for electrostatic problem

$$\boxed{\nabla \cdot (\varepsilon(\mathbf{r})\nabla\Phi) = -\rho}$$

Could we put permittivity out of divergence operator?



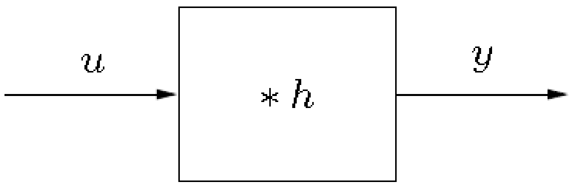
Optoelectronic device is inhomogeneous!

ETL: electron transport layer
HTL: hole transport layer
BHJ: bulk heterojunction
Red line: boundary conditions imposed

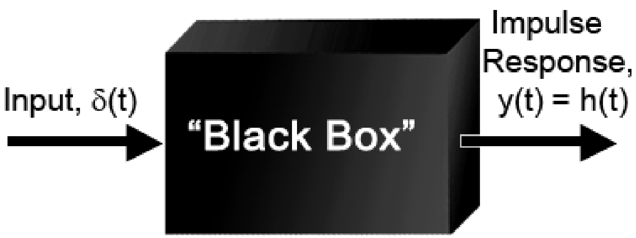
4. Poisson's Equation (2)

input $u \ (u(t) = 0, \ t < 0)$

output y



$$y(t) = \int_0^t h(t-\tau)u(\tau)\, d\tau$$

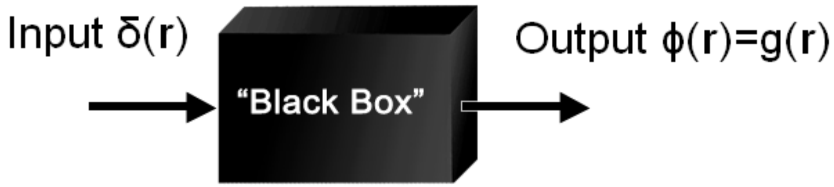


input ρ

output Φ

solution of Poisson's equation in free space

$$\Phi(\mathbf{r}) = \int_{v'} \rho(\mathbf{r}') \frac{1}{4\pi\varepsilon_0 |\mathbf{r}-\mathbf{r}'|} dv'$$



Ref: Chew, Section 3.3.2 and 3.3.3

4. Poisson's Equation (3) —— Green's function (Optional)

$$\nabla\cdot\left(\varepsilon_0\nabla g\left(\mathbf{r},\mathbf{r}'\right)\right)=-\delta(\mathbf{r}-\mathbf{r}')$$

$$g(\mathbf{r},\mathbf{r}')=\frac{1}{4\pi\varepsilon_0|\mathbf{r}-\mathbf{r}'|}$$

$$\int_{v'}\nabla\cdot\left(\varepsilon_0\nabla\frac{1}{4\pi\varepsilon_0|\mathbf{r}-\mathbf{r}'|}\right)dv'=-\int_{v'}\delta(\mathbf{r}-\mathbf{r}')dv'$$

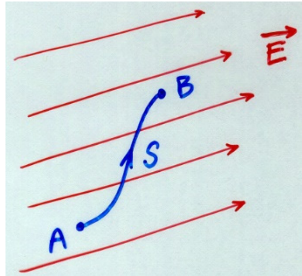
$$\int_{S'}\frac{1}{4\pi}\nabla\frac{1}{R}\cdot d\mathbf{S}'=-1$$

$$\int_{S'}\frac{1}{4\pi}\frac{-\mathbf{a}_\mathbf{R}}{R^2}\cdot d\mathbf{S}'=-1$$

$$\frac{-1}{4\pi R^2}\int_{S'}\mathbf{a}_\mathbf{R}\cdot d\mathbf{S}'=-1$$

5. Electrostatic Energy and Capacitance (1)

The work done is equal to the change in electrostatic energy (move a positive charge from one point to the other)



$$W = Q\int_{\Gamma} \mathbf{E} \cdot d\mathbf{l} = -Q\int_{\Gamma} \nabla\Phi \cdot d\mathbf{l} = Q(\Phi_A - \Phi_B)$$

1. The electrostatic energy of a positive charge Q at position r in the presence of a potential Φ

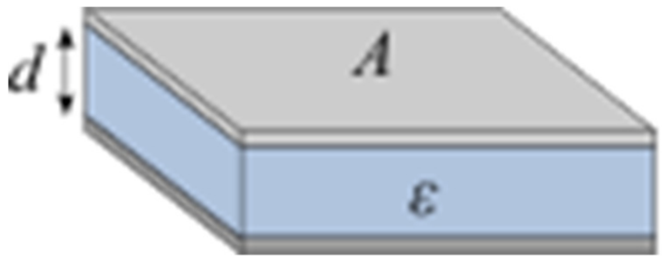
$$U_E = Q\Phi(\mathbf{r})$$

2. The electrostatic energy stored in a system of three and N point charges

$$U_E = \frac{1}{4\pi\varepsilon_0}\left(\frac{Q_1Q_2}{R_{12}} + \frac{Q_1Q_3}{R_{13}} + \frac{Q_2Q_3}{R_{23}}\right) \qquad U_E = \frac{1}{2}\sum_{i=1}^{N} Q_i \sum_{j=1}^{N(j\neq i)}\left(\frac{1}{4\pi\varepsilon_0}\frac{Q_j}{R_{ij}}\right)$$

5. Electrostatic Energy and Capacitance (2)

The total electrostatic energy stored in a capacitor is



$$U_E = \frac{1}{2}QV = \frac{1}{2}CV^2$$

Capacitance (C)

Energy density (energy per unit volume) of the electrostatic field

$$U_E = \int_v \frac{1}{2}\rho\Phi dv = \int_v \frac{1}{2}\nabla\cdot\mathbf{D}\Phi dv = \int_v \frac{1}{2}\mathbf{D}\cdot(-\nabla\Phi)dv$$

$$= \int_v \frac{1}{2}\mathbf{D}\cdot\mathbf{E}dv = \int_v \frac{1}{2}\varepsilon\mathbf{E}\cdot\mathbf{E}dv$$

6. Debye (Screening) Length

Debye length (Thomas–Fermi screening length) is a measure of a charge carrier's net electrostatic effect and how far its electrostatic effect persists.

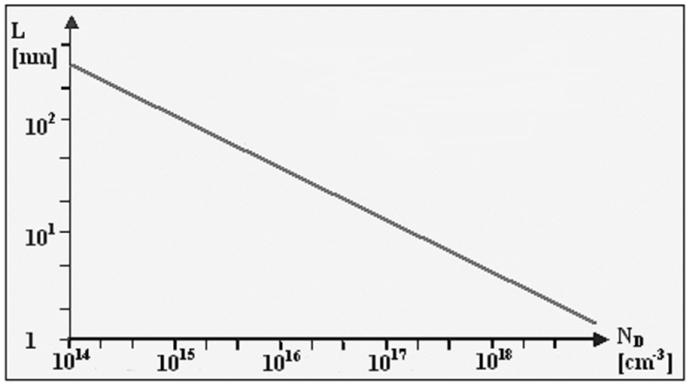
The Debye length of semiconductors is given $L_D = \sqrt{\dfrac{\varepsilon k_B T}{q^2 N_{dop}}}$

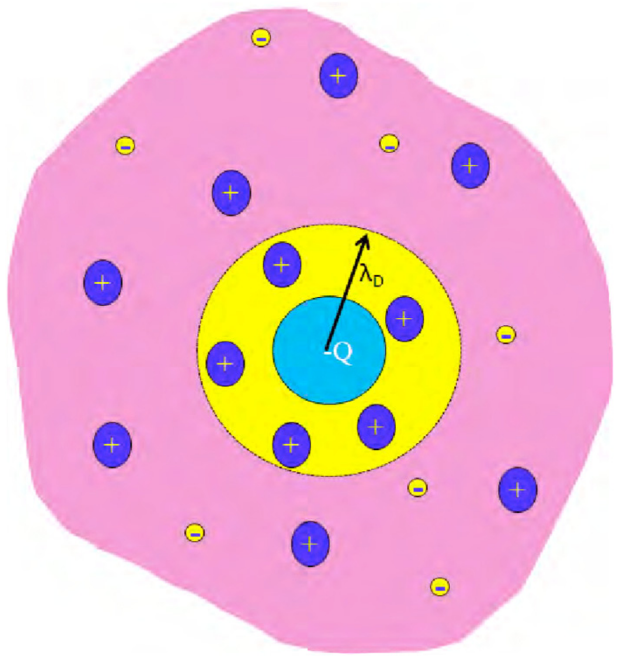
ε is the dielectric constant

k_B is the Boltzmann's constant

T is the kelvins temperature

N_{dop} is the net density of dopants





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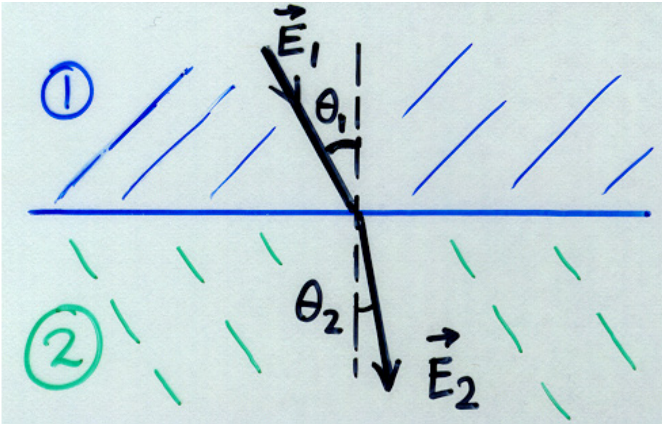
7. Boundary Conditions (1)

Tangential component of E field is continuous across dielectric boundary

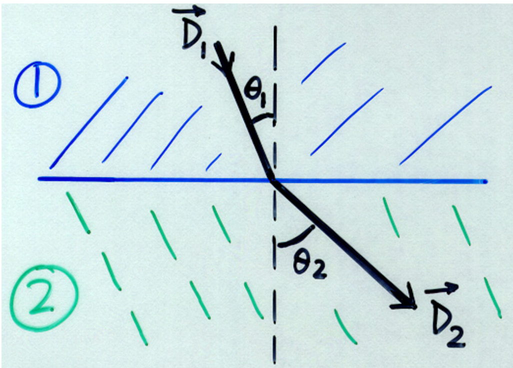


$$\oint_{\Gamma} \mathbf{E} \cdot d\mathbf{l} = 0$$

$$E_1 \sin\theta_1 = E_2 \sin\theta_2$$

$$E_{1t} = E_{2t}$$

Normal component of D field is continuous across dielectric boundary



$$\oint_{S} \mathbf{D} \cdot d\mathbf{S} = 0$$

$$D_1 \cos\theta_1 = D_2 \cos\theta_2$$

$$D_{1n} = D_{2n}$$

 Ref: Xie, Section 3.1.1 and 3.4

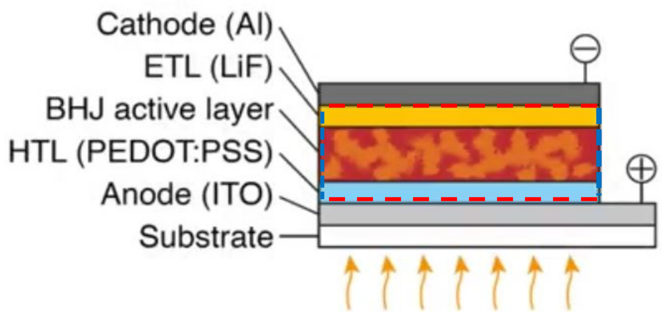
7. Boundary Conditions (2)

Dirichlet boundary condition (Red line)

$$\Phi(\mathbf{r})\,|_{r\to\infty} = 0$$ → unbounded problem (reference potential)

$$\Phi(\mathbf{r})\,|_{r=r_e} = V$$ → electrodes (optoelectronics)

Neumann boundary condition (Blue line)



$$\varepsilon \frac{\partial \Phi(\vec{r})}{\partial n}\Big|_{\vec{r}\in S} = \sigma_s$$ → surface charge

$$\frac{\partial \Phi(\vec{r})}{\partial n}\Big|_{\vec{r}\in S} = 0$$ → non-electrodes (floating BC, optoelectronics)