Electromagnetic Force Density in Condensed Matter

(a numerical test)

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Motivation

- Electromagnetic forces in condensed matter are still subject of debates (see “Abraham-Minkowski controversy” and related papers)
- Total force acting on a rigid body: mostly settled but there are ambiguities when magnetization is present in time-varying fields. This talk is not about this problem
- In case of non-magnetic materials, the total force is all but settled but the spatial distribution of force density is not. There are several competing relations
- S.M Barnett and R. Loudon, “On the electromagnetic force on a dielectric medium,” J.Phys.B **39** S671, 2006. Compares two most popular force densities in a macroscopic setting (inconclusive). Many more papers published to date. But macroscopic theory is in principle insufficient for a determination.
- Making a tractable microscopic model that can allow one to make a determination is actually difficult. But we will try

Competing Expressions

Same total force and torque on a rigid body, for arbitrary fields (stays true beyond statics and beyond linear approximation)

Total electric field

$$\mathbf{f}_a = \rho\mathbf{E} = -(\nabla \cdot \mathbf{P})\mathbf{E}$$

Induced charge density

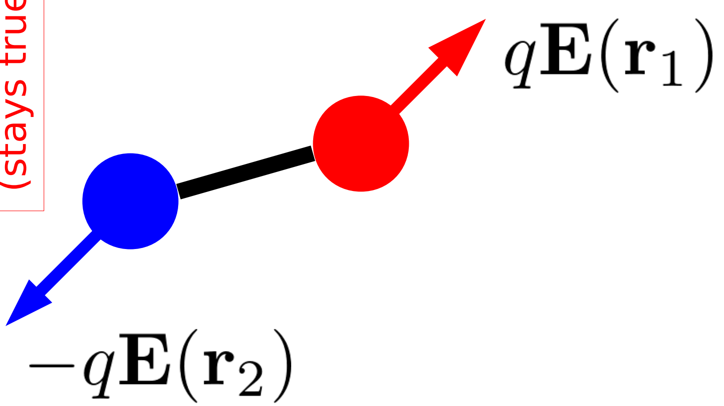
Lorentz (actually, Coulomb) force acting on the induced charge

(what about free and bound charges?)

$$\mathbf{f}_b = (\mathbf{P} \cdot \nabla)\mathbf{E}$$

The medium is assumed to be made of rigid “dipoles”

(why is the link between the opposite charges rigid? how is then the medium polarized?)



There are Other Expressions

$$\mathbf{f}(\mathbf{r}) \longrightarrow \mathbf{f}(\mathbf{r}) + \underbrace{\nabla \cdot \hat{T}(\mathbf{r})}_{\text{Zero total force and torque}}$$

This transformation of the force density does not change the total force and torque*

$$\mathbf{f}_b = \mathbf{f}_a + \nabla \cdot (\mathbf{E} \otimes \mathbf{P})$$

What if we take $\hat{T} = (1/2)(\mathbf{E}\cdot\mathbf{P})\hat{I}$? Although this expression is simple, it can not be developed into anything familiar ***in general***. However, if we assume (a) linearity§ and (b) statics (irrotational electric field), then:

$$\nabla \cdot \hat{T} = \frac{1}{2}\nabla(\mathbf{E}\cdot\mathbf{P}) = \mathbf{f}_b + \frac{\nabla\epsilon}{8\pi}E^2$$

$$\mathbf{f}_c = \mathbf{f}_b - \nabla\cdot\hat{T} = -\frac{\nabla\epsilon}{8\pi}E^2$$

⟺ Another commonly encountered force density (i.e., Landau and Lifshitz, v.8)

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* Divergence of a tensor is defined as $\nabla \cdot \hat{T} = \sum_{\alpha\beta} \hat{\mathbf{e}}_\alpha [\partial T_{\alpha\beta}/\partial r_\beta]$

§ Linearity and statics imply that $\mathbf{P} = \frac{\epsilon - 1}{4\pi}\mathbf{E}$

Electrostriction Force

But wait, there is more... Electrostriction force is often introduced independently

$$\mathbf{f}_{\text{elstr}} = \frac{1}{8\pi}\nabla\left[E^2\rho\left(\frac{\partial\epsilon}{\partial\rho}\right)_T\right]$$

Assume that $\epsilon = 1 + \beta\rho$ → $\mathbf{f}_{\text{elstr}} = \nabla\left[\frac{\epsilon - 1}{8\pi}E^2\right]$

$$\mathbf{f}_d = \mathbf{f}_c + \mathbf{f}_{\text{elstr}} = \frac{\epsilon - 1}{8\pi}\nabla E^2$$

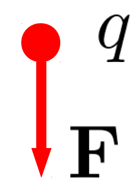
← Another commonly encountered form

Medium is linear and electric field is irrotational → $\mathbf{f}_d(\mathbf{r}) = \mathbf{f}_b(\mathbf{r})$

But in general there is no such equivalence

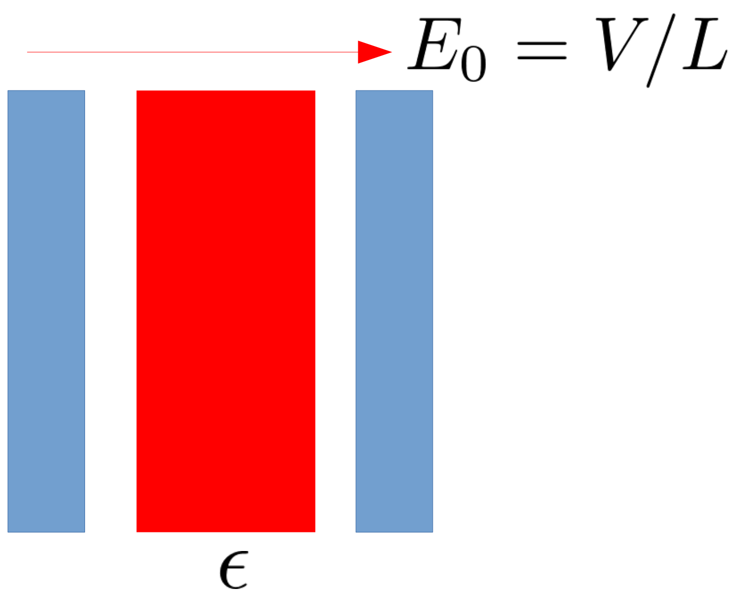
How to Compare?

a) Charge over a half-space
(S.M Barnett and R. Loudon, J.Phys.B **39** S671, 2006)



Since the half-space is infinite, the force on the charge is (minus) the total force on the medium. All proposed expressions predict the same total force.

a) Slab in a capacitor



The total force is the same for all expressions (zero). But ***stress*** is different.

We can potentially use this setup to test different expressions.

Different Predictions for Surface Pressure

$$\mathbf{f}_a = -(\nabla \cdot \mathbf{P})\mathbf{E} \longrightarrow P_a = -\frac{E_0^2}{8\pi}\frac{\epsilon^2 - 1}{\epsilon^2}$$

$$\mathbf{f}_b = (\mathbf{P} \cdot \nabla)\mathbf{E} \longrightarrow P_b = -\frac{E_0^2}{8\pi}\frac{(\epsilon - 1)^2}{\epsilon^2}$$

$$\mathbf{f}_c = -\frac{E^2}{8\pi}\nabla\epsilon \longrightarrow P_c = -\frac{E_0^2}{8\pi}\frac{\epsilon - 1}{\epsilon}$$

Negative pressure (extension)

Keep in mind that this is an approximation. We will use a more rigorous result a bit later

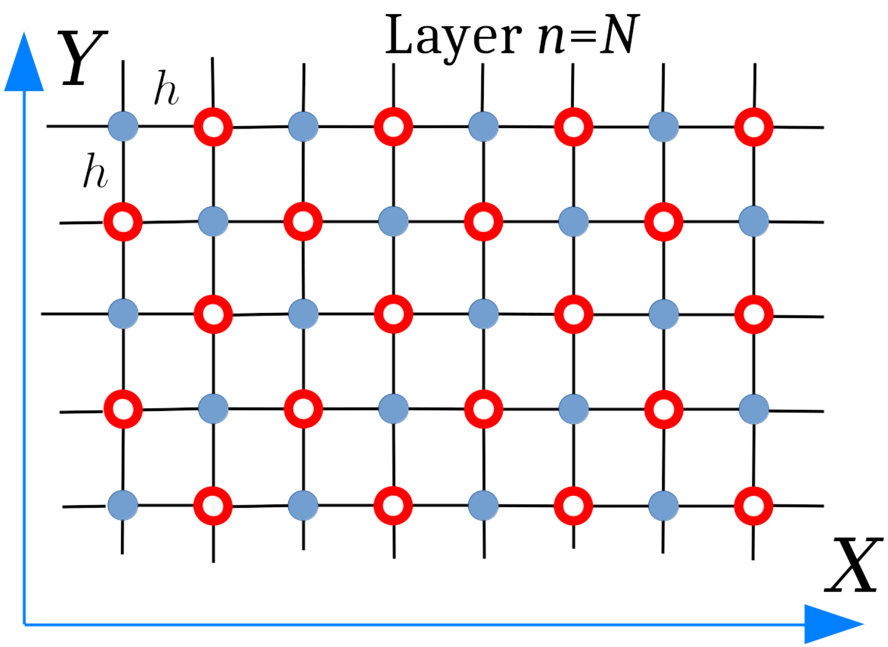
$$\mathbf{f}_{\mathrm{elstr}} = \nabla\left[\frac{\epsilon - 1}{8\pi}E^2\right] \longrightarrow P_{\mathrm{elstr}} = \frac{E_0^2}{8\pi}\frac{\epsilon - 1}{\epsilon^2}$$

Positive pressure (contraction)

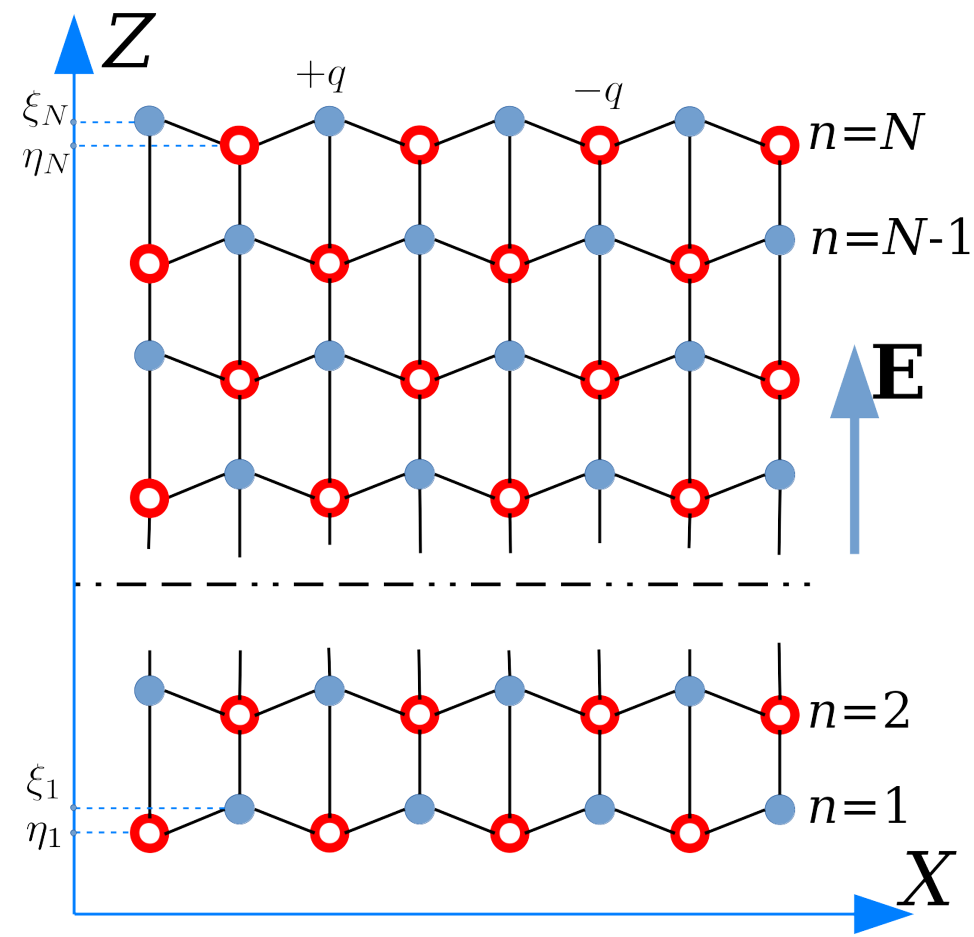
$$\mathbf{f}_d = \mathbf{f}_c + \mathbf{f}_{\mathrm{elstr}} = \frac{\epsilon - 1}{8\pi}\nabla E^2 \longrightarrow P_d = P_c + P_{\mathrm{elstr}} = P_b$$

Equivalence holds only in statics, linear electrodynamics, and if the approximate Electrostriction term is used

Model: Ionic Crystal (e.g., NaCl)



Top View



Side View

Each link (aka chemical bond) is a spring of constant k and equilibrium length h

The model has only one scalar parameter $\kappa = q^2/kh^3 \lesssim 0.25$ ← Due to the requirement of stability

Features of the Model

- The model is essentially 3D and discrete
- Electrostatic interaction between ions is accounted for rigorously. It is essential (no effect without it).
- All elastic bonds (in *X*, *Y* and *Z*) are accounted for
- The model has only one parameter: $\kappa = q^2/kh^3$. It quantifies the relative strength of electrostatic interaction
- System of many nonlinear equations, can be solved by relaxation

Constant vector (i.e. force of the external field)

Linear, easily invertible

$$Ax = b + F[x]$$

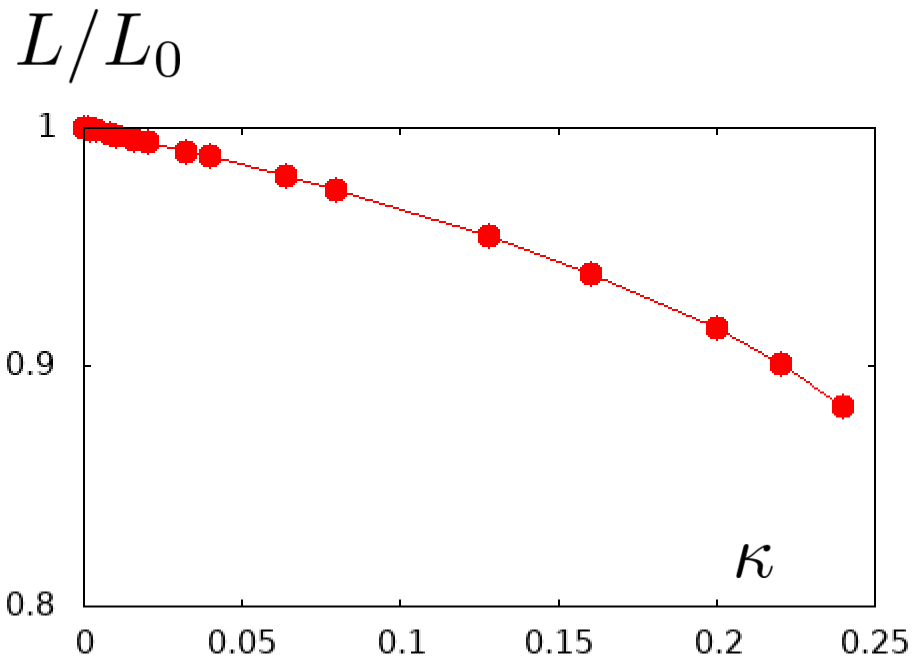
Nonlinear functional of positions (all other forces)

Vector of *z*-positions of all sub-layers

$$x_{n+1} = A^{-1}\left(b + F[x_n]\right)$$

If the iterations are set up correctly, there is a fixed point

Equilibrium for no External Field or Pressure



$$\kappa = q^2/kh^3$$

$$N = 150$$

(this value was used in the simulation but really results are independent of the number of layers)

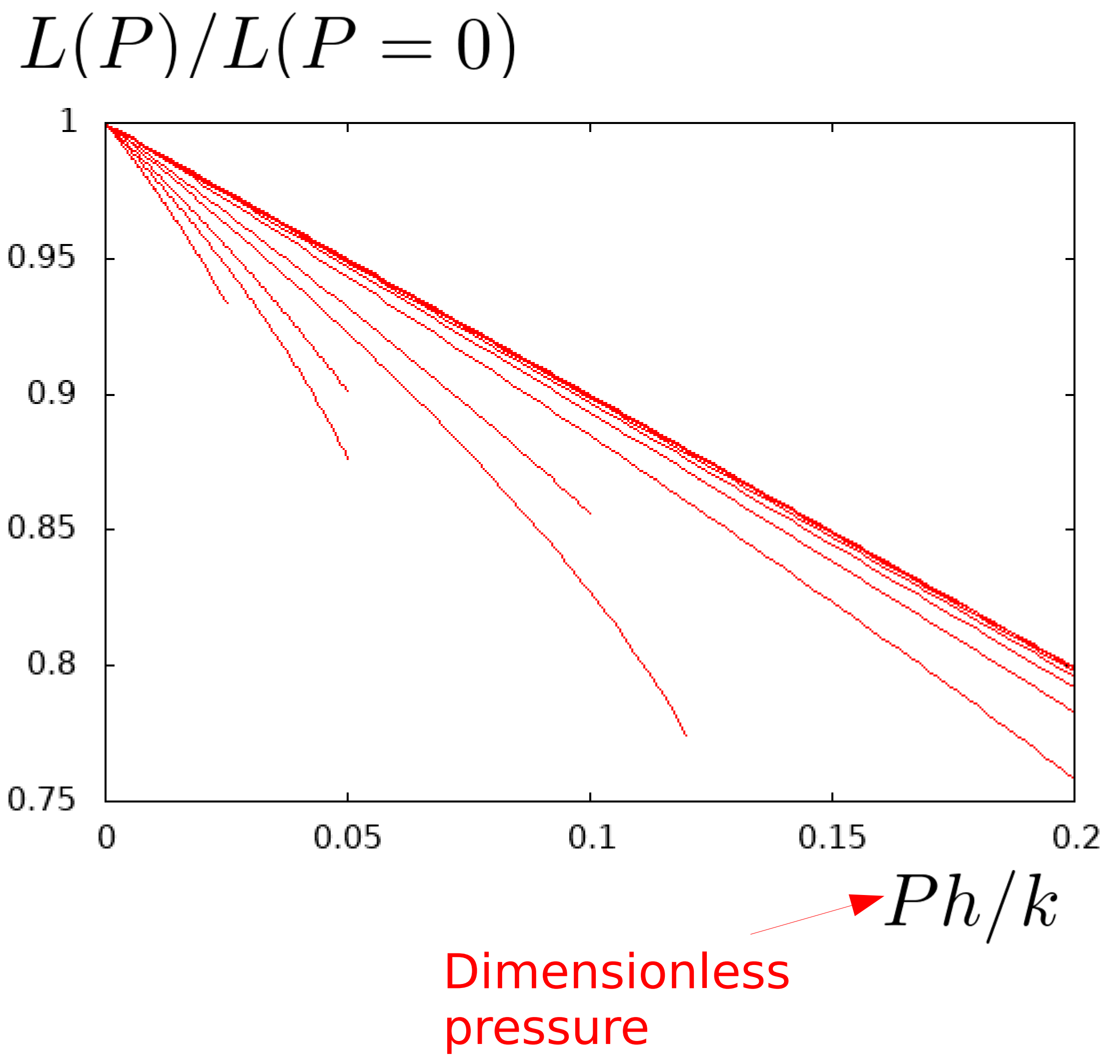
$$L_0 = (N-1)h$$ ← Width of the slab without electrostatic interaction of atom layers

$$L$$ ← Width of the slab with electrostatic interaction

a) Lattice unit is smaller in the Z-direction (unit cell is not a cube). Is this possible?

b) Surface cells are different from bulk cells

Elastic Deformations due to Pressure

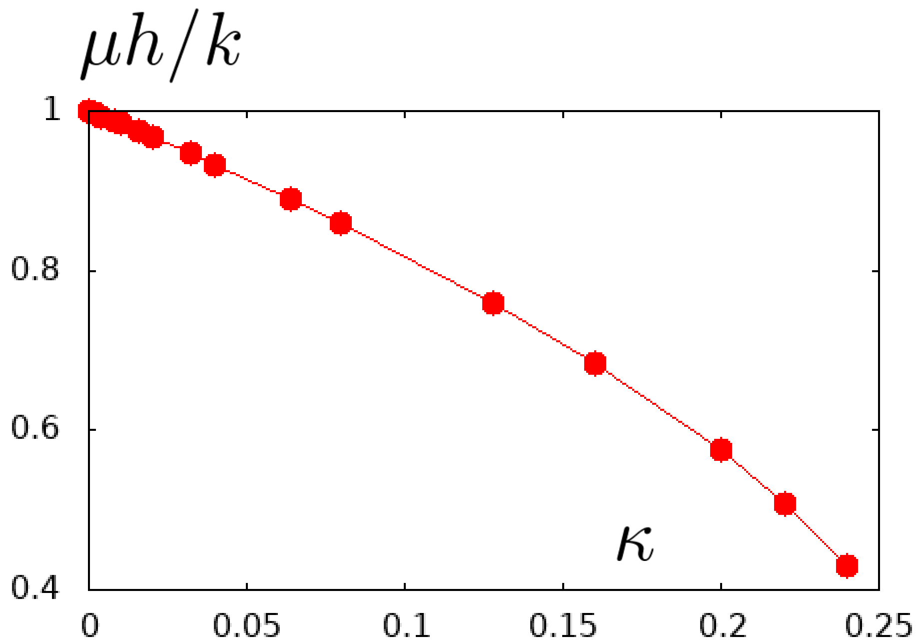


Curves from top to bottom correspond to the following values of κ :

0.001
0.002
0.004
0.008
0.016
0.032
0.064
0.128
0.160
0.200
0.220
0.240

At larger values of κ the structure collapses for smaller values of P

Young's Modulus μ



$$\frac{L(P)}{L(P=0)} = 1 - \frac{1}{\mu} P$$

Electrostatic interaction tends to reduce the modulus because nearest atom layers always attract

If the modulus is too small, the structure can collapse

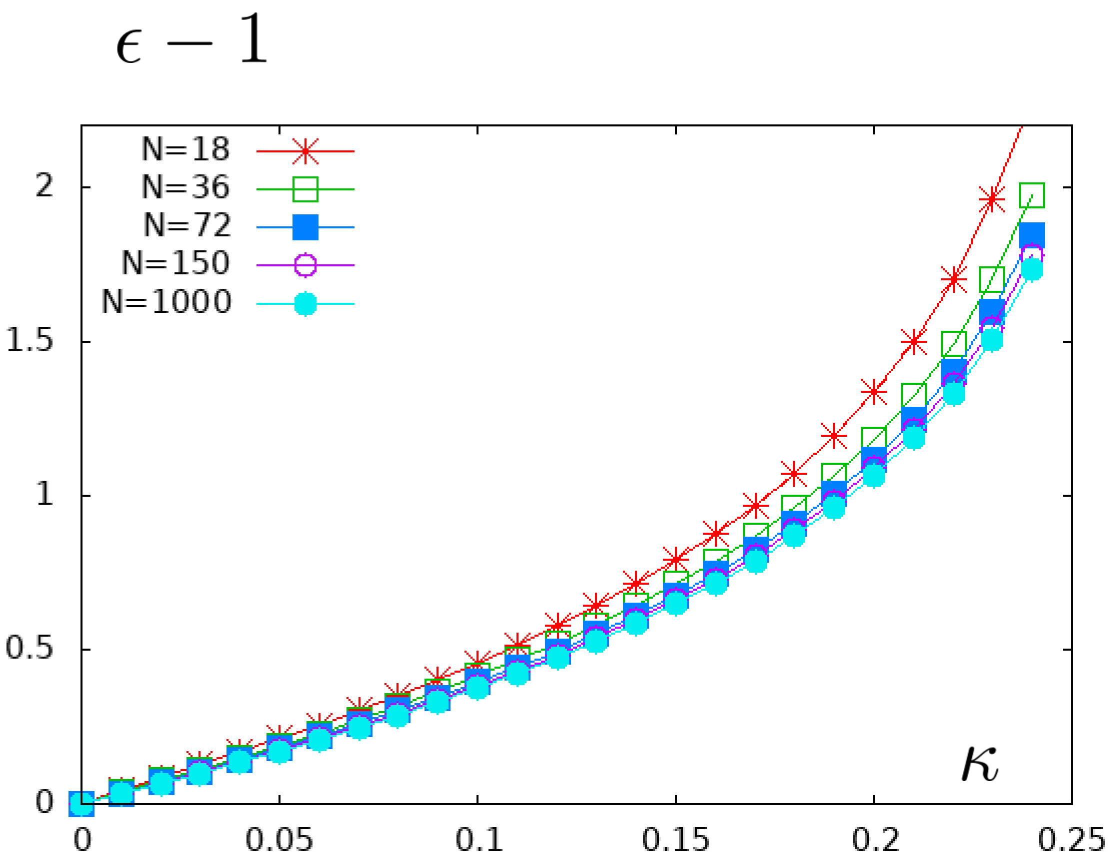
a) Pressure is assumed to be positive if it acts to compress the slab

b) Modulus has the dimensionality of pressure

c) In the absence of electrostatic interaction

$$\mu = \mu_0 = k/h$$

Dielectric Constant at Zero Pressure



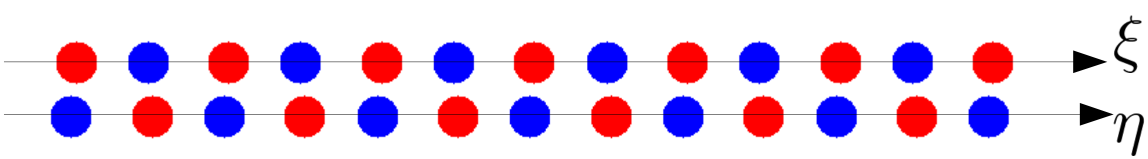
Definition in terms of dimensionless quantities:

$$\epsilon = \frac{1}{1 - 2\pi\mathcal{D}/\mathcal{L}\mathcal{E}}$$

$$\mathcal{D} = \sum_{n=1}^{N} (-1)^n \frac{\xi_n - \eta_n}{h}$$

$$\mathcal{E} = E_0 h^2/q$$

$$\mathcal{L} = \frac{\xi_N - \xi_1 + \eta_N - \eta_1}{2h}$$

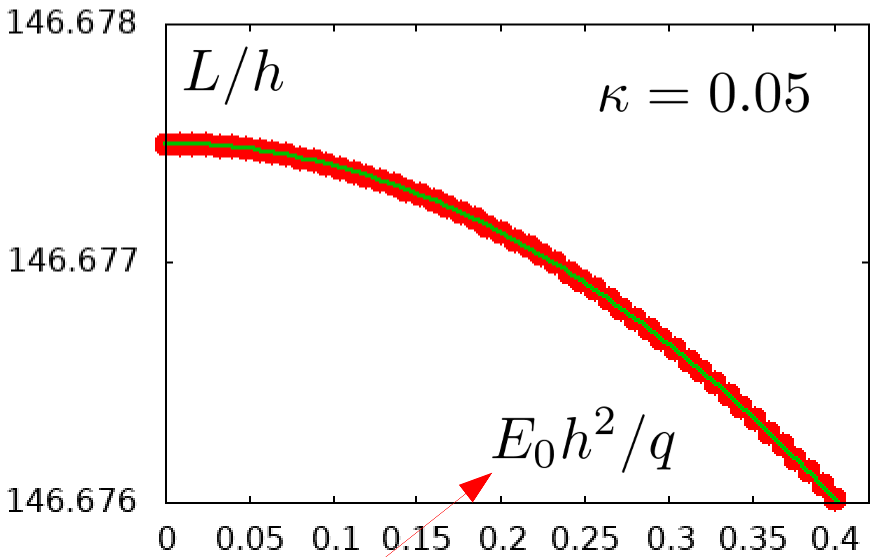


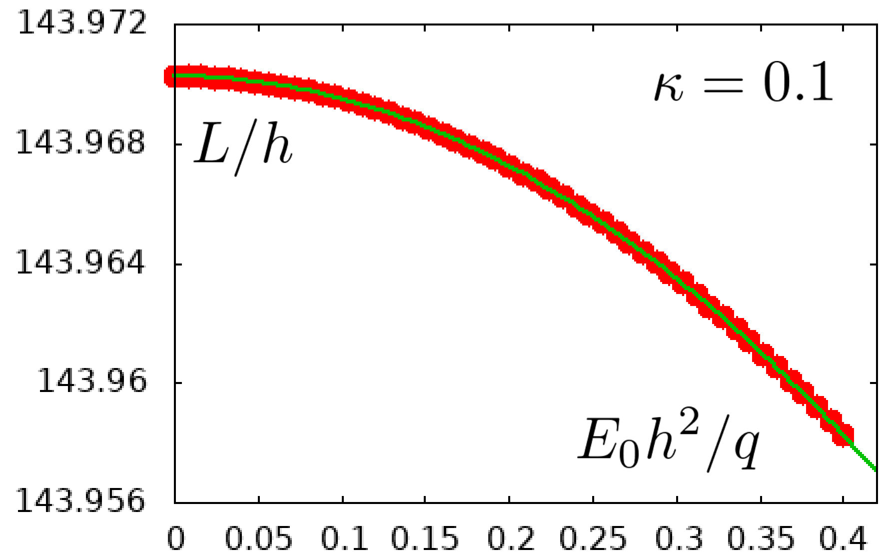
Note:

a) Dielectric constant depends on the film width!

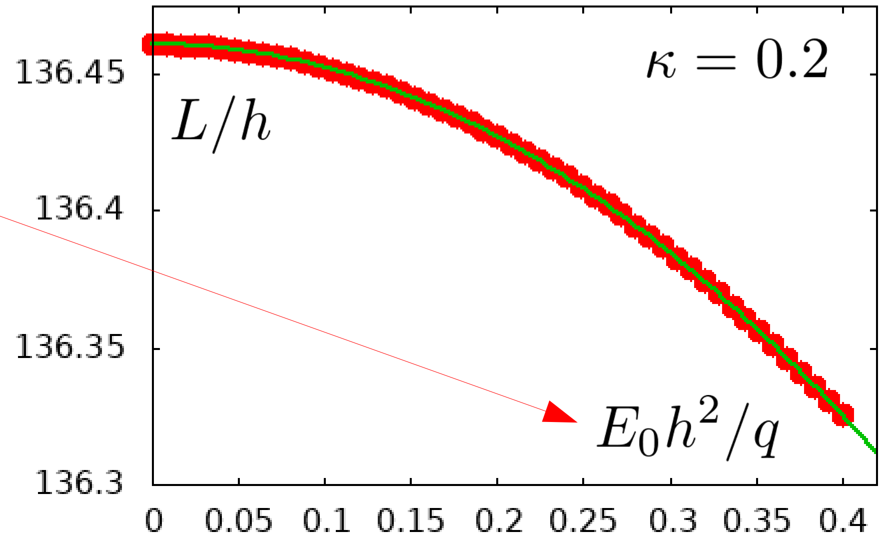
b) Bulk limit is reached around N=1000 atom layers

Elastic Deformation due to Applied Field (N=150)





Applied field in atomic units



Conclusion 1:
It's always contraction

Conclusion 2:
Dependence on applied field is almost perfectly quadratic (as expected theoretically)

Comparing Pressures with Approximate Electrostriction

$$P_{\rm eq} = \mu \left(1 - \frac{L(E_0)}{L(E_0 = 0)}\right)$$

This is the equivalent pressure that is needed to compress the slab to the computed value $L(E_0)$

$$P_{\rm th} = \beta E_0^2$$

This is the theoretical pressure due to the applied field

$$\beta_a = -\frac{\epsilon^2 - 1}{8\pi\epsilon^2} \qquad \beta_b = -\frac{(\epsilon - 1)^2}{8\pi\epsilon^2}$$

$$\beta_c = -\frac{\epsilon - 1}{8\pi\epsilon} \qquad \beta_{\rm elstr} = +\frac{\epsilon - 1}{8\pi\epsilon^2}$$

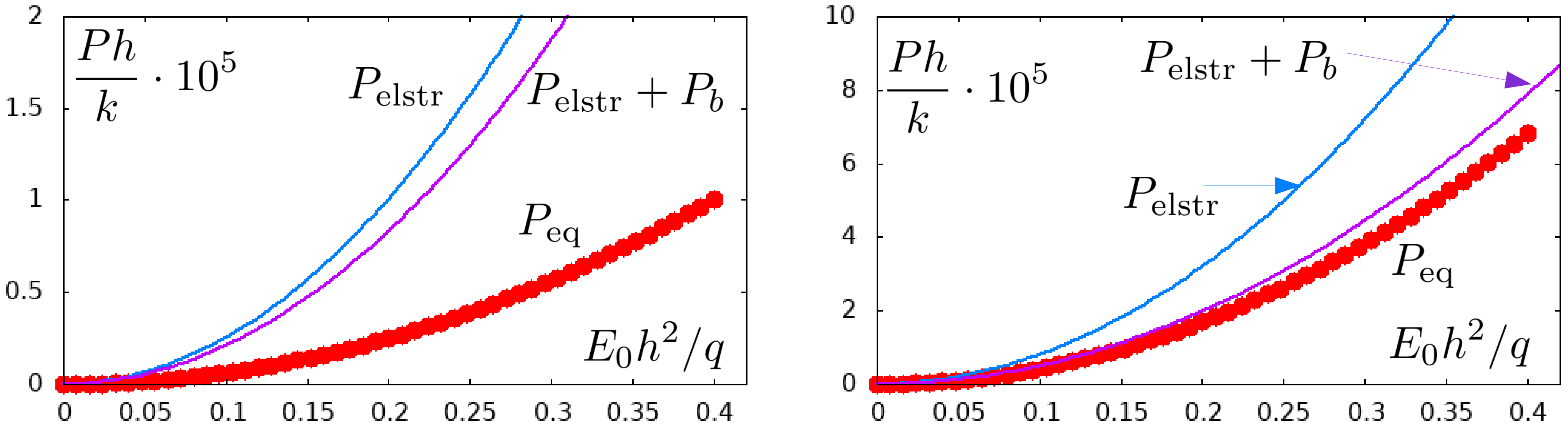
Dimensionless Young's modulus. We have already computed it.

Dimensionless Form

$$\frac{P_{\rm eq} h}{k} = \frac{\mu h}{k}\left(1 - \frac{L(E_0)}{L(E_0 = 0)}\right) \qquad \frac{P_{\rm th} h}{k} = \kappa \beta \mathcal{E}^2 \qquad \mathcal{E} = \frac{E_0 h^2}{q}$$

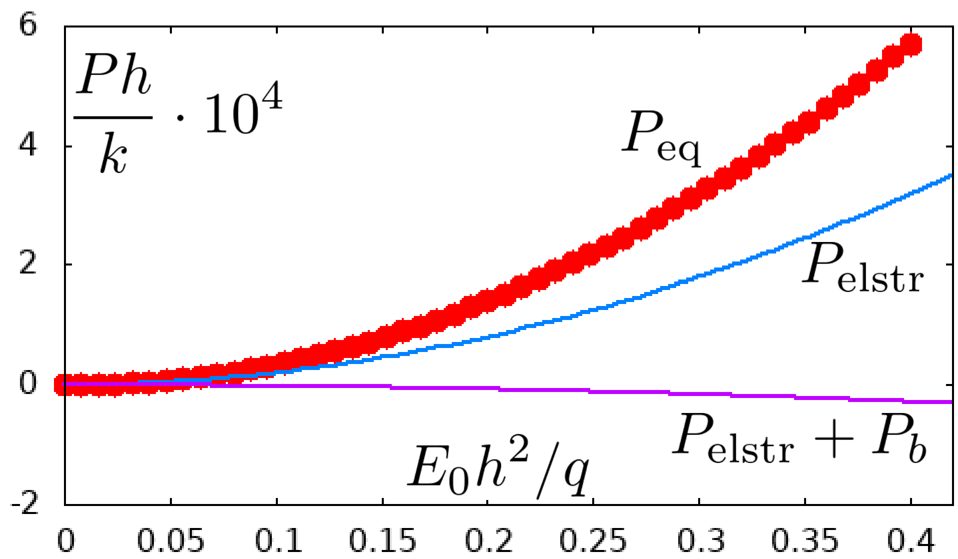
Comparing Pressures with Approximate Electrostriction (Cont., Data for N=150)

$\kappa = 0.05,\ \mu h/k = 0.9915,\ \epsilon = 1.174$ $\qquad$ $\kappa = 0.1,\ \mu h/k = 0.818\ \epsilon = 1.383$



System of many nonlinear equations, can be solved by relaxation

$\kappa = 0.2,\ \mu h/k = 0.575\ \epsilon = 2.088$



Rigorous Derivative in the Electrostriction Term

$$\mathbf{f}_{\text{elstr}} = \frac{1}{8\pi}\nabla\left[E^2\rho\left(\frac{\partial\epsilon}{\partial\rho}\right)_T\right]$$ ← Basic definition

We have used so far:

$$\epsilon = 1 + \beta\rho \quad \Rightarrow \quad \mathbf{f}_{\text{elstr}} = \nabla\left[\frac{\epsilon - 1}{8\pi}E^2\right]$$ ← Approximation, which is really applicable to gaseous media, and beyond that it is dubious

We can try to compute the derivative numerically by applying external pressure and changing the slab width, *L*

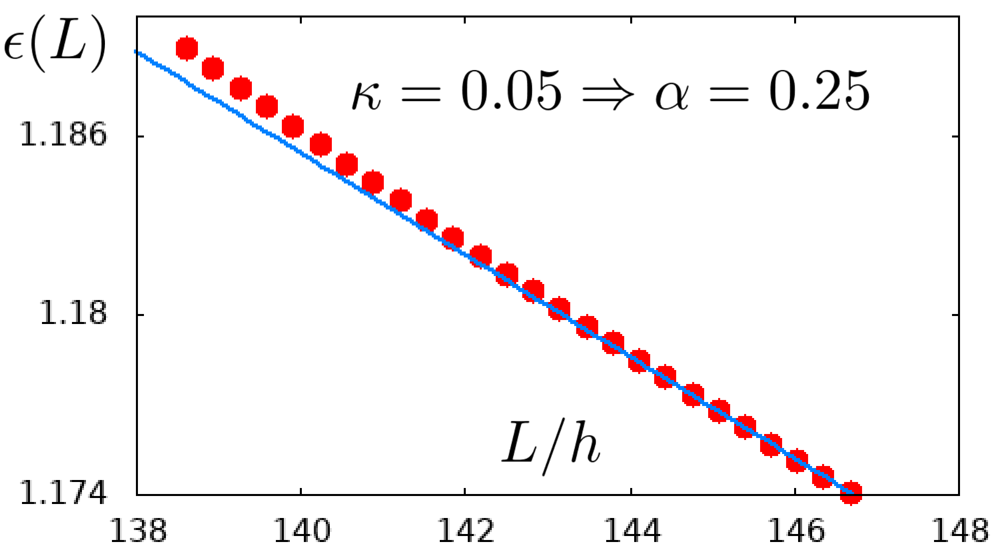
$$\rho = \rho_0\frac{L_0}{L} \quad \Rightarrow \quad \alpha \equiv \rho\frac{\partial\epsilon}{\partial\rho} = -L\frac{\partial\epsilon}{\partial L} \quad \Rightarrow \quad \beta_{\text{elstr}} = +\frac{\alpha}{8\pi\epsilon^2}$$

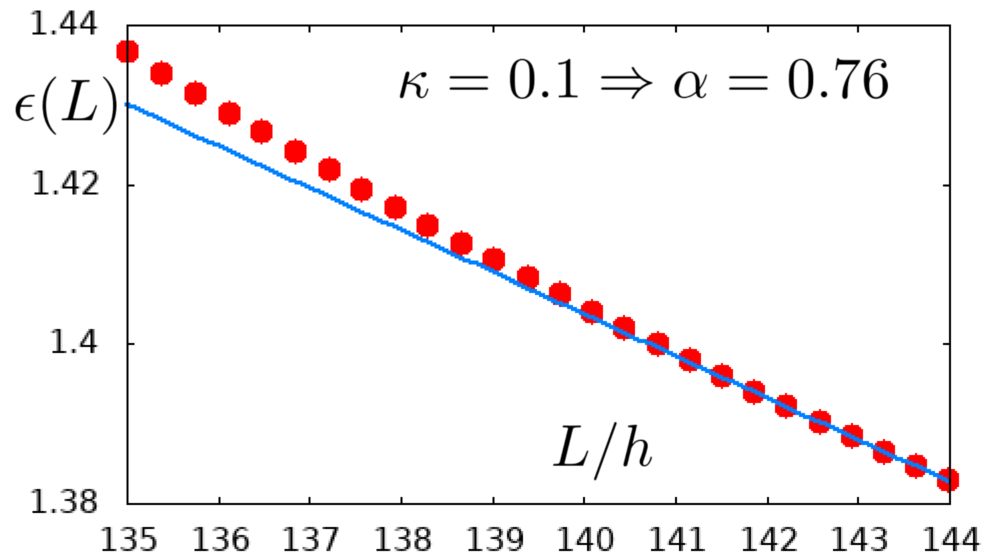
L_0 → Equilibrium width at zero pressure and zero field

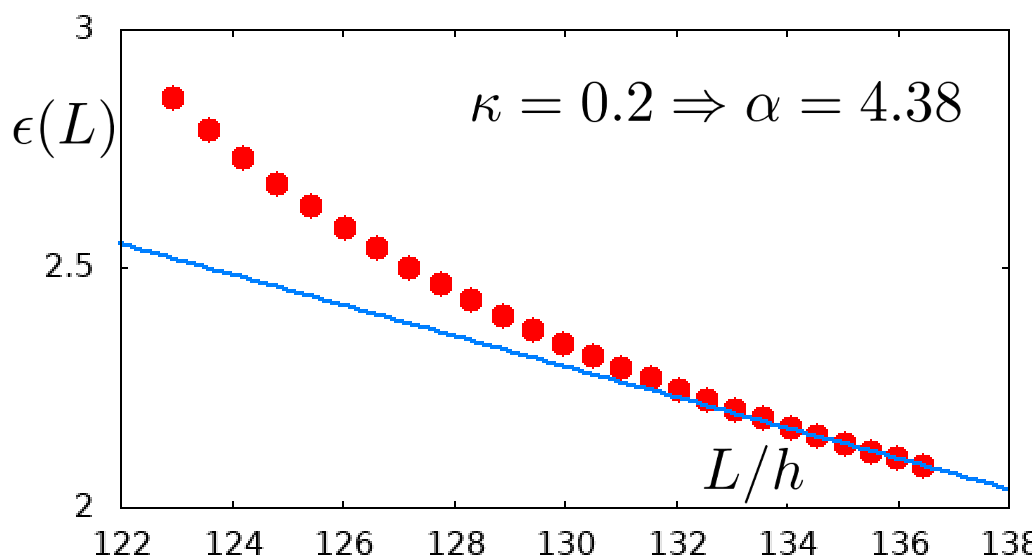
L → Equilibrium width at non-zero pressure and zero field

Computing the Derivative by Changing External Pressure and thus Changing L

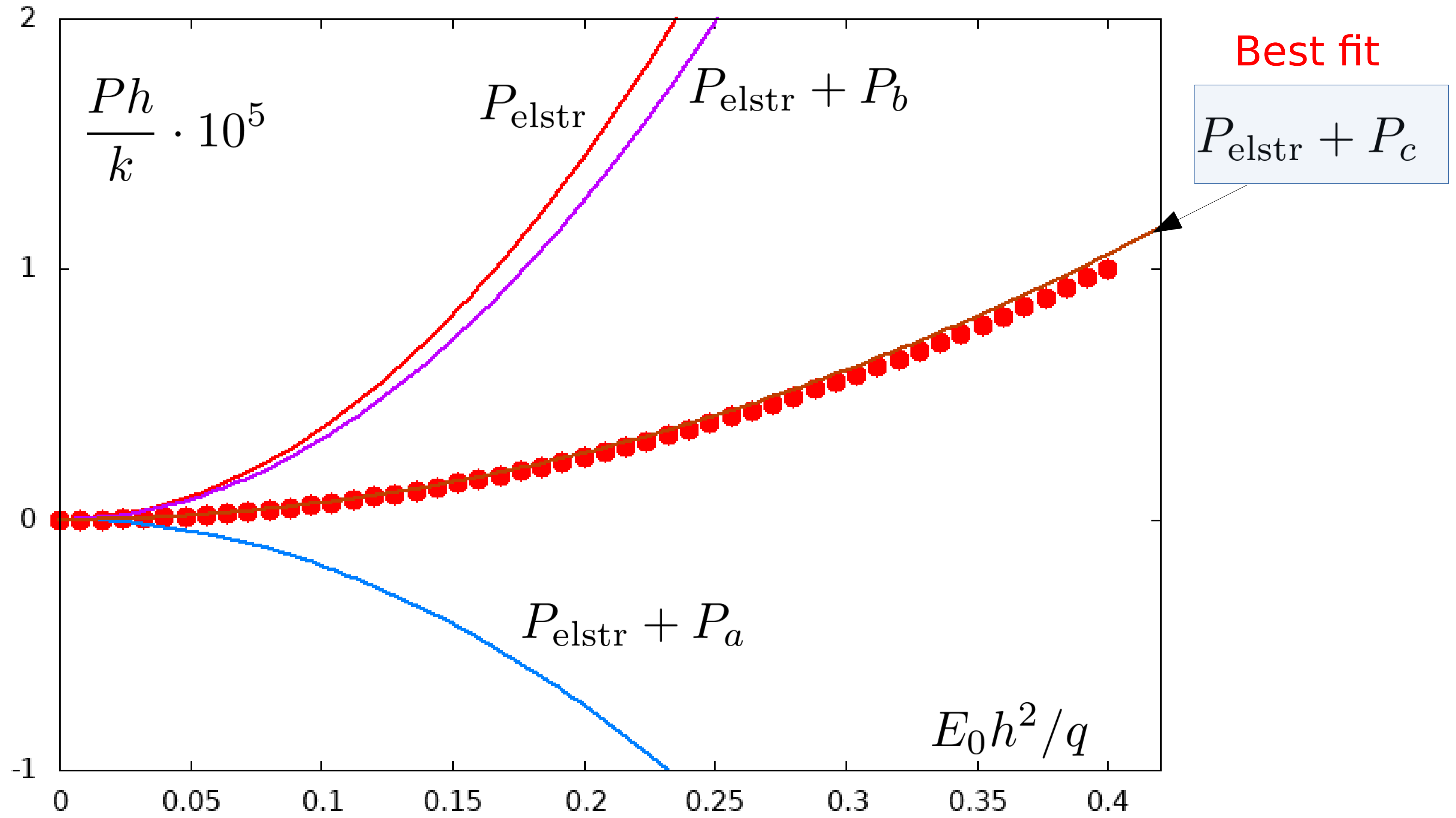
$$\alpha = -L\frac{\partial \epsilon}{\partial L}$$



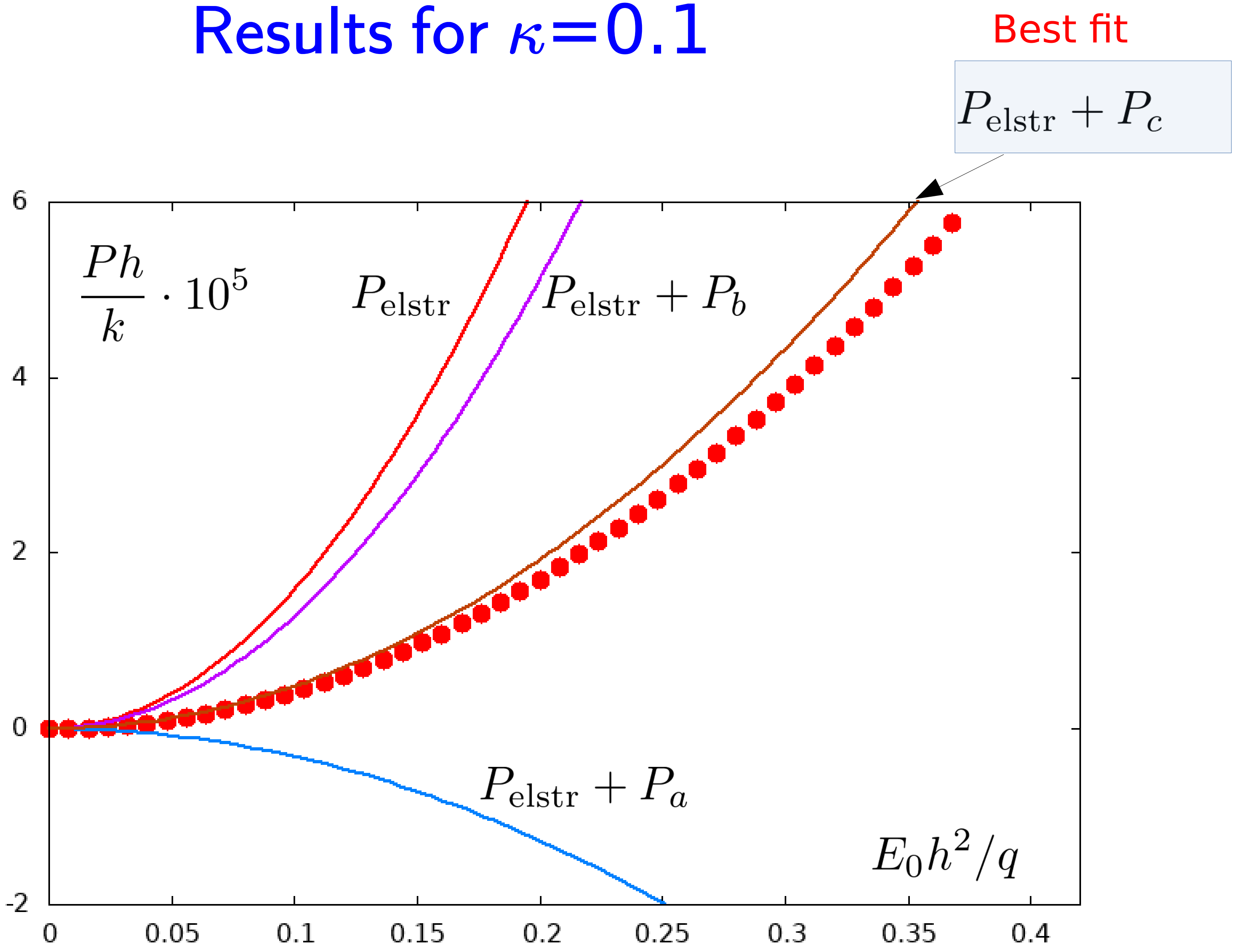




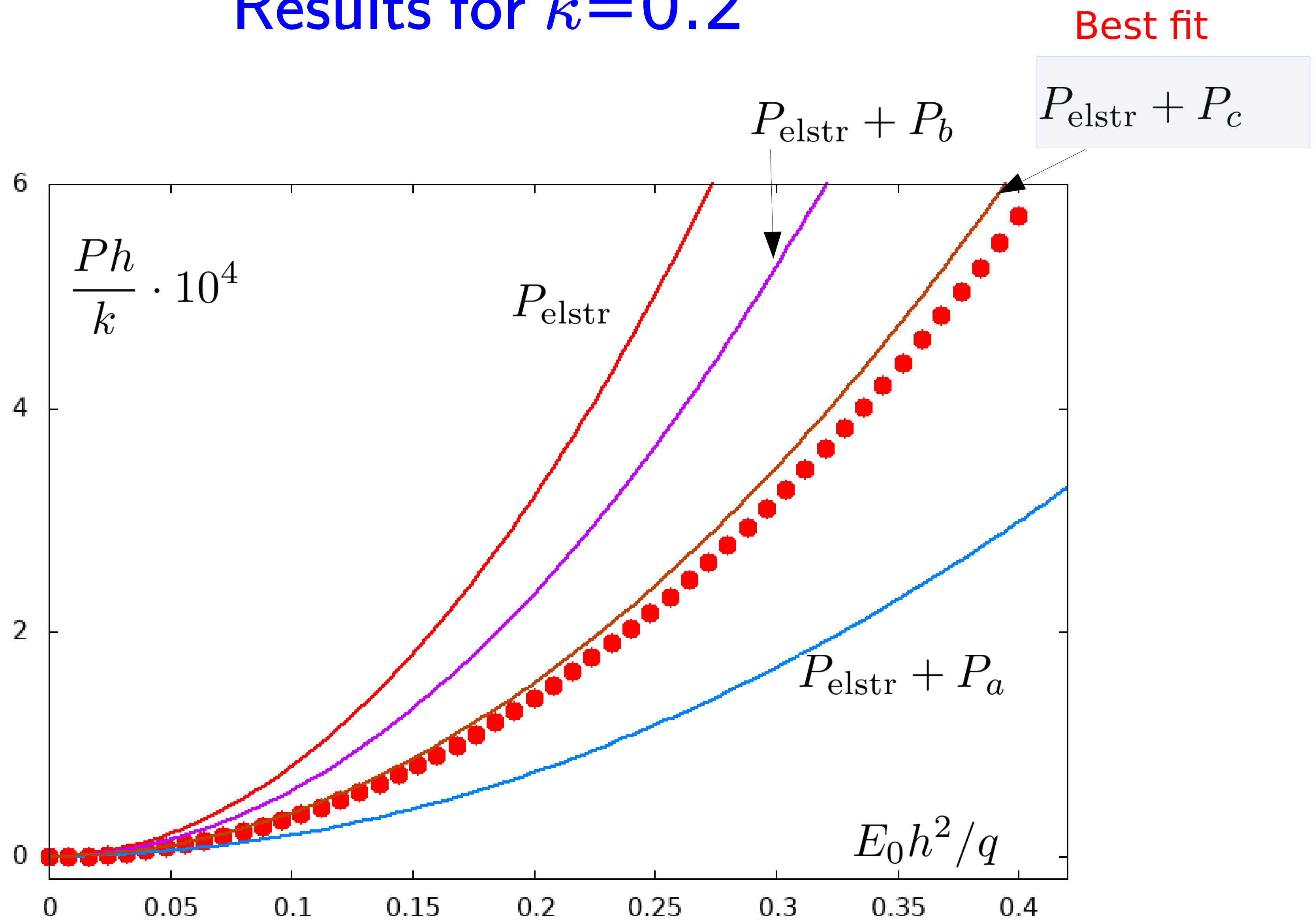
Results for κ=0.05



Results for κ=0.1



Results for κ=0.2



CONCLUSIONS

- The model considered is most consistent with the following force density:

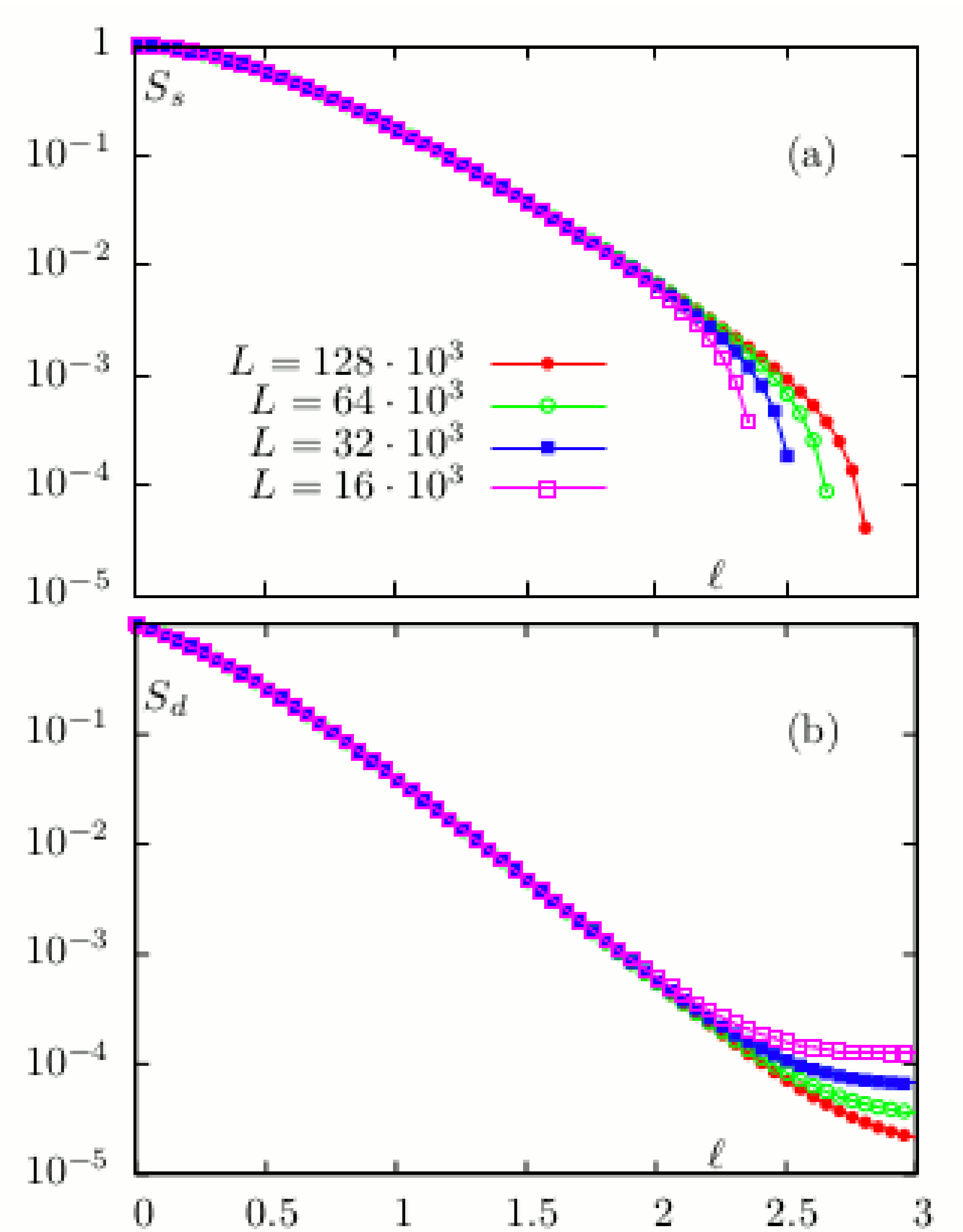
$$\mathbf{f}_c + \mathbf{f}_{\text{elstr}} = -\frac{\nabla\epsilon}{8\pi}E^2 + \frac{1}{8\pi}\nabla\left[\alpha E^2\right] \quad \text{where} \quad \alpha = \rho\left(\frac{\partial\epsilon}{\partial\rho}\right)_T$$

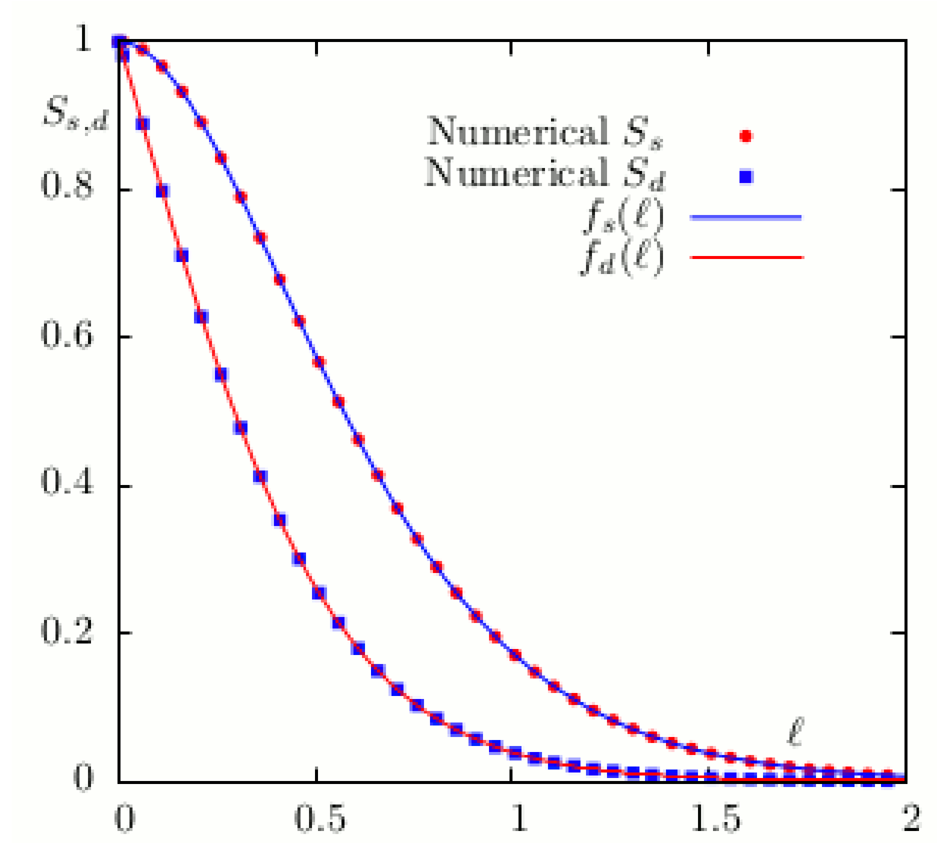
- This force is only reduced to $\mathbf{f}_b$ under several assumptions, the strongest of which is that the medium is gaseous with $\alpha = \epsilon - 1$. The model used suggests $\alpha \neq \epsilon - 1$. But in this case a tangential electric field will create normal pressure on a flat surface, which seems to be nonsensical. It is difficult to verify this prediction numerically.
- It's always contraction, so account of electrostriction is essential
- Electrostatic interaction of sub-layers is essential. Without it, the slab width is independent of external field and the predicted pressure is zero

A Few Additional Remarks

- The model is not easy to generalize beyond statics
- Not clear how this will work in other types of media (electronic polarization, liquids, etc.) Generalizations are dubious
- Computation of derivatives is hard. May be this explains imperfect fit of theoretical and computed pressures
- More generally, there are many numerical issues at play. Finding equilibrium by iterative relaxation is very tricky (there are many instabilities). But I verified the solution almost with the machine precision
- We disregarded the side surfaces. But surface effects can propagate deep into the bulk of a crystal
- It is not easy to verify results for tangential field because this requires consideration of shapes that are finite in all directions such as a truncated cylinder
- This work is not finished . . .

Appendix: Electrostatic Forces





$$f_s(\ell) = \frac{1 + (p - a_1)\ell}{1 - a_1\ell + a_2\ell^2 - a_3\ell^3 + a_4\ell^4} e^{-p\ell}$$

$$f_d(\ell) = \frac{1 + (q - A)\ell + r\ell^2}{1 + b_2\ell^2 + b_3\ell^3 + b_4\ell^4} e^{-q\ell}$$