Electrostatics

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Course Overview

1. Charges in Optoelectronic Devices
2. Electric Displacement and Polarization Density
3. Poisson’s Equation
4. Boundary Conditions
5. Green’s Function
6. Electrostatic Energy and Capacitance
7. Analogy between Electrostatics and Magnetostatics
8. Debye (Screening) Length
9. Nanogenerator (Optional)

1. Charges in Optoelectronic Devices

What are the charges in optoelectronic devices?

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

Interplay of charges is essential to optoelectronics.

charges appear everywhere in devices

How to control the positions of charges?

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. Poisson's Equation

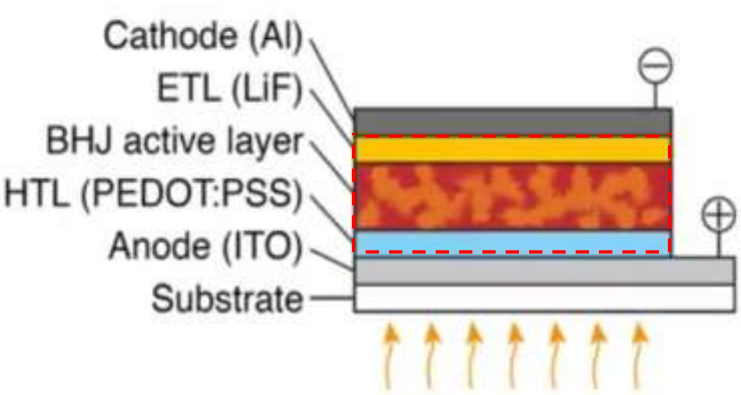
$$\mathbf{D} = \varepsilon(\mathbf{r})\mathbf{E} \qquad \mathbf{E} = -\nabla\Phi \qquad \nabla\cdot\mathbf{D} = \rho \longrightarrow \text{free charge}$$

Poisson equation: governing equation for electrostatic problem

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

Does similar equation exist?

Could we put permittivity out of divergence operator?



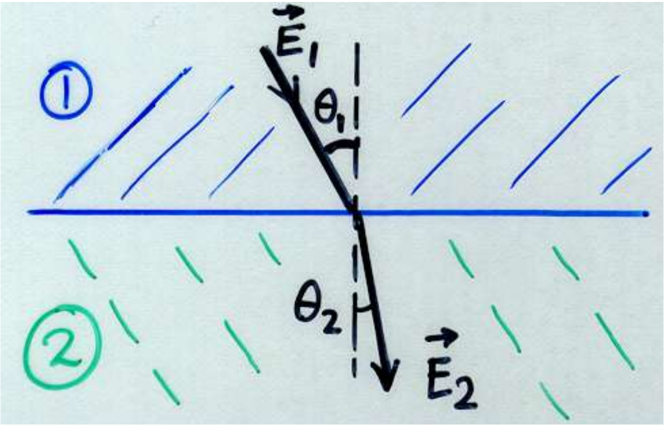
Optoelectronic device is inhomogeneous!

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

 Ref: Xie, Section 3.1 and 3.4

4. Boundary Conditions (1)

Tangential component of E field is continuous across dielectric boundary



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

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

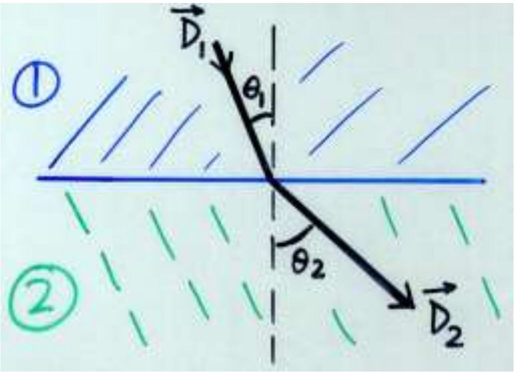
$$E_{1t} = E_{2t}$$

→ Electrostatic field is conservative.

Is there other field is conservative?

<u>If no free charge appears at the boundary</u>, then

Normal component of D field is continuous across dielectric boundary



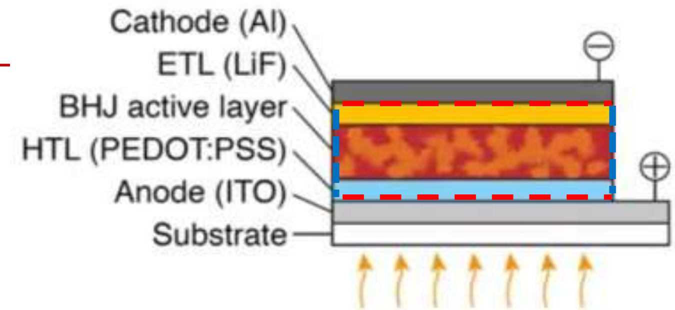
$$\oint_S \mathbf{D} \cdot d\mathbf{S} = 0$$

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

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

Ref: Xie, Section 3.1 and 3.4

4. Boundary Conditions (2)



Dirichlet type (Red line: metal electrode)

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

$$\Phi(\mathbf{r})\big|_{r=r_e} = V \longrightarrow$$ electrodes (**optoelectronics**)

Neumann type (Blue line: truncation boundary)

$$\frac{\partial \Phi(\vec{r})}{\partial n}\bigg|_{\vec{r}\in S} = 0 \longrightarrow$$ non-electrode (truncation) boundaries (floating BCs, **optoelectronics**)

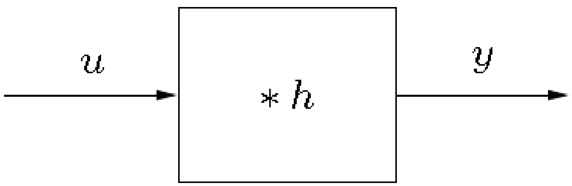
$$\varepsilon_s \frac{\partial \Phi(\vec{r})}{\partial n}\bigg|_{\vec{r}\in S} - \varepsilon_i \frac{\partial \Phi(\vec{r})}{\partial n}\bigg|_{\vec{r}\in S} = \sigma_s \longrightarrow$$ n is directed to insulator side
surface charge
(semiconductor-insulator interface)

 Ref: Xie, Section 3.1 and 3.4

5. Green's Function (1) — How about the complex nonlinear system?

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

output y



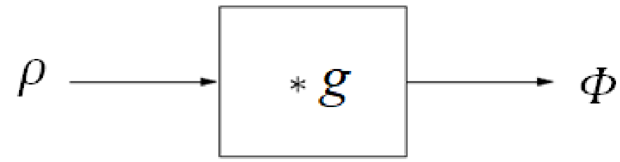
linear time-invariant

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

input ρ

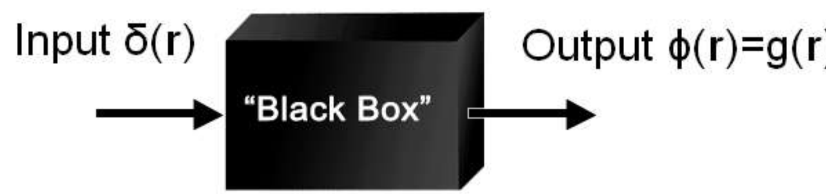
output Φ

linear space-invariant



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

5. Green's Function (2)

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

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

$\mathbf{r}\neq\mathbf{r}'$

$$\nabla\cdot\left(\nabla\frac{c}{|\mathbf{r}-\mathbf{r}'|}\right)=0$$

$\mathbf{r}=\mathbf{r}'$ singular problem

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

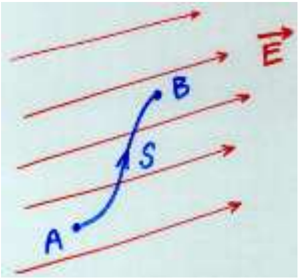
$$\int_{S'}\frac{1}{4\pi}\nabla\frac{1}{R}\cdot d\mathbf{S}'=-1$$

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

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

6. 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

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

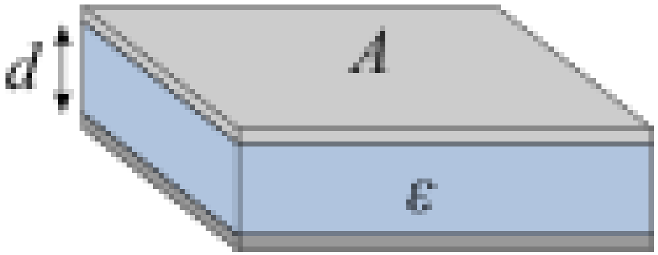
2. The electrostatic energy stored in a system of three and N point charges

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

How about self-energy?

6. 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

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

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

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

Integration by part and symmetry of operators are important tricks!

7. Analogy between Electrostatics and Magnetostatics

Stored electric energy

$$U_E = \mathbf{p} \cdot \mathbf{E}$$

$$U_E = \int_v \frac{1}{2} \mathbf{D} \cdot \mathbf{E} dv = \int_v \frac{1}{2} \varepsilon |\mathbf{E}|^2 \, dv$$

$$= \int_v \frac{1}{2} \rho \phi dv$$

Electric energy density

$$u_E = \frac{1}{2} \varepsilon |\mathbf{E}|^2$$

Stored magnetic energy

$$U_H = \mathbf{m} \cdot \mathbf{B}$$

$$U_H = \int_v \frac{1}{2} \mathbf{B} \cdot \mathbf{H} dv = \int_v \frac{1}{2} \mu |\mathbf{H}|^2 \, dv$$

$$= \int_v \frac{1}{2} \mathbf{A} \cdot \mathbf{J} dv$$

Magnetic energy density

$$u_H = \frac{1}{2} \mu |\mathbf{H}|^2$$

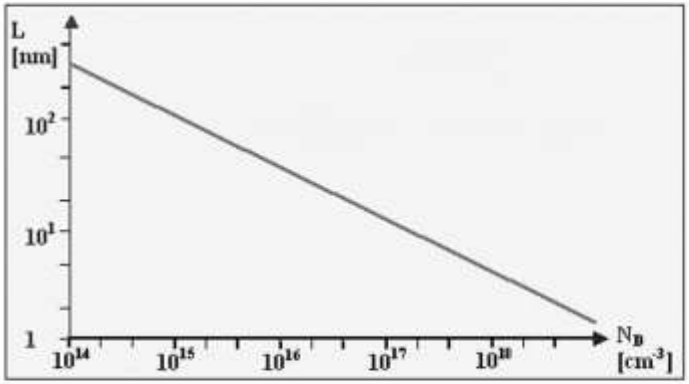
How about electric torque and magnetic torque?

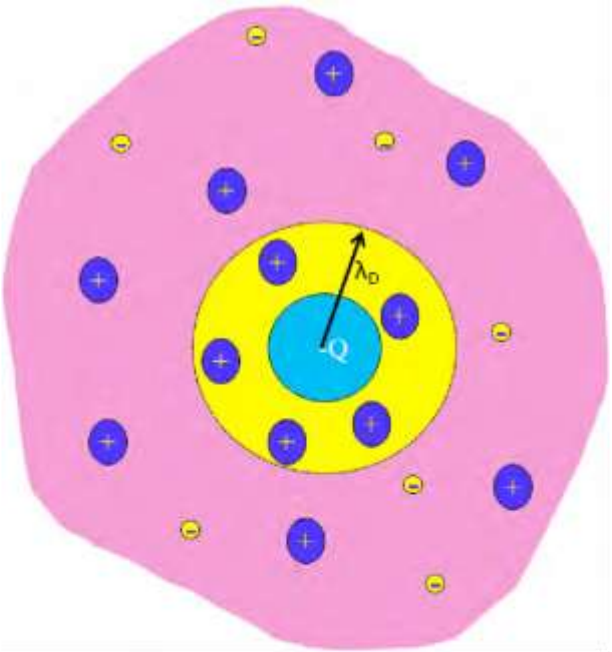
8. Debye (Screening) Length

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 $L_{\mathrm{D}} = \sqrt{\frac{\varepsilon k_{\mathrm{B}} T}{q^2 N_{\mathrm{dop}}}}$

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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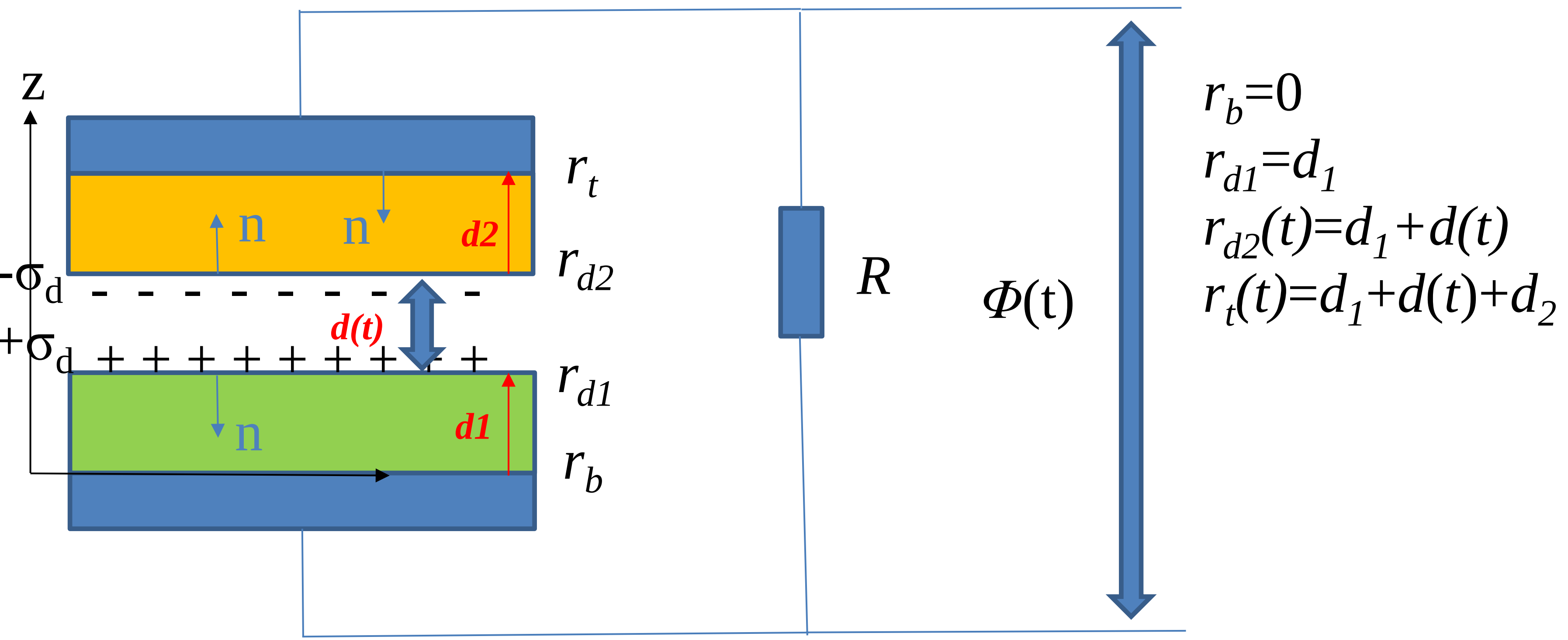
9. Nanogenerator (Optional)

Figure by Qun Wang Group at USTC; Concept proposed by Zhonglin Wang



$$\nabla\cdot(\varepsilon(\mathbf{r})\nabla\Phi(t))=0$$

$$\Phi_t(t)=RA\frac{d\sigma_t(t)}{dt},\ \sigma_t(t)=-\varepsilon(\mathbf{r})\frac{\partial\Phi(t)}{\partial n}\Big|_{r=r_t(t)},\ \Phi_b=0$$

$$\varepsilon(\mathbf{r})\frac{\partial\Phi(t)}{\partial n}\Big|_{r=r_{d_1}^{+}}-\varepsilon(\mathbf{r})\frac{\partial\Phi(t)}{\partial n}\Big|_{r=r_{d_1}^{-}}=\sigma_d,\ \varepsilon(\mathbf{r})\frac{\partial\Phi(t)}{\partial n}\Big|_{r=r_{d_2(t)}^{-}}-\varepsilon(\mathbf{r})\frac{\partial\Phi(t)}{\partial n}\Big|_{r=r_{d_2(t)}^{+}}=-\sigma_d$$