(I) Saltation energy of a charged sphere

Here we refer energy of interaction between equilibrated mobile ions and permanent charges of the solute as "saltation energy". In case of a charged sphere one can calculate the energy of interaction between the charged sphere and surrounding ions using Eqn. 5.

$$I_B = \frac{e_c^2}{(4\pi\epsilon_0\epsilon_{ext}k_BT)} \quad (1)$$

$$\kappa^{-1} = \sqrt{\left(\frac{\epsilon_0\epsilon_{ext}k_BT}{2\times10^3 N_A e_c^2}\right)} \quad (2)$$

$$\Delta G_{nz}([salt], R) = \frac{1}{2}k_BT\left(\frac{Q}{e_c}\right)^2 \frac{I_B\kappa^{-1}}{R(R+\kappa^{-1})} \quad (3)$$

$$\Delta G_z([salt], R) = \frac{1}{2}k_BT\left(\frac{Q}{e_c}\right)^2 \frac{I_B}{R} \quad (4)$$

$$\Delta\Delta G_{nz}([salt]) = \Delta G_{nz}([salt], R) - \Delta G_z(R) \quad (5)$$

where I_B is Bjerrum length, c is ionic strength in M, k_B is Boltzman constant, T is absolute temperature, e_c is the electronic charge, κ^{-1} is Debye length, ε_0 is the electric permititivity of free space, ε_{ext} is the external dielectric constant of the medium, R is the radius of charged sphere, ΔG_{nz} ([salt], R) is electrical energy of charged sphere in solvent with salt, $\Delta G_z(R)$ is the electrical energy of charged sphere in solvent without salt, $\Delta\Delta G_{nz}$ ([salt]) is the saltation energy of charged sphere. Thus, using the following parameters R=10 Å, internal and external dielectric constants 1 and 80, respectively, and varying salt concentration from 0.02 M until 0.2 M, the analytical and numerical (using DelPhi) solutions are calculated and plotted against logarithm of salt concentration (Figure 1). For example, with salt concentration 0.02 M and external dielectric constant 80 the analytical and numerical (using DelPhi) solutions for the saltation energy of the charged sphere are -2.77 kT and -2.92 kT, respectively.

These calculations are done by using prepared files in the folder `Example_3.1.2/Ex1/`. To run these examples on your own machine, execute python script Run-saltation-charged-sphere.py as:

```
python3 Run-saltation-charged-sphere.py
```

On Running this script, the above mentioned analytical and DelPhi calculations are performed and plot (`plot-salt-ele-sphere.png`) and csv(`saltation_charged_sphere.csv`) file

containing results are created. As is shown in the Figure 1, the calculated “saltation energy” is in excellent agreement with the analytical solution.

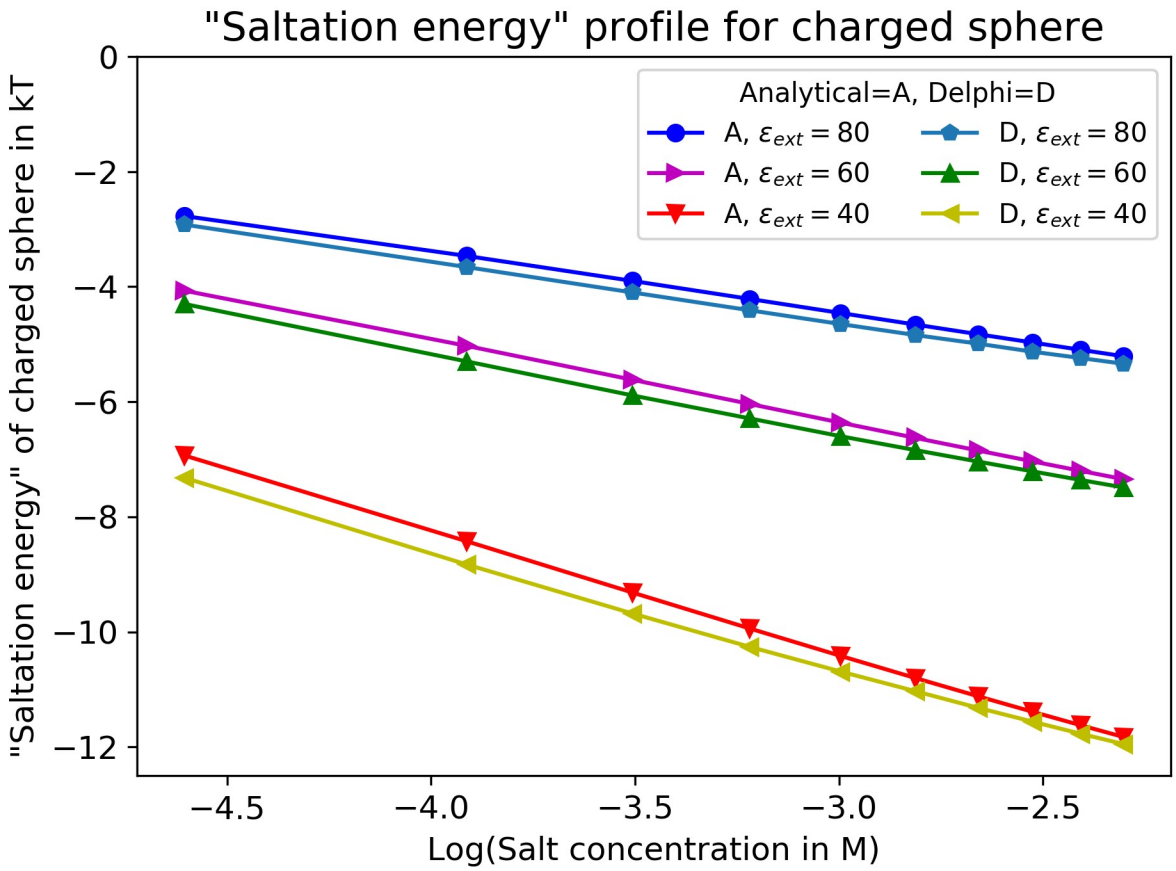

Figure 1: Analytical and DelPhi result for the saltation energy of the charged sphere in different salt concentration and different external dielectric constants.