

Supporting information to the article A self-consistent mean-field model for polyelectrolyte gels

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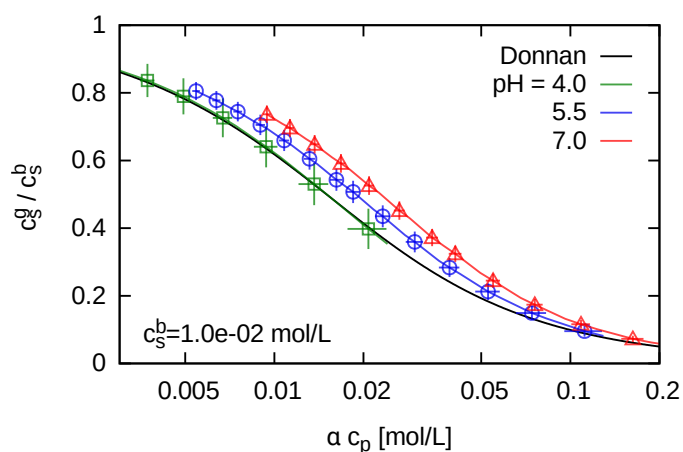


Figure 1. The average salinity inside the weak gels as a function of the charge density of the gel, αc_p , for different pH values. Solid curve is the Donnan prediction.

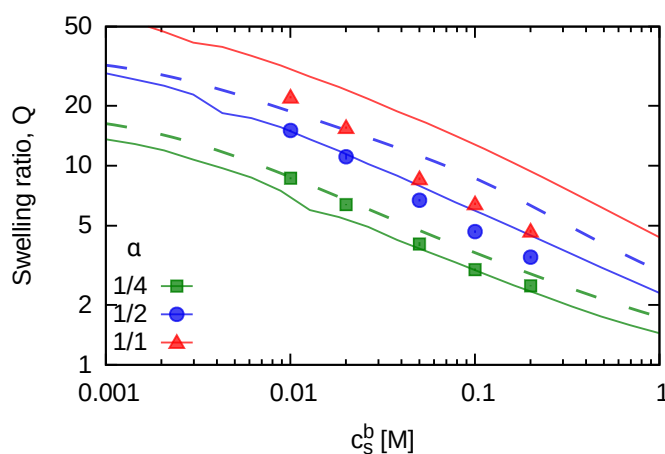


Figure 2. The equilibrium swelling ratio of the strong gels as a function of salt concentration in the bulk, c_s^b . The dashed curves represent the analytical model, solid curves the mean-field model and data points are simulation results. The kinks on the mean-field curves are discretization artifacts.

A. Density profiles from simulations and SF-SCF

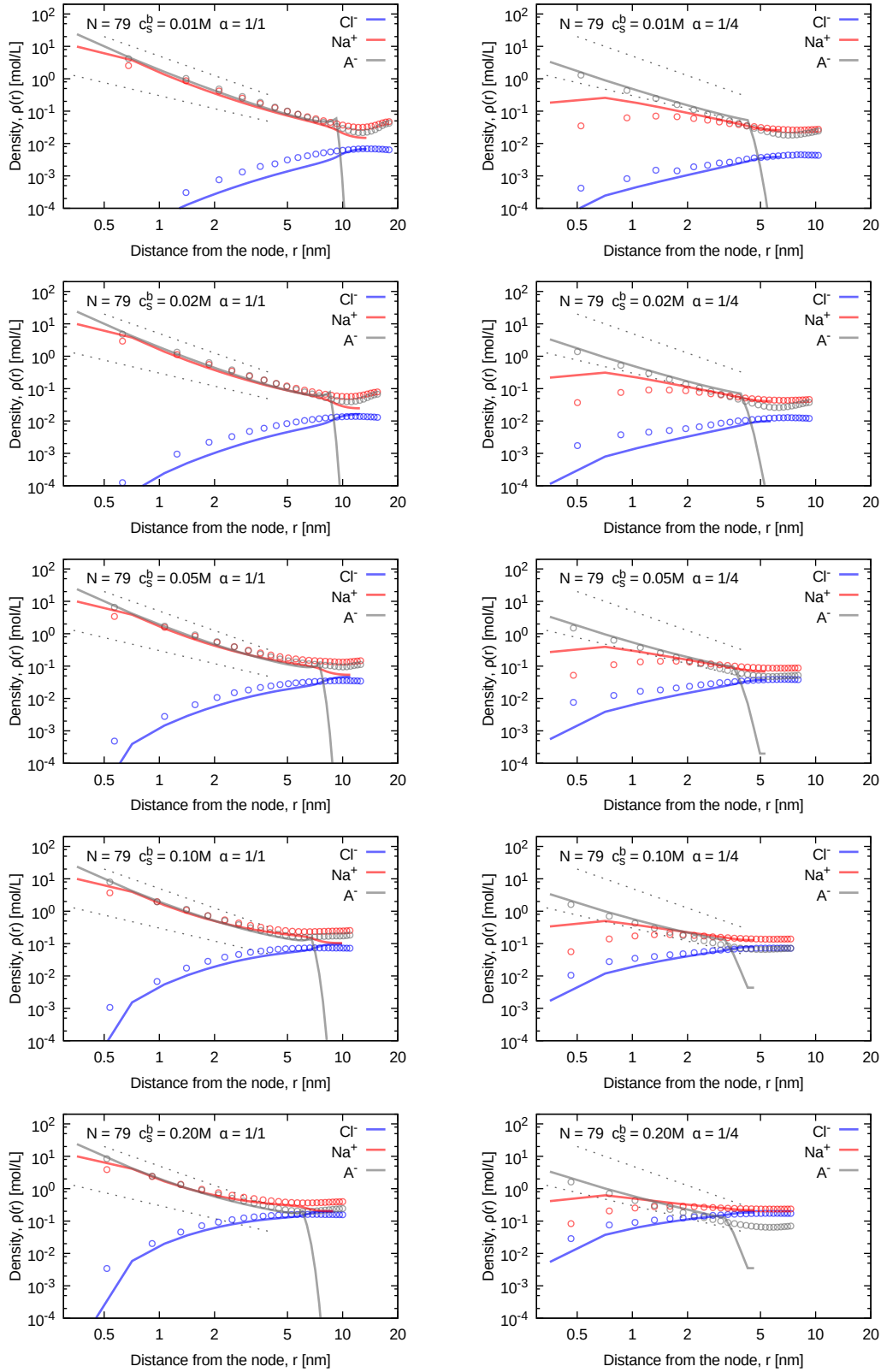


Figure 3. Density profiles from simulations (points) and from the SF-SCF method (lines) at various salt concentrations, and two representative ionization degrees: $\alpha = 1$ (left), and $\alpha = 1/4$ (right). Different particle types (monomers, counterions, coions) are distinguished by colour. The two gray lines with slopes $-4/3$ (lower one) and -2 (upper one) show the scaling prediction for the neutral star and highly charged star, respectively.

B. The Pressure-extension curves

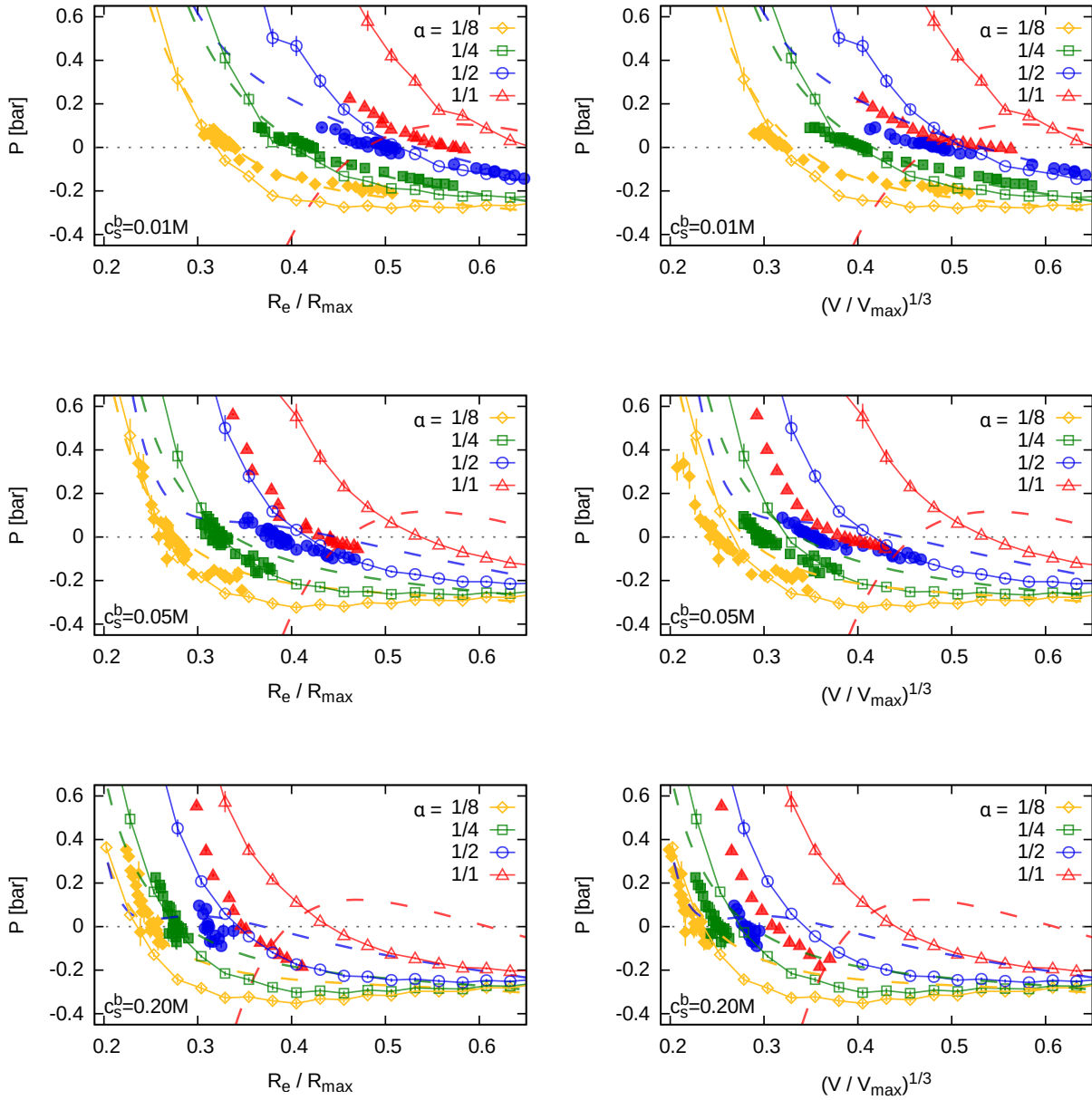


Figure 4. The pressure-extension curves, where each plot represents a fixed salt content and different degrees of ionization. The salt content increases from top to bottom. The empty points connected with lines represent the SF-SCF results. Full points of matching colour and shape are the corresponding simulation results. Dashed lines of matching colour are the corresponding predictions of the modified model of Katchalsky and Michaeli [1, 2]. Plots in the left column use R_e measured from the simulations, while the right column uses the gel volume, V . The values of $(V/V_{\max})^3$ from the SF-SCF and from the analytical model were obtained with the assumption of affine deformation. The difference between the two columns is due to the violation of the affine deformation.

C. Salinity inside and outside the gel versus molar volume of the gel

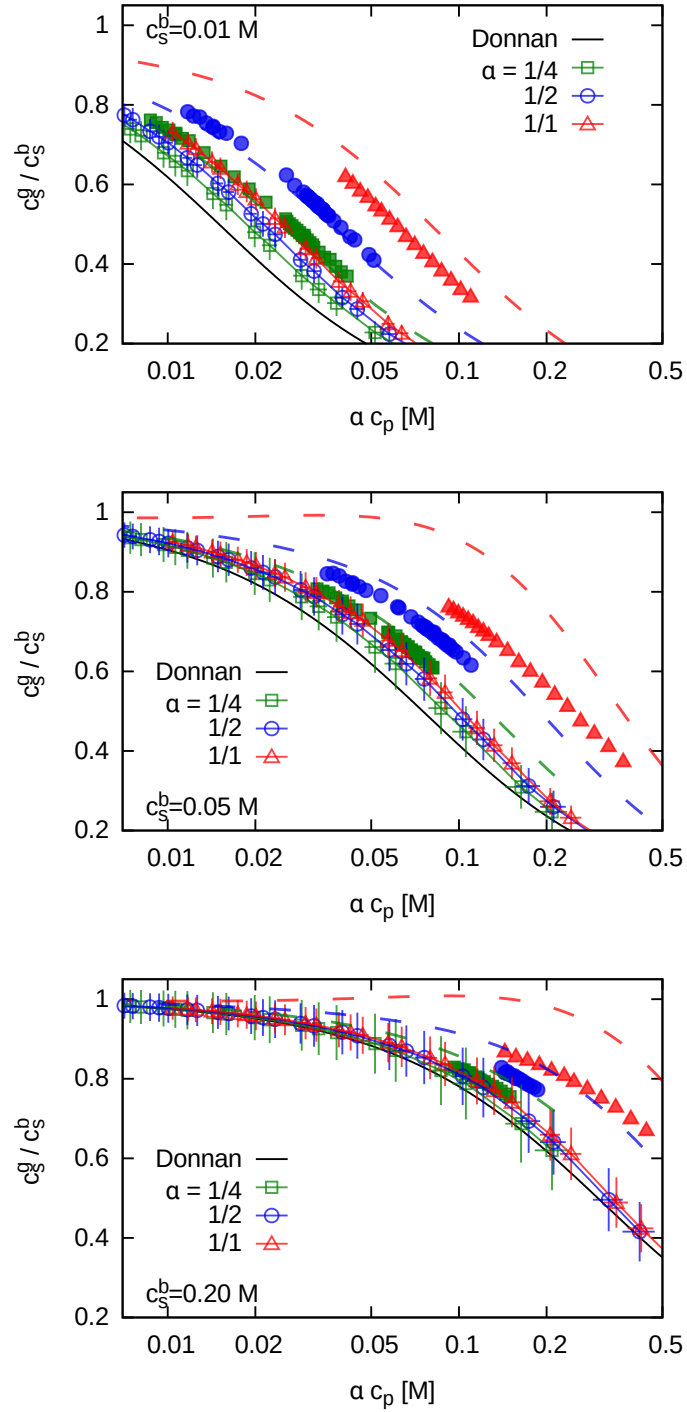


Figure 5. The ratio of salt concentration in the gel and salt concentration in the bulk, c_s^g/c_s^b , as a function of the total concentration of charged groups in the gel, αc_p , of the gel with strand length $N = 79$. Each panel includes three degrees of ionization indicated in the legend. The different panels correspond to different salt concentrations in the bulk.

D. Density profiles of weak gels

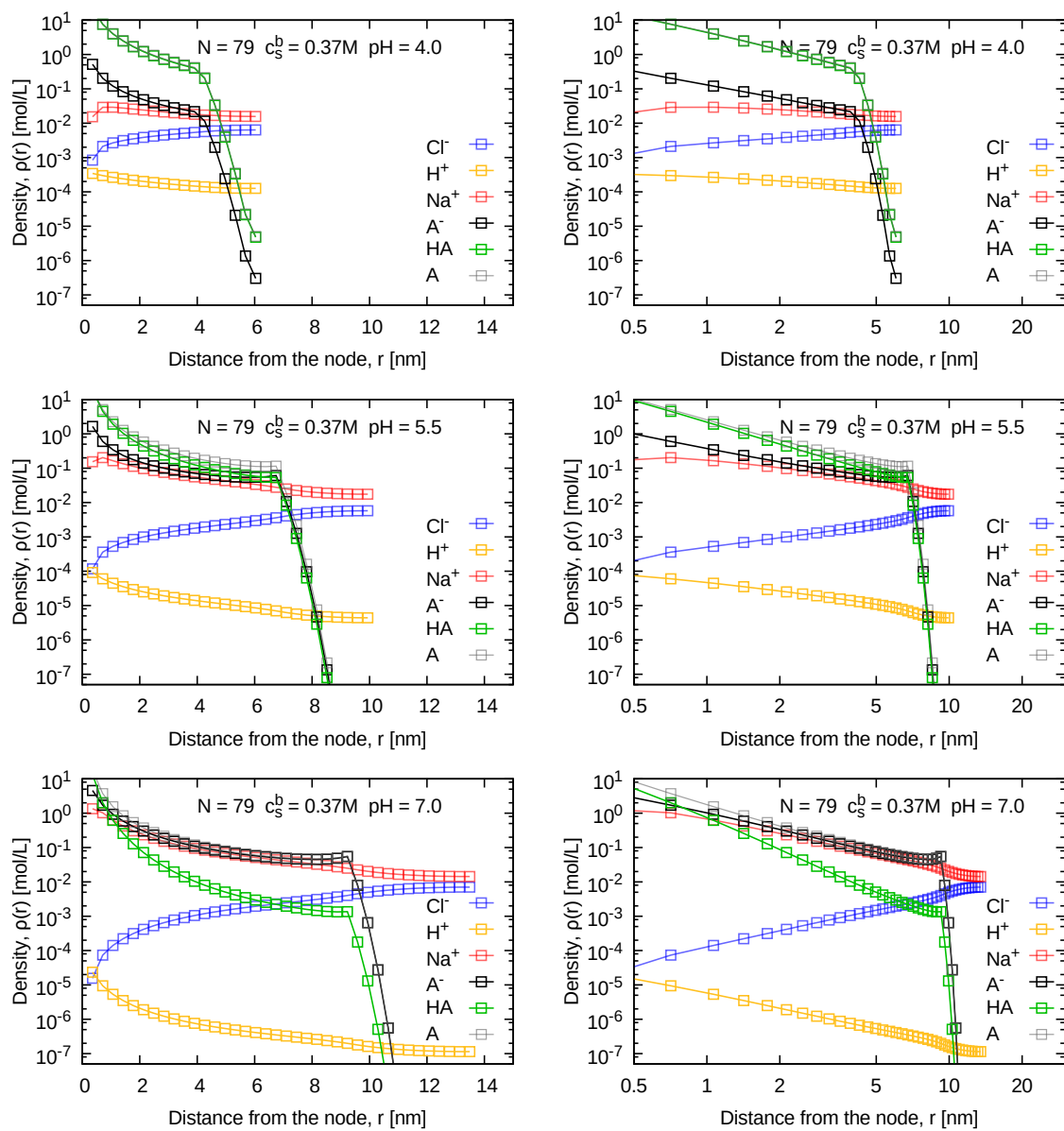


Figure 6. Density profiles of weak polyelectrolyte gels at selected pH values in semilogarithmic (left) and logarithmic representation (right). The symbols denote polymer segments A, their deprotonated form, A^- , protonated form HA, counterions Na^+ , co-ions Cl^- , and protons H^+ .

E. Mean-field predictions for neutral gels

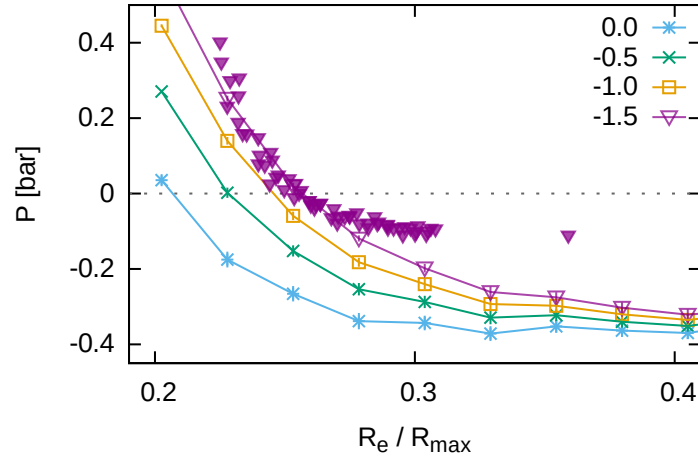


Figure 7. The pressure-extension curves for neutral gels from the mean-field model (points connected with lines) at different values of χ indicated in the caption, compared to the simulation data for the neutral gel (data points). Qualitatively, the mean-field predictions agree with the simulations for any value of χ . By tuning the χ parameter, the mean-field model can be calibrated to yield quantitative agreement with the simulation data close to free swelling equilibrium and under compression $P_{\text{ext}} \gtrsim 0$.

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- [1] Katchalsky, A. and Michaeli, I. (1955). Polyelectrolyte gels in salt solutions. *Journal of Polymer Science*, 15:69.
 [2] Kořovan, P., Richter, T., and Holm, C. (2015). Modeling of polyelectrolyte gels in equilibrium with salt solutions. *Macromolecules*, 48(20):7698–7708.