Two treatments within particle-based simulations for modeling a charged surface are using explicit, discrete charges and continuous, uniform charges. The computational cost can be substantially reduced if, instead of explicit surface charges, one uses an electric field to describe continuous surface charges. In addition, many electrolyte theories, including the Poisson–Boltzmann theory, are developed on the assumption of uniform surface charges \[1\]. However, recent simulations have demonstrated that with discrete surface charges, when the lattice constant becomes notably larger than the charge diameter, one observes much stronger charge reversal, compared to the surfaces with continuous charges \[2–5\]. These examples show that the two treatments for modeling a charged dielectric interface can lead to substantially different results. In this note, we calculate the electrostatic force for a single charge above an infinite plate, and compare the differences between discrete and continuous representations of surface charges.

We consider a charged, planar substrate located at \(z = 0\) and a test charge with valence \(q\) (\(q > 0\)) located at \((\delta_x l, \delta_y l, z)\) where \(z > 0\), and without loss of generality, \(\delta_x \in [0, 1/2]\) and \(\delta_y \in [0, 1/2]\). A schematic of the discrete charged surface is presented in Fig. 1. The surface charges are distributed uniformly, forming a 2D-square lattice with a spacing constant \(l\). The interface carries a uniform charge density \(\sigma\) (\(\sigma < 0\)), so that each surface bead carries a charge of \(\sigma l^2\). The interface is also characterized by a dielectric contrast \(\Delta = (\varepsilon_{\text{sol}} - \varepsilon_{\text{sub}})/(\varepsilon_{\text{sol}} + \varepsilon_{\text{sub}})\), where \(\varepsilon_{\text{sol}}\) and \(\varepsilon_{\text{sub}}\) correspond to the dielectric permittivity of solvent medium and substrate, respectively. This produces images of the surface charges which overlap with themselves, such that the effective surface charge of each bead is \((1 + \Delta)\sigma l^2\).

**FIG. 1:** Schematic of a point charge located above a charged, dielectric interfaces. (a) The surface is characterized by a charge density \(\sigma\) and an lattice spacing \(l\) on an infinite square lattice. (b) The red and purple spheres above the plate represent test charge and surface charges, respectively, for the situation of \(\varepsilon_{\text{sub}} < \varepsilon_{\text{sol}}\). Their image charges with the magnitude weakened by \(\Delta\) (see text for definitions) are also sketched.
The electrostatic energy $U_s$ between the test charge and the substrate is expressed as

$$
\beta U_s(z) = \sum_{n_x=-\infty}^{\infty} \sum_{n_y=-\infty}^{\infty} \frac{(1 + \Delta)(2\pi\mu)^{-1}}{\sqrt{(n_x l - \delta_x l)^2 + (n_y l - \delta_y l)^2 + z^2}},
$$

where $\beta$ is the Boltzmann factor, $\mu = (2\pi q l_B |\sigma|)^{-1}$ the Gouy–Chapman length, and $l_B$ the Bjerrum length. From $\beta U_s(z)$, we derive the corresponding electrostatic force $\beta F_s(z)$, which is

$$
\beta F_s(z) = -\frac{\partial(\beta U_s)}{\partial z} = \sum_{n_x=-\infty}^{\infty} \sum_{n_y=-\infty}^{\infty} \frac{(1 + \Delta)(2\pi\mu)^{-1}}{(n_x - \delta_x)^2 + (n_y - \delta_y)^2 + (z/l)^2\frac{3}{2}}.
$$

When $l \ll z$, $\beta F_s(z)$ can be approximated by a 2D-integral,

$$
\beta F_s(z) \simeq \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy \frac{(1 + \Delta)q\sigma l_B(z/l)}{(x^2 + y^2 + (z/l)^2)^{3/2}} = (1 + \Delta)\mu^{-1} \equiv \beta F^c_s(z),
$$

where $\beta F^c_s(z)$ represents the force of a point charge above a charged surface with an “effective” charge density of $(1 + \Delta)\sigma$ in the continuum representation.

To compare the differences of electrostatic forces in discrete and continuous model, we calculate the ratio between $F_s(z)$ and $F^c_s$,

$$
\Gamma = \frac{F_s}{F^c_s} = \sum_{n_x=-\infty}^{\infty} \sum_{n_y=-\infty}^{\infty} \frac{(2\pi)^{-1}(z/l)}{\frac{3}{2}}.
$$

Fig. 2 shows the numerical results of $\Gamma$ as a function of $z/l$ for various $\delta_x$ and $\delta_y$ values. We are particularly interested in the region where $z/l \ll 1$. When $\delta_x = \delta_y = 0$, $\gamma$ is dominant by the $n_x = n_y = 0$ term, and diverges as $(2\pi)^{-1}(z/l)^{-2}$.

Clearly, as $z/l \ll 1$, the electrostatic force of a point charge near the discretely charged interface can become significantly larger compared to that of the continuum model, meaning discretely charged pattern enhances the ion–surface correlation. This provides an intuitive understanding of stronger charge reversal in the model of discrete surface charges.
When $\delta_x$ and $\delta_y$ are nonzero, the numerical data suggests that the lateral ion distribution should be different in the two models. For discretely charged surfaces with a large lattice spacing, the surface counterions are mainly trapped near the surface charges. However, for the continuous model, the lateral distribution is uniform. This argument has been confirmed by simulations where they observe strong counterion binding (or localization) around the surface charged groups [2, 4].

In addition, the test point charge also interacts with its own image, leading to the force $\beta F_i$ expressed as

$$\beta F_i(z) = \Delta \frac{q^2 B \mu}{4 \pi^2}. \quad (5)$$

To compare the relative magnitude between ion-surface interaction and self-image interaction, in Fig. 3 we plot the absolute dimensionless force $|F_i|/F_s$ in comparison with $F_s/F_s$, or in other words, we choose to use $|F_s|$ as the characteristic force scale. It follows that

$$\frac{|F_i|}{F_s} = \frac{|\Delta|}{1 + \Delta} \frac{q^2 B \mu}{4 \pi^2} = \frac{|\Delta|}{1 + \Delta} \frac{q^2 B \mu}{4 \pi^2} (z/l)^{-2} = K (z/l)^{-2}, \quad (6)$$

where the dimensionless number $K$ is introduced to denote the strength of self-image interactions:

$$K = \frac{|\Delta|}{1 + \Delta} \frac{q^2 B \mu}{4 \pi^2}. \quad (7)$$

Compared to the asymptotic behavior of Eq. (4) when $\delta_x = \delta_y = 0$, we find a critical coupling of

$$K^* = (2\pi)^{−1}. \quad (8)$$

For strong coupling $K \gg K^*$, the self-image interaction is dominant compared to the ion-surface interaction for a wide range of $z/l$, whereas for weak coupling $K \ll K^*$, the relative strength between self-image interaction and ion-surface interaction depends on the position $z/l$. Obviously, at the far field $z/l \gg 1$, the ion-surface interaction is always the dominant one.

Considering the overall interaction between a test charge and the charged dielectric interface, Fig. 3 shows that while the continuous, uniform surface charge model gives a quite simple picture, the discrete surface charge model can offer a range of different cases (even for such a simple problem!) depending on the values of $z/l$ and $K$.

The finite size of the surface ionic groups and that of the counterions sets a lower bound of $z$ close to the surface. Let $a$ be diameter of the surface ionic groups and that of the counterions. The two treatments for modeling a charged dielectric interface can indeed lead to substantially different results for $a/l \ll 1$ ($l$ is the large lattice spacing), especially when $K \ll K^*$ (weak self-image coupling) as well.
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