Random batch Quasi-Ewald method for the simulations of charged particles under dielectric confinement (arXiv: 2207.04687)

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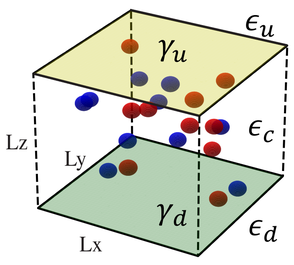
Abstract

We derive an analytic, fast convergent lattice summation formula for the interaction energy/force of dielectric confined charged particles based on a novel Quasi-Ewald splitting strategy, then further achieving O(N) scaling for N-particle simulations via random batch importance sampling in the reciprocal space. The singularity in the analytical expression is carefully renormalized, thus extending our method to the case of metamaterials confinement, characterized by negative permittivity values.

An open-source package **QuasiEwald.jl** is published.

Dielectric Confined Quasi-2D Charged Systems

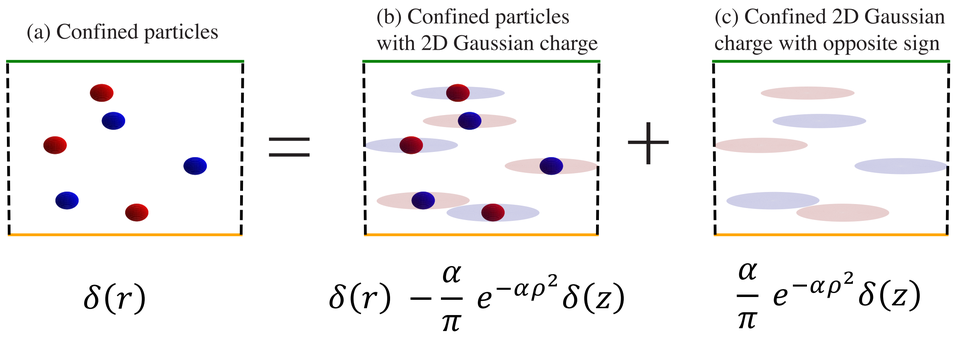


- Red/blue spheres represent cations/anions;
- Yellow/green planes represent upper/lower boundary with dielectric mismatches;
- $\epsilon_u/\epsilon_c/\epsilon_d$ represent the piece-wise dielectric constants of the upper/central/lower region $\Omega_u/\Omega_c/\Omega_d$;
- γ_u/γ_d represent the reflection rate of the upper/lower substrates.

$$\begin{cases} -\nabla_{\boldsymbol{r}}\left[\epsilon(\boldsymbol{r})\nabla_{\boldsymbol{r}}G(\boldsymbol{r},\ \boldsymbol{r}_0)\right] = \delta(\boldsymbol{r}-\boldsymbol{r}_0) & r \in \mathbb{R}^3\ , \\ G(\boldsymbol{r},\ \boldsymbol{r}_0)|_- = G(\boldsymbol{r},\ \boldsymbol{r}_0)|_+ & \text{on } \partial\Omega_c\ , \\ \epsilon_c\partial_z G(\boldsymbol{r},\ \boldsymbol{r}_0)|_- = \epsilon_u\partial_z G(\boldsymbol{r},\ \boldsymbol{r}_0)|_+ & \text{on } \partial\Omega_c \cap \partial\Omega_u\ , \\ \epsilon_c\partial_z G(\boldsymbol{r},\ \boldsymbol{r}_0)|_- = \epsilon_d\partial_z G(\boldsymbol{r},\ \boldsymbol{r}_0)|_+ & \text{on } \partial\Omega_c \cap \partial\Omega_d\ , \\ G(\boldsymbol{r},\ \boldsymbol{r}_0) \to 0 & \text{as } r \to \infty\ . \end{cases}$$

Quasi-Ewald Splitting

We develop **a novel splitting strategy** to handle the long-range electrostatic interaction in Quasi-2D systems:



The splitted Green's functions:

$$G_1(r,r') = -\sum_m \int_0^\infty 2k\ g(k,z,z')\left[1 - \exp\left(-\frac{k^2}{4\alpha}\right)\right] J_0(k\rho)\ dk\ .$$

$$G_2(r,r') = -\frac{4\pi}{L_x L_y}\sum_k g(k,z,z')\exp\left(-\frac{k^2}{4\alpha} - ik\rho\right)\ .$$

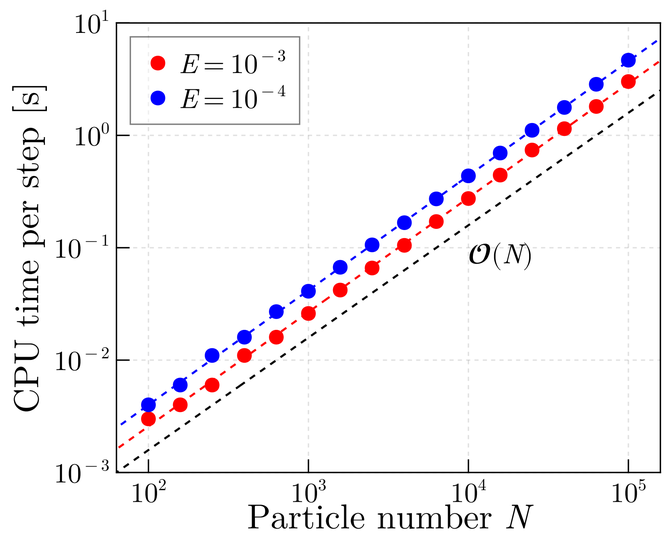
Corresponding to short-range and long-range terms, respectively.

Random Batch Sampling

The summation in the reciprocal space is estimated via **Importance Sampling**:

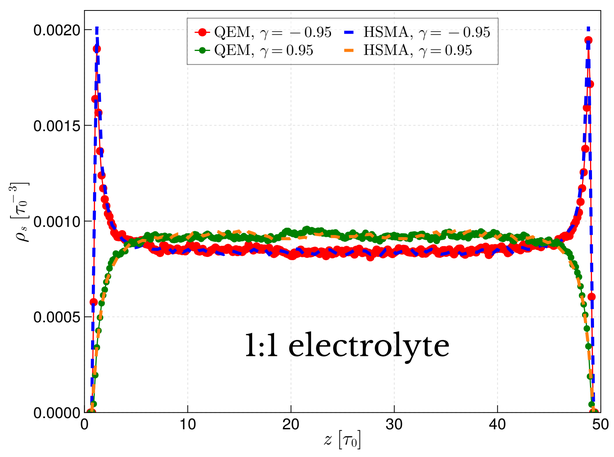
$$\sum_k f(k)e^{-\frac{k^2}{4\alpha}} \to \frac{S}{p}\sum_{k_p \in K} f(k_p)\ ,$$

where p is constant of $O(1)$ [1], which leads to a linear complexity.

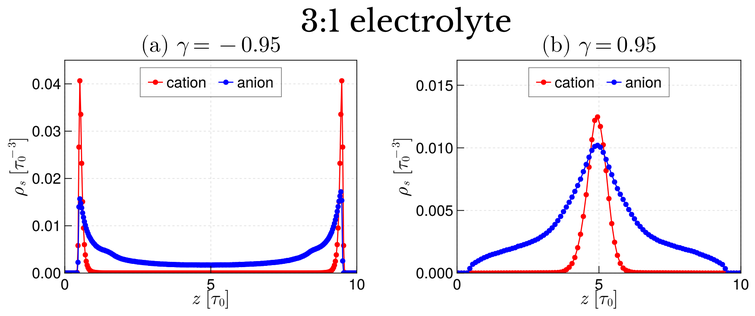


Highlights

I. Accurate Simulations for Quasi-2D Charged Particle Systems

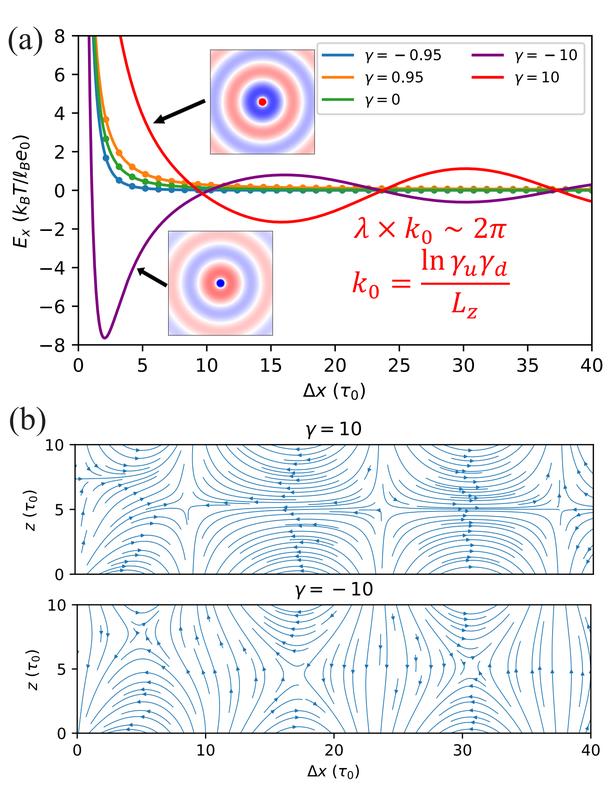


3:1 electrolyte



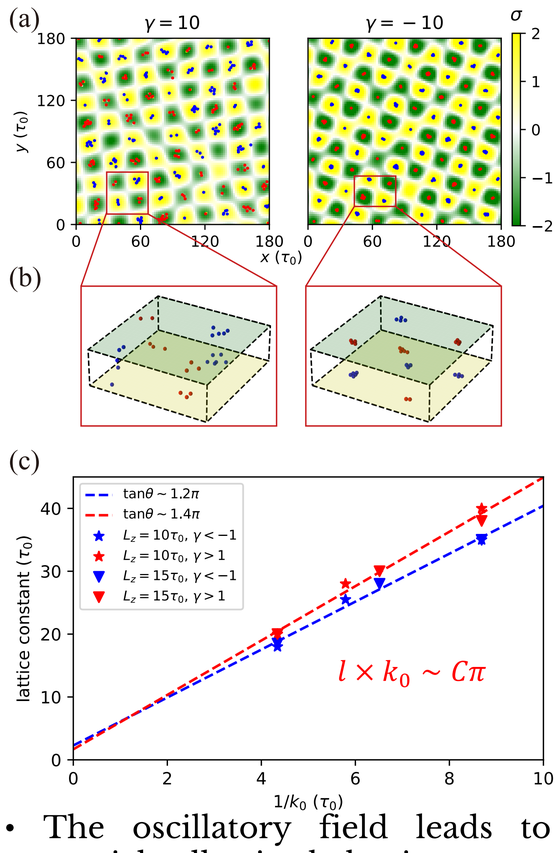
- Our method accurately reproduce the density profile of confined electrolyte [2].

II. Oscillatory Electrostatic Field via Dielectric Confinements



- Via confinement, the electrostatic field shown to be oscillatory.

III. Spontaneous Charge Oscillations and Lattice Formation



- The oscillatory field leads to special collective behavior

arXiv:2207.04687

ArrogantGao/QuasiEwald.jl

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References

[1] S. Jin, L. Li, Z. Xu, and Y. Zhao, A random batch Ewald method for particle systems with Coulomb interactions, SIAM J. Sci. Comput. 43, B937 (2021)
[2] J. Liang, J. Yuan, E. Luijten, and Z. Xu, Harmonic surface mapping algorithm for molecular dynamics simulations of particle systems with planar dielectric interfaces, J. Chem. Phys. 152, 134109 (2020).