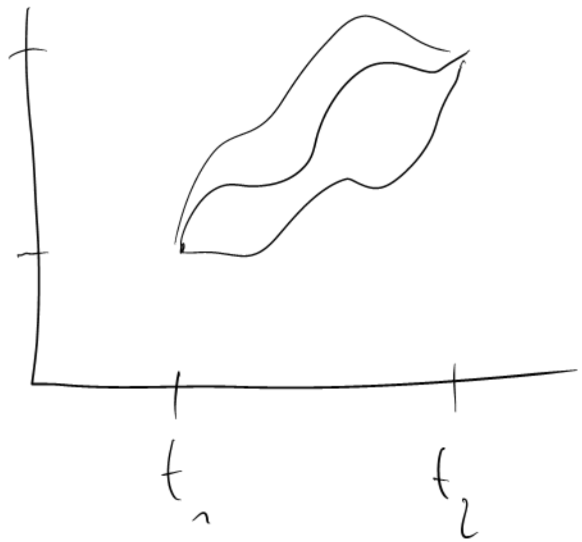
3. Variational Electrostatics

ODE $\rightarrow$ solution $q(t)$



$$S = \int_{t_1}^{t_2} dt \, L(q, \dot{q}) \overset{!}{=} \text{Min.}$$

S: action functional

L: Lagrange function

field theory PDE. scalar field $\phi(\vec{r})$

$\mathcal{L}(\phi, \vec{\nabla}\phi)$ "Lagrange density"

$S = \int d^3\vec{r}\ \mathcal{L}(\phi, \vec{\nabla}\phi)$ "action"

$\stackrel{!}{=}$ Min.

write $\phi = \phi_0 + \delta\phi$

solution ↵ ↳ deviation

$$\delta S = \int d^3\vec{r} \left(\frac{\partial \mathcal{L}}{\partial \phi}\bigg|_{\phi_0} \delta\phi + \frac{\partial \mathcal{L}}{\partial(\partial_\alpha \phi)}\bigg|_{\phi_0} \underbrace{\delta(\partial_\alpha \phi)}_{\partial_\alpha \delta\phi} \right)$$

$$\partial_\alpha \phi \equiv \frac{\partial \phi}{\partial x_\alpha} \qquad \alpha = 1, 2, 3$$

partial int.

Einstein Σ-convention: Greek indices that occur twice are to be summed over

$$\delta S = \int d^3\vec{r} \left[\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\alpha \left(\frac{\partial \mathcal{L}}{\partial(\partial_\alpha \phi)} \right) \right] \delta\phi \overset{!}{=} 0$$

for any $\delta\phi$

$$\underbrace{\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\alpha \frac{\partial \mathcal{L}}{\partial(\partial_\alpha \phi)}}_{\displaystyle = \frac{\delta S}{\delta \phi}} = 0$$

PDE

Euler-Lagrange equation

"functional derivative"

Assume that charge distribution ρ is given

$$F := \int d^3r \left\{ -\frac{\varepsilon}{2} \left(\vec{\nabla} \phi \right)^2 + \rho \phi \right\} \qquad \frac{\delta F}{\delta \phi} = 0$$

potential

$$\rho + \varepsilon \, \vec{\nabla} \cdot \left(\frac{1}{2} \cdot 2 \vec{\nabla} \phi \right) = 0$$

$$\Leftrightarrow \quad \boxed{ -\vec{\nabla}^2 \phi = \frac{1}{\varepsilon} \rho } \qquad \text{Poisson equation}$$

$\phi_0 \equiv$ solution

$$F[\phi_0] = \int d^3\vec{r}\,\left\{-\frac{\varepsilon}{2}\underbrace{(\vec{\nabla}\phi_0)^2}_{\vec{\nabla}\phi_0\cdot\vec{\nabla}\phi_0} + \rho\,\phi_0\right\}$$

p. I.

$$= \int d^3\vec{r}\,\left\{+\frac{\varepsilon}{2}\,\phi_0\,\vec{\nabla}^2\phi_0 + \rho\,\phi_0\right\} \overset{\text{Poisson}}{=}$$

$$= \int d^3\vec{r}\,\left\{\frac{1}{2}\,\phi_0\,(-\rho) + \rho\,\phi_0\right\} = +\frac{1}{2}\int d^3\vec{r}\,\rho\,\phi_0$$

electrostatic field energy

A C Maggs (inspired by R. Feynman).

This is <u>not</u> a minimum, but a <u>maximum</u>!

$$\phi = \phi_0 + \delta\phi$$

$$(\vec{\nabla}\phi)^2 = (\vec{\nabla}\phi_0)^2 + 2(\vec{\nabla}\phi_0)\cdot\vec{\nabla}\delta\phi + (\vec{\nabla}\delta\phi)^2$$

$$F[\phi] = F[\phi_0] + \underbrace{\text{linear term}}_{\substack{(\text{in } \delta\phi) \\ = 0}} + \underbrace{\int d^3\vec{r}\left(-\frac{\varepsilon}{2}(\vec{\nabla}\delta\phi)^2\right)}_{<0}$$

base the formulation <u>not</u> on the potential ϕ,

but rather the electric field $\vec{E}$!

$$\frac{\varepsilon}{2} \int d^3\vec{r}\; \vec{E}^2 \overset{!}{=} \text{Min.} + \underline{\text{constraint}}$$

$$\vec{\nabla} \cdot \vec{E} = \frac{1}{\varepsilon} \rho$$

$$F = \int d^3\vec{r} \left\{ \frac{\varepsilon}{2} \vec{E}^2 - \underbrace{\phi}_{\substack{\text{Lagrange} \\ \text{multiplier}}} \left(\varepsilon \vec{\nabla} \cdot \vec{E} - \rho \right) \right\} =$$

$$F = \int d^3r \left\{ \frac{\varepsilon}{2} E_\alpha E_\alpha - \phi\left(\varepsilon \delta_{\alpha\beta} \partial_\beta E_\alpha - \rho \right) \right\}$$

$$\frac{\delta F}{\delta \phi} \stackrel{!}{=} 0 \quad \rightsquigarrow \quad \underbrace{\varepsilon \vec{\nabla} \cdot \vec{E} - \rho = 0} \quad \text{Gauß' law}$$

$$\frac{\delta F}{\delta E_\alpha} \stackrel{!}{=} 0 \quad \Rightarrow \quad \varepsilon E_\alpha + \partial_\beta\left(\phi \varepsilon \delta_{\alpha\beta} \right) = 0$$

$$E_\alpha + \partial_\alpha \phi = 0 \Rightarrow \vec{E} = -\vec{\nabla}\phi$$

$\rightsquigarrow$ ϕ has interpretation as potential

$$\Rightarrow \underbrace{\vec{\nabla} \times \vec{E} = -\vec{\nabla} \times \vec{\nabla}\phi = 0}$$

$\hookrightarrow$ electrostatics is recovered!

$$F[\vec{E}_0] = \frac{\varepsilon}{2}\int d^3r\, \vec{E}_0^2$$ indeed field energy!

solution

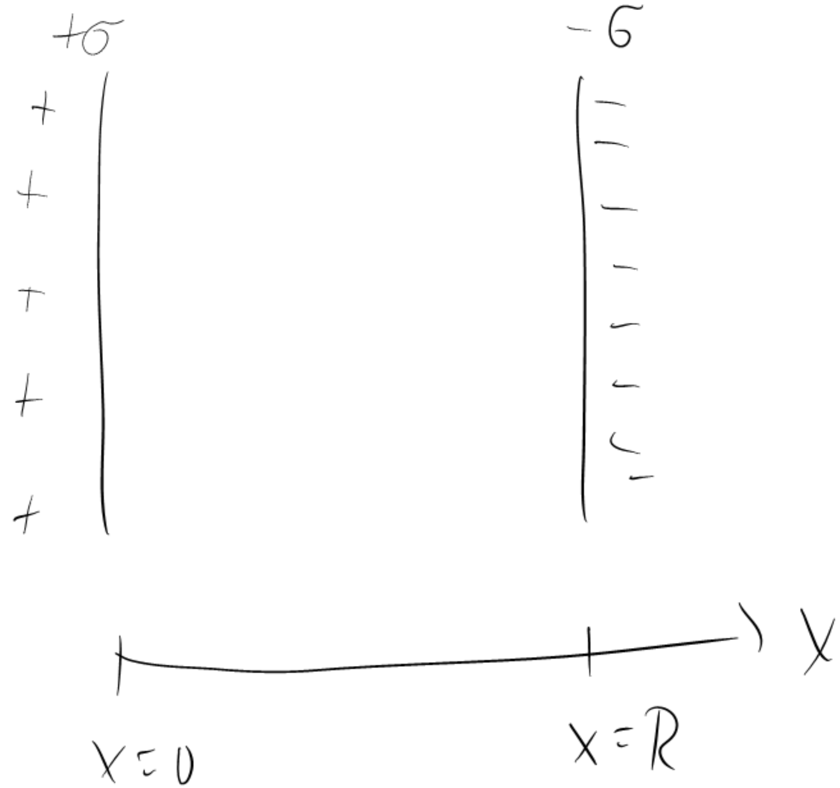
$$F[\vec{E}_0 + \delta\vec{E}_0] = F[\vec{E}_0] + \overbrace{\text{linear term}}^{=0} + \underbrace{\frac{\varepsilon}{2}\int d^3r\, (\delta\vec{E})^2}_{>0}$$

$$\vec{E}^2 = (\vec{E}_0 + \delta\vec{E})^2 = \vec{E}_0^2 + (\delta\vec{E})^2 + \text{linear term}$$

$\downarrow$ we do get a minimum!

4. Some capacitors

a) Two infinite parallel walls



$$\sigma = \frac{\text{charge}}{\text{area}}$$

$E_y = E_z = 0$

(translational invariance)

$$\varepsilon \frac{d}{dx} E_x = \rho = \sigma \left[\delta(x) - \delta(x-R) \right]$$

$$E_x = \text{const. } \underline{\text{except}} \text{ at } \begin{cases} x = 0 \\ x = R \end{cases}$$

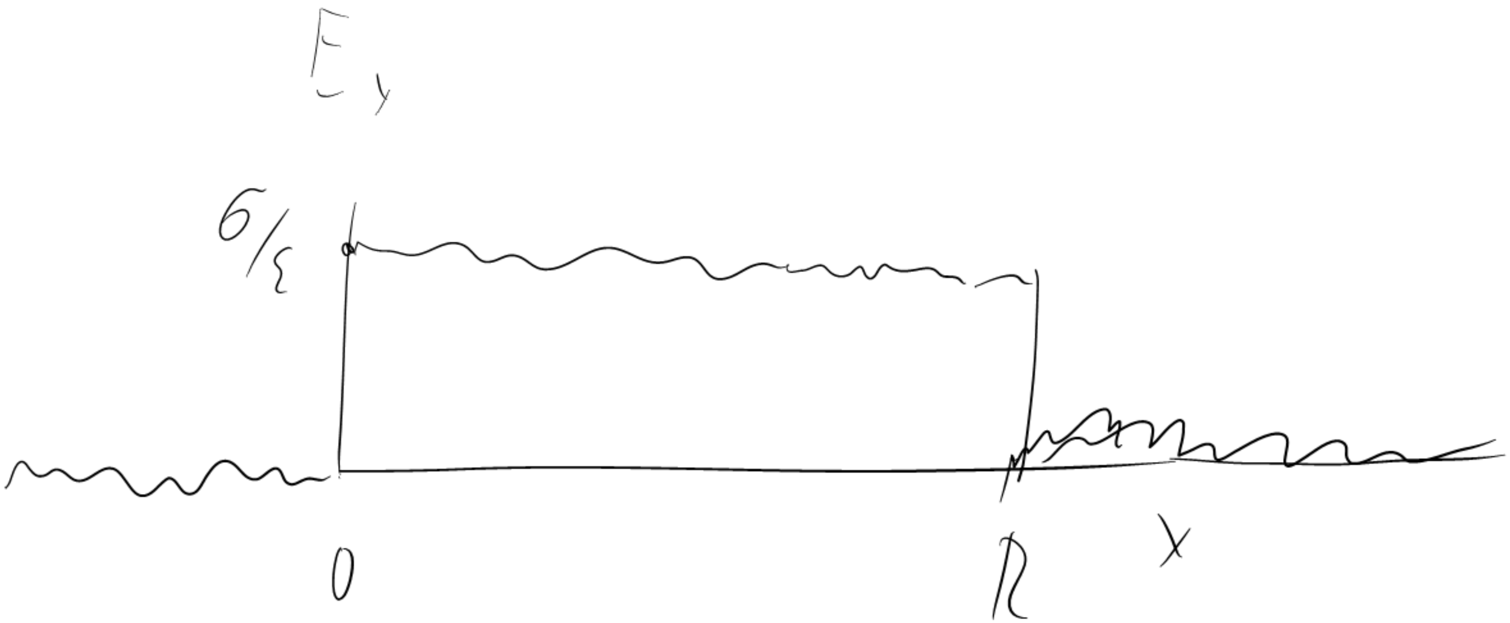
integrate over a small interval

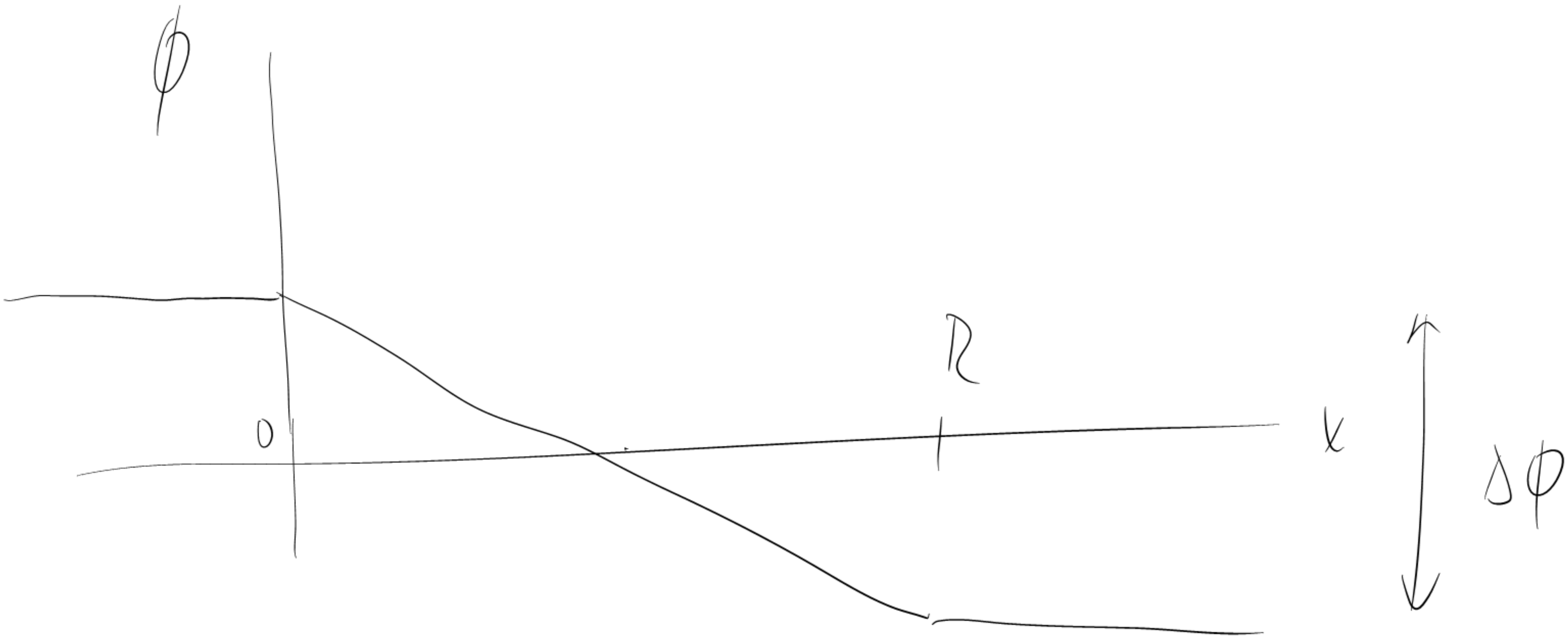
$$\varepsilon \left[E_x(0+) - E_x(0-) \right] = \sigma \qquad E_x(R+) = 0$$

$$\varepsilon \left(E_x(R+) - E_x(R-) \right] = -\sigma \qquad E_x(0-) = 0$$

$$\left.\begin{aligned} \varepsilon\, E_y(0+) &= +\sigma \\ -\varepsilon\, E_x(R-) &= -\sigma \end{aligned}\right\} \quad E_x(0+) = E_y(R-) = \frac{\sigma}{\varepsilon}$$

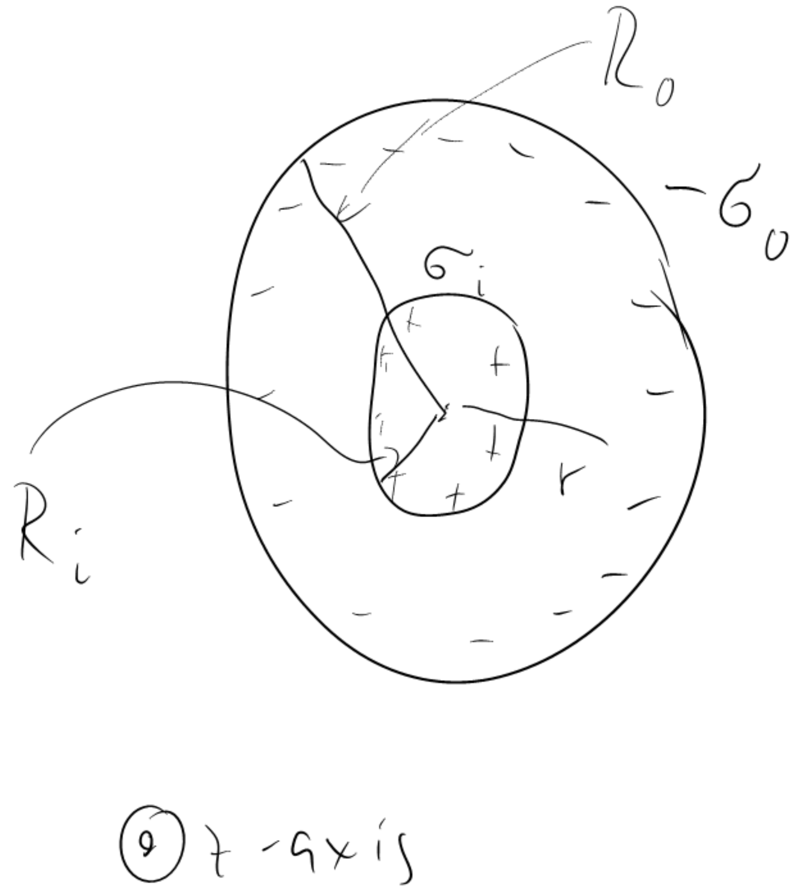
$$= E_x(\text{interior})$$





$$\frac{\Delta\phi}{R} = E_x = \frac{\sigma}{\varepsilon} \qquad \Delta\phi = \frac{\sigma R}{\varepsilon}$$

Infinite straight coaxial cable



cylinder coordinates

$\underbrace{r, \varphi, z}_{\text{do not matter}} \rightsquigarrow \phi = \phi(r)$

charge neutral

$$\sigma_i \, dz \, R_i \, d\varphi = \sigma_0 \, dz \, R_0 \, d\varphi$$

$$\sigma_0 = \sigma_i \frac{R_i}{R_0}$$

$\vec{\nabla}^2 \phi = 0$ in the interior

$$\vec{\nabla}^2 = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \underbrace{\varphi\text{-dep.} + z\text{-dep.}}_{\text{do not matter}}$$

$$0 = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r}\phi$$

$$0 = \frac{\partial}{\partial r} r \frac{\partial}{\partial r}\phi$$

$$A = r\frac{\partial}{\partial r}\phi$$

$$\frac{\partial}{\partial r}\phi = \frac{A}{r} \qquad A = ??$$

$$\vec{E} = E\,\hat{e}_r$$

unit vector in r direction

$$E = -\frac{\partial}{\partial r}\phi = -\frac{A}{r}$$

interior of cable: $\underline{\underline{\vec{E} = 0}}$

$$\int d^3r\, \vec{\nabla}\cdot\vec{E} = \frac{1}{\varepsilon} \underbrace{\int d^3r\, \rho}_{= Q} = \frac{1}{\varepsilon} Q$$

contained charge

$$\overset{\text{Gauß' theorem}}{=} \int_{\text{surf}} d\vec{A}\cdot\vec{E}$$

$$-\frac{A}{R_i} \cdot dz\, R_i\, d\varphi = \frac{1}{\varepsilon} \sigma_i\, dz\, R_i\, d\varphi$$

$$A = -\frac{\sigma_i R_i}{\varepsilon} \qquad \frac{\partial}{\partial r}\phi = -\frac{\sigma_i R_i}{\varepsilon}\frac{1}{r}$$

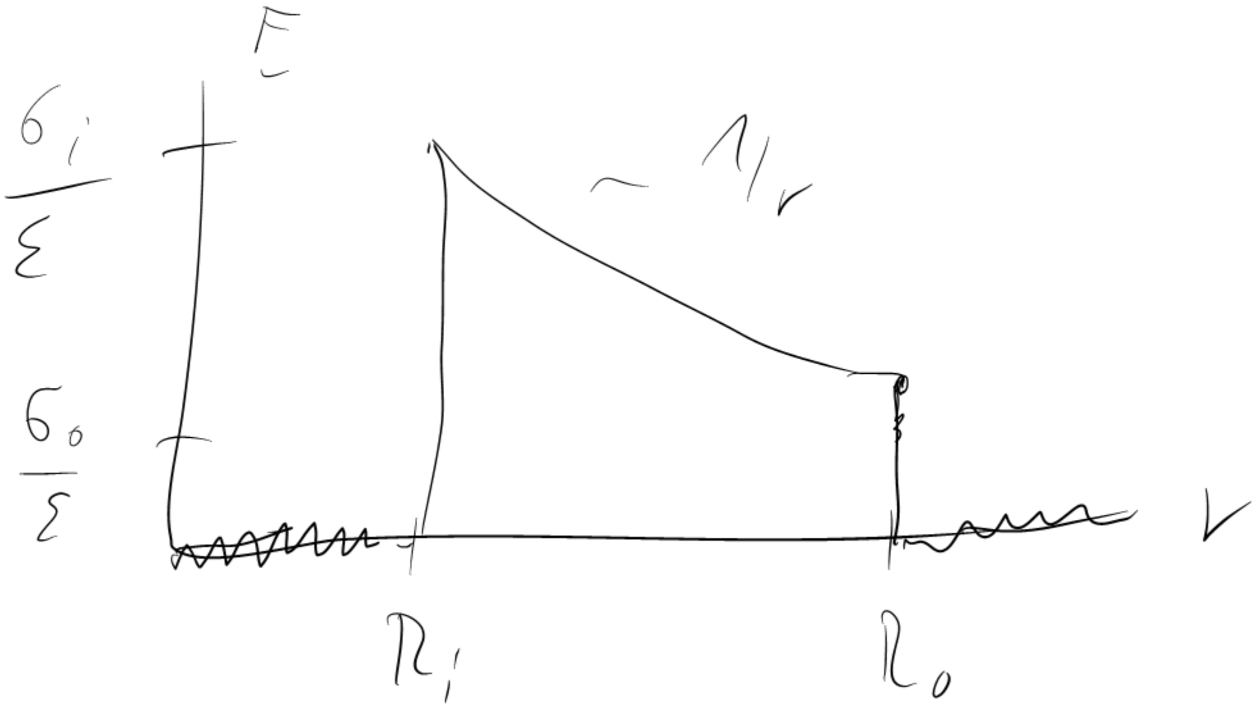
$$\phi = -\frac{\sigma_i R_i}{\varepsilon}\ln r + B \qquad E = +\frac{\sigma_i R_i}{\varepsilon}\frac{1}{r}$$

normalization: $\phi(R_0) = 0$

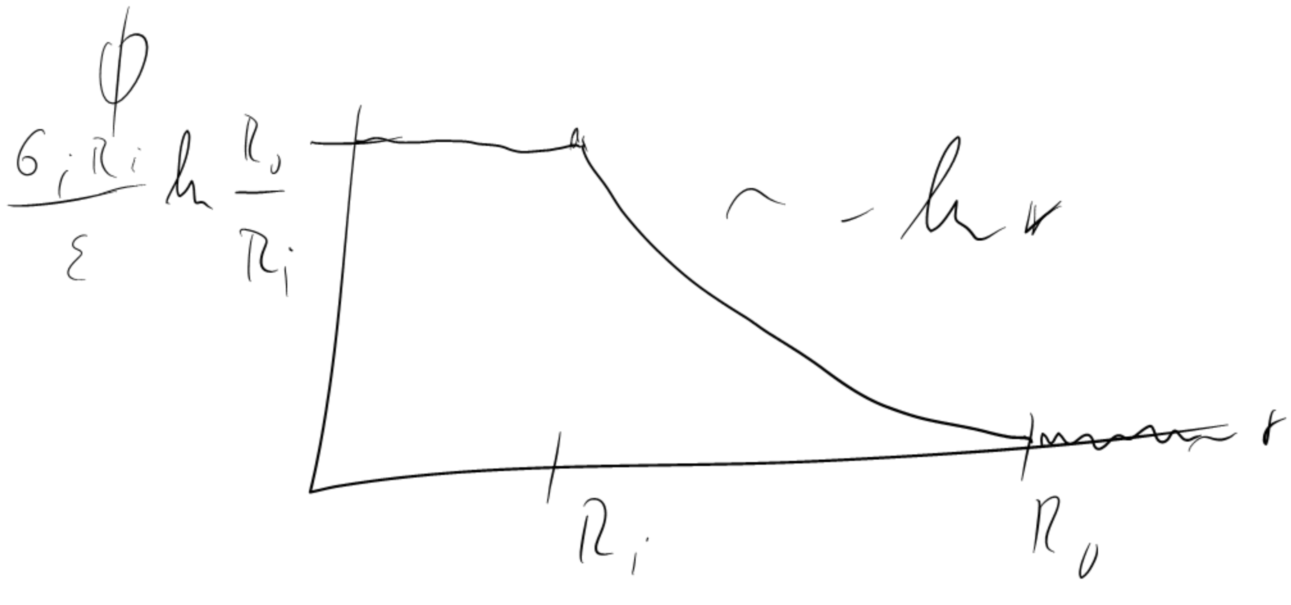
$$0 = -\frac{\sigma_i R_i}{\varepsilon}\ln R_0 + B \qquad E(r=R_0) = \frac{\sigma_i R_i}{\varepsilon}\frac{1}{R_0}$$

$$= \frac{\sigma_0}{\varepsilon} \quad \text{OK}$$

$$\underbrace{\phi = -\frac{\sigma_i R_i}{\varepsilon}\ln\frac{r}{R_0}}$$

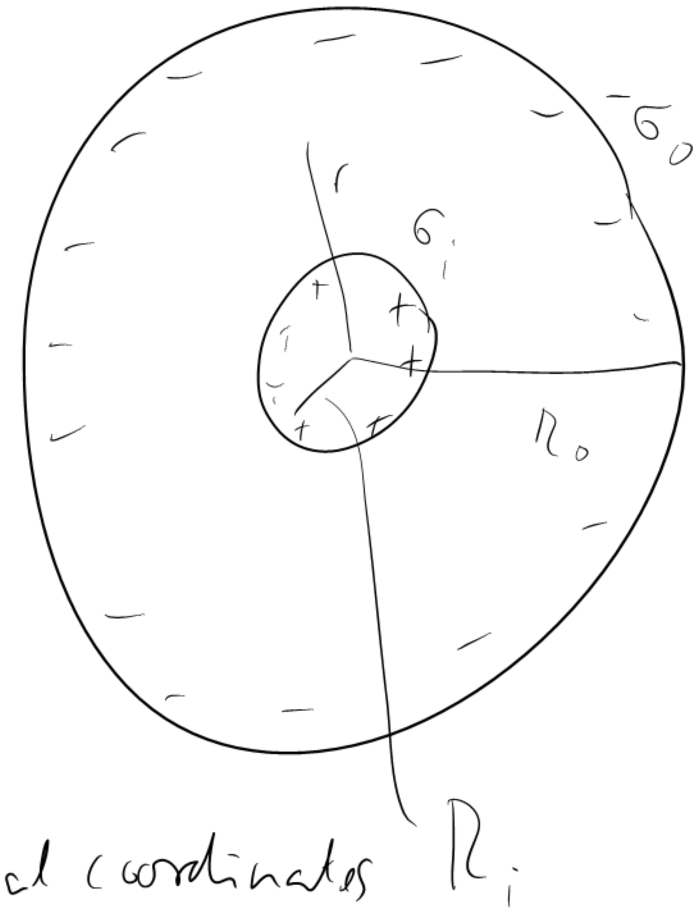


E
$\frac{\sigma_i}{\varepsilon}$
$\frac{\sigma_o}{\varepsilon}$
$\sim 1/r$
r
R_i
R_o



ϕ
$\frac{\sigma_i R_i}{\varepsilon} \ln \frac{R_o}{R_i}$
$\sim -\ln r$
r
R_i
R_o

Spherical capacitor



$R_i < r < R_0$

charge neutrality:

$$\sigma_i R_i^2 \underbrace{d\Omega}_{\text{solid angle}} = \sigma_0 R_0^2 \, d\Omega$$

$$\sigma_0 = \sigma_i \left(\frac{R_i}{R_0}\right)^2$$

Spherical coordinates

r, θ, φ only r matters, $\Phi = \Phi(r)$

$$\vec{\nabla}^2 = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \underbrace{\text{angle terms}}_{\text{don't matter}}$$

$$0 = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \phi$$

$$0 = \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \phi$$

$$A = r^2 \frac{\partial}{\partial r} \phi$$

$$-\frac{\partial}{\partial r}\phi = -\frac{A}{r^2} = E$$

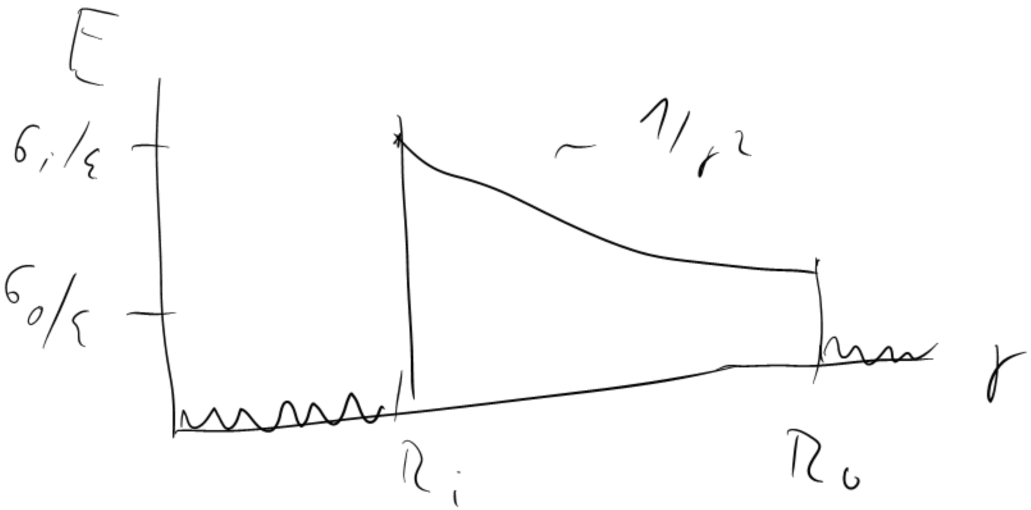
$$-\frac{A}{R_i^2} R_i^2 \, d\Omega = \frac{1}{\varepsilon} \sigma_i R_i^2 \, d\Omega$$

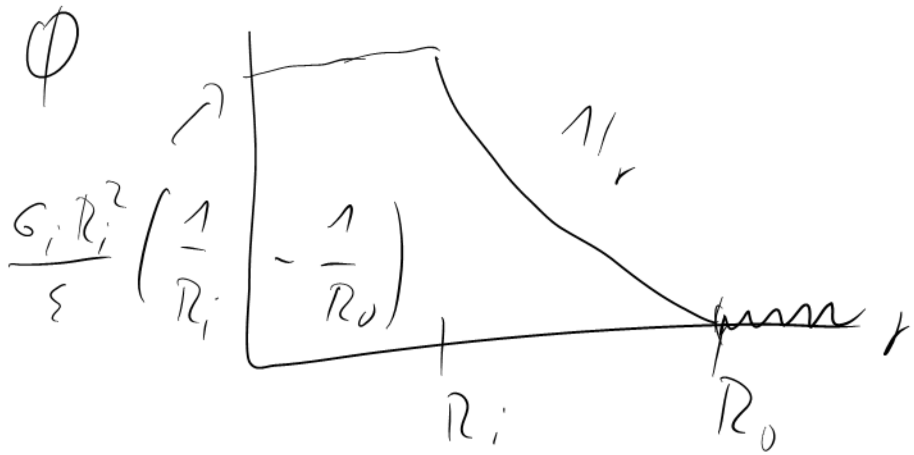
$$\boxed{A = -\frac{\sigma_i R_i^2}{\varepsilon}}$$

$$E = \frac{\sigma_i R_i^2}{\varepsilon r^2} \quad \frac{\partial}{\partial r}\phi = -\frac{\sigma_i R_i^2}{\varepsilon}\frac{1}{r^2} = \frac{\sigma_i R_i^2}{\varepsilon}\frac{\partial}{\partial r}\left(\frac{1}{r}\right)$$

$$\phi(r) = \frac{\sigma_i R_i^2}{\varepsilon}\frac{1}{r} + B \qquad \phi(R_0) = 0 \text{ (norm.)}$$

$$B = -\frac{\sigma_i}{\varepsilon}\frac{R_i^2}{R_0} \qquad \phi(r) = +\frac{\sigma_i R_i^2}{\varepsilon}\left(\frac{1}{r} - \frac{1}{R_0}\right)$$





5. Poisson-Boltzmann theory

System of N charges $e z_i$ at positions $\vec{r}_i$

$$\mathcal{H}(\{\vec{r}_i\}) = \frac{e^2}{4\pi\varepsilon} \frac{1}{2} \sum_{i \neq j} \frac{z_i z_j}{|\vec{r}_i - \vec{r}_j|}$$

Stat. Mech.

$$\beta = \frac{1}{k_B T}$$

$$Z = \int d^3\vec{r}_1 \int d^3\vec{r}_2 \ldots \int d^3\vec{r}_N \; \exp\left[-\beta \mathcal{H}\right]$$

HARD !

$$\beta \mathcal{H} = \underbrace{\frac{e^2}{4\pi\varepsilon k_B T}}_{\ell_B} \frac{1}{2} \sum_{i \neq j} \frac{z_i z_j}{|\vec{r}_i - \vec{r}_j|}$$

abbrev:

$$\boxed{\ell_B = \frac{e^2}{4\pi\varepsilon k_B T}}$$

Bjerrum length

$\sim 7\,\text{Å}$ for water and room temperature

$\varepsilon \simeq 80$

$$\beta \mathcal{H} = l_B \frac{1}{2} \sum_{i \neq j} \frac{z_i z_j}{|\vec{r}_i - \vec{r}_j|}$$

Mean Field Theory: neglect fluctuations

$\langle \ldots \rangle$ statistical average of ...

$$\rho(\vec{r}) = \sum_i z_i e \, \delta(\vec{r} - \vec{r}_i)$$

$$\langle \rho(\vec{r}) \rangle = \sum_i z_i e \, \langle \delta(\vec{r} - \vec{r}_i) \rangle$$

$$\langle \vec{E}(\vec{r}) \rangle \qquad \vec{\nabla} \cdot \langle \vec{E} \rangle = \frac{1}{\varepsilon} \langle \rho \rangle$$

$$\langle \phi(\vec{r}) \rangle \qquad -\vec{\nabla}^2 \langle \phi \rangle = \frac{1}{\varepsilon} \langle \rho \rangle$$

$$\rho(\vec{r}) = \langle \rho \rangle + \delta\rho \quad \leftarrow \text{fluctuation}$$

$$\mathcal{H} = \frac{\varepsilon}{2} \int d^3\vec{r}\, \vec{E}^2$$

$$\vec{E}(\vec{r}) = \langle \vec{E} \rangle + \delta \vec{E}$$

$$\phi(\vec{r}) = \langle \phi \rangle + \delta \phi$$