

AN $\mathcal{O}(N)$ QUASI-EWALD SPLITTING METHOD FOR NANOCONFINED ELECTROSTATICS*

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Abstract. Simulating the dynamics of charged particles in quasi-two-dimensional (quasi-2D) nanoconfined systems presents a significant computational challenge due to the long-range nature of electrostatic interactions and the geometric anisotropy. To address this, we introduce a novel *quasi-Ewald splitting* strategy tailored for particle-based simulations in this geometry. Our splitting strategy seamlessly integrates a collection of advanced numerical techniques, including optimal quadrature rules [L. N. Trefethen, *SIAM Rev.*, 64 (2022), pp. 132–150], fast pairwise kernel summation methods [S. Jiang and L. Greengard, *Commun. Comput. Phys.*, 31 (2022), pp. 1–26], and the random batch method with importance sampling in k -space [S. Jin et al., *SIAM J. Sci. Comput.*, 43 (2021), pp. B937–B960]. The resulting algorithm achieves an $\mathcal{O}(N)$ overall computational complexity, where N denotes the total number of confined particles. Simulations of several prototype systems validate the accuracy and efficiency of our method. Furthermore, we present numerical observations specifically related to nanoconfined charged many-body systems, highlighting phenomena such as dielectric boundary effects, anisotropic diffusion, and the structure of the electrical double layer (EDL) under conditions of charge asymmetry.

Key words. molecular dynamics, charged system, nanoconfinement, sharp dielectric interfaces, random batch Ewald

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1. Introduction. In recent years, the modeling, simulation, and experimental investigation of quasi-two-dimensional (quasi-2D) systems have gained significant attention across various disciplines [6, 9, 68, 67, 28, 70, 86, 90]. Typically, such systems possess a nano-sized longitudinal thickness in the z direction, achieved through confinement; they are bulk-like and modeled as doubly periodic in the transverse xy directions, hence endowed with an inherent *multiscale* nature. Among quasi-2D systems, charged many-body systems under dielectric nanoconfinement are of particular interest to us, such as graphene [71], metal dichalcogenide monolayers [49], semiconductors, and solid-state battery systems [53]. A key observation in these systems is the *dielectric confinement effect* [34, 47], which arises from the discontinuity in dielectric properties at the boundaries and leads to distinct electrostatic screening

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behaviors. This effect plays a pivotal role in governing the properties of charged systems and has been implicated in a wide range of phenomena, including ion transport in nanochannels [1, 48, 16, 40], the structural organization of polymer brushes [92], and the pattern formation observed in confined dipolar systems [83, 24]. Despite significant advancements in simulation techniques over the past few decades, achieving accurate and efficient representations of the dielectric confinement effect remains a formidable challenge [24]. Moreover, the intrinsic multiscale nature of quasi-2D systems, combined with the long-range interactions inherent to electrostatic forces, presents profound difficulties for both theoretical modeling and numerical simulation approaches.

Linear-scaling algorithms have been extensively developed for the efficient simulation of isotropic, nonconfined N -particle systems under periodic or free-space boundary conditions. These approaches primarily follow three strategies: (1) Fourier spectral methods, (2) tree-based methods, and (3) random batch sampling methods. Fourier spectral methods combine kernel splitting with the Fast Fourier Transform (FFT) to achieve $\mathcal{O}(N \log N)$ complexity, including the Particle-Mesh Ewald (PME) [13] method and the u -series method [77]. Tree-based methods, such as the Fast Multipole Method (FMM) [31, 30, 10, 19, 27, 32, 89, 94] and the dual-space multilevel kernel-splitting (DMK) framework [39], utilize hierarchical data structures to reach $\mathcal{O}(N)$ complexity. Random batch sampling methods, such as the random batch Ewald (RBE) [46] and random batch sum-of-Gaussians (RBSOG) [61], leverage importance sampling in Fourier space to provide $\mathcal{O}(N)$ stochastic acceleration, which is particularly effective for capturing ensemble averages in molecular dynamics simulations [43, 44, 45]. While these methods are robust for isotropic Coulomb systems, quasi-2D systems with confined geometries introduce unique challenges due to reduced symmetry, necessitating either significant modifications to existing algorithms or the development of new methodologies.

Various methods have been developed to reduce the $\mathcal{O}(N^2)$ complexity inherent in quasi-2D confined systems. For systems with a homogeneous dielectric background, early contributions include the Lekner summation-based MMM2D method [2], which achieves $\mathcal{O}(N^{5/3})$ complexity. More recent developments include the Ewald3DC method [88], the spectral Ewald method [64], periodic FMMs [85, 74], SoEwald2D [22], and the fast sum-of-Gaussians method [25]. These approaches typically leverage the FFT, FMM, or random batch sampling to reach $\mathcal{O}(N \log N)$ or $\mathcal{O}(N)$ complexity. However, the requirement of a homogeneous dielectric background limits their general applicability. To address sharp dielectric interfaces, one approach involves solving for the induced charge density or surface potential through various optimization techniques [8, 82, 36, 37, 5, 4]. Alternatively, the Image Charge Method (ICM) can be integrated with established electrostatic solvers [80, 81, 17, 93, 62, 63, 23], and its error can be controlled accurately [26]. Despite their potential, these methods still face significant challenges in strongly confined quasi-2D systems.

This difficulty is particularly pronounced for large aspect ratio systems, with $L_x, L_y \gg L_z$, as commonly encountered in simulations of charged particles confined in narrow channels or membranes. In such settings, the thickness in the z direction is fixed, whereas the domain in the xy plane must often be enlarged to reduce finite-size effects, thereby increasing the aspect ratio. As a result, the computational cost of ICM-based Ewald3D summations, such as ICM-PPPM [93], scales with the aspect ratio [26], while boundary integral-based approaches often become ill-conditioned in quasi-2D geometries [5], leading to substantial overhead in these regimes, complicating the balance between computational accuracy and efficiency.

Notably, in recent years, methods have also been developed for electrostatic problems with undulating dielectric interfaces [84, 76], which present additional challenges for modeling and simulations.

In this work, we propose an $\mathcal{O}(N)$ simulation algorithm, namely the quasi-Ewald method (QEM), for doubly periodic charged particle systems with dielectric mismatches at the confinement boundaries. To overcome the difficulties caused by the geometry of quasi-2D systems, we propose a tailored quasi-Ewald splitting strategy, which divides the original Coulomb kernel into short-range real space and long-range Fourier space components. Through the Dirichlet-to-Neumann map, we derive the Green's function for quasi-2D nanoconfined electrostatics and thereby arrive at an analytic, fast-converging lattice summation formula for this class of systems. We further develop a set of efficient and accurate methods to numerically evaluate these components. We apply analytic reduction combined with a tailored Gauss quadrature rule [78] to numerically evaluate the zeroth-order Hankel transform [75] in the short-range components, and develop a *separation via sorting* technique [38, 22] to accelerate the pairwise summation in the long-range components. Finally, by introducing the *random batch sampling* [43, 46, 41, 29, 44, 57, 55, 42] in k -space, we achieve linear complexity, making QEM suitable for molecular dynamics simulations of large-scale, nanoconfined quasi-2D systems. Notably, QEM is *mesh-free*, requires no image charges to handle dielectric mismatches at the boundaries, and does not require zero-padding to handle the nonperiodicity in the z direction. Consequently, this approach is capable of addressing challenges posed by extremely thin systems with polarizable boundaries, which are difficult to handle with existing approaches.

2. The model: concepts and mathematical preliminaries. In this section, we introduce the key model concepts and mathematical notations that will be used throughout this paper. First, Figure 1 provides a schematic representation of the quasi-2D charged many-body system under confinement. We note that quasi-2D systems [67] are essentially three-dimensional (3D) systems, with a characteristic length scale in z much smaller than that in the xy plane. Physically, these systems model charged many-body interactions with dielectric confinement effects [15, 24].

To accurately compute electrostatic interactions in quasi-2D systems, they are usually modeled as doubly periodic in the xy directions to mimic a bulk-like

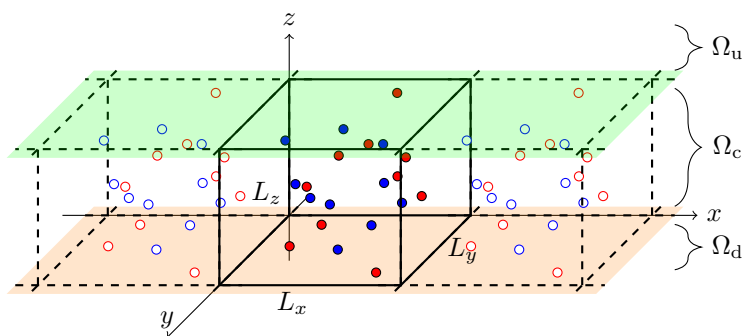


FIG. 1. A schematic of the quasi-2D nanoconfined particle system. The filled circles denote the charged particles confined within the central simulation box, while the empty circles represent their periodic replicas in the xy directions. The green and orange regions highlight the sharp dielectric interfaces, i.e., $\partial\Omega_c \cap \partial\Omega_u$ and $\partial\Omega_c \cap \partial\Omega_d$, respectively. Note that the system is periodic in both x and y , but for clarity, only the periodic replicas along the x axis are sketched here. (Figure in color online.)

environment, while incorporating appropriate dielectric confinement interfaces and boundary conditions in the z direction [66, 62]. Specifically, we consider a simulation box with dimensions (L_x, L_y, L_z) in $\mathbb{R}^3$, where dielectric confinement interfaces are positioned at $z = 0$ and $z = L_z$. As shown in Figure 1, the two dielectric interfaces divide $\mathbb{R}^3$ into three distinct subdomains, denoted as Ω_u , Ω_c , and Ω_d from top to bottom, respectively. The dielectric permittivity is piecewise constant over the three subdomains:

$$(2.1) \quad \epsilon(\mathbf{r}) = \begin{cases} \epsilon_u, & \mathbf{r} \in \Omega_u, \\ \epsilon_c, & \mathbf{r} \in \Omega_c, \\ \epsilon_d, & \mathbf{r} \in \Omega_d, \end{cases}$$

where ϵ_u , ϵ_c , and ϵ_d are positive material-specific constants.

Next, we describe molecular dynamics (MD) simulations of quasi-2D charged systems in a canonical (NVT) ensemble. Consider N charged particles inside the simulation box with positions $\mathbf{r}_i = (x_i, y_i, z_i)$, carrying charges q_i ($i = 1, 2, \dots, N$), and satisfying the overall charge-neutrality condition (if not, the electrostatic interaction will be ill-defined under doubly periodic boundary conditions [22]):

$$(2.2) \quad \sum_{i=1}^N q_i = 0.$$

An MD simulation of the N charged particles in a canonical ensemble essentially requires numerically integrating the following $6N$ -dimensional Newton's equations with a Langevin thermostat [20],

$$(2.3) \quad \begin{aligned} d\mathbf{r}_i &= \mathbf{v}_i dt, \\ m_i d\mathbf{v}_i &= \mathbf{F}_i dt + d\boldsymbol{\eta}_i, \end{aligned}$$

where $\mathbf{F}_i$ represents the force exerted on the i th particle, and $d\boldsymbol{\eta}_i = -\gamma \mathbf{v}_i dt + \sqrt{\frac{2\gamma}{\beta}} d\mathbf{W}_i$ represents the coupling with the environment (heat bath), where $\mathbf{W}_i$ are i.i.d. Wiener processes, γ is the reciprocal characteristic time associated with the thermostat, and $\beta = \frac{1}{k_B T}$. It is understood that for Langevin dynamics, the damping term $-\gamma \mathbf{v}_i dt$ and thermal fluctuation term $\sqrt{\frac{2\gamma}{\beta}} d\mathbf{W}_i$ are balanced by the fluctuation-dissipation relationship, thus approximating an NVT ensemble. Finally, the force $\mathbf{F}_i$ is computed via $\mathbf{F}_i := -\nabla_{\mathbf{r}_i} U$, where U is the potential energy of the system. Specifically, for the electrostatic energy of quasi-2D systems, the potential energy U reads

$$(2.4) \quad U = \frac{1}{2} \sum_{\mathbf{m}}' \sum_{i,j=1}^N q_i q_j G(\mathbf{r}_i; \mathbf{r}_j + \mathbf{L}_{\mathbf{m}}),$$

where $\mathbf{m} = (m_x, m_y, 0)$ with $(m_x, m_y) \in \mathbb{Z}^2$, $\mathbf{L}_{\mathbf{m}} := (m_x L_x, m_y L_y, 0)$ denotes the quasi-2D lattice vectors, and the lattice sum $\sum_{\mathbf{m}}'$ is defined such that the singular contribution in the bare Coulomb interaction for $i = j$, $\mathbf{m} = \mathbf{0}$ is excluded. Finally, we define $G(\mathbf{r}; \mathbf{r}')$ to be Green's function in a quasi-2D geometry, governed by Poisson's equation subject to dielectric interface conditions:

$$(2.5) \quad \begin{cases} -\nabla_{\mathbf{r}} \cdot [\epsilon(\mathbf{r}) \nabla_{\mathbf{r}} G(\mathbf{r}; \mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'), & \text{for } \mathbf{r} \in \mathbb{R}^3, \\ G(\mathbf{r}; \mathbf{r}')|_- = G(\mathbf{r}; \mathbf{r}')|_+, & \text{on } \partial\Omega_c, \\ \epsilon_c \partial_z G(\mathbf{r}; \mathbf{r}')|_- = \epsilon_u \partial_z G(\mathbf{r}; \mathbf{r}')|_+, & \text{on } \partial\Omega_c \cap \partial\Omega_u, \\ \epsilon_c \partial_z G(\mathbf{r}; \mathbf{r}')|_- = \epsilon_d \partial_z G(\mathbf{r}; \mathbf{r}')|_+, & \text{on } \partial\Omega_c \cap \partial\Omega_d, \\ G(\mathbf{r}; \mathbf{r}') \rightarrow 0, & \text{as } r \rightarrow \infty, \end{cases}$$

where $r := \|\mathbf{r}\| = \sqrt{x^2 + y^2 + z^2}$, and $\|\cdot\|$ represents the Euclidean norm.

The ICM can be applied to analytically solve the above set of equations, which expresses Green's function as an infinite series of image charges, constructed through an iterative process of image-charge reflections [35, 63]. Note that after each reflection, the magnitude of image charges is weakened by a dimensionless factor γ_u (or γ_d), measuring the dielectric contrasts for the upper and lower dielectric interfaces, defined as

$$(2.6) \quad \gamma_u := \frac{\epsilon_c - \epsilon_u}{\epsilon_c + \epsilon_u}, \quad \gamma_d := \frac{\epsilon_c - \epsilon_d}{\epsilon_c + \epsilon_d}.$$

Since the dielectric constants are all positive, γ_u and γ_d satisfy $|\gamma_u| < 1$ and $|\gamma_d| < 1$. Hence, the following infinite-series ICM representation of Green's function $G(\mathbf{r}; \mathbf{r}')$ is guaranteed to converge:

$$(2.7) \quad G(\mathbf{r}; \mathbf{r}') = \frac{1}{4\pi\epsilon_c} \left[\frac{1}{\|\mathbf{r} - \mathbf{r}'\|} + \sum_{l=1}^{\infty} \left(\frac{\gamma_l^+}{\|\mathbf{r} - \mathbf{r}'_{+}^{(l)}\|} + \frac{\gamma_l^-}{\|\mathbf{r} - \mathbf{r}'_{-}^{(l)}\|} \right) \right],$$

where the factors for the l th level image charges read $\gamma_l^+ := \gamma_d^{[l/2]} \gamma_u^{[l/2]}$ and $\gamma_l^- := \gamma_d^{[l/2]} \gamma_u^{[l/2]}$. Here the superscript $+$ ($-$) indicates the location of image charges in Ω_u (Ω_d). The notations $\lceil x \rceil$ and $\lfloor x \rfloor$ represent the “ceiling” and “floor” functions, respectively, and the positions of the l th-level images are given by

$$(2.8) \quad \mathbf{r}'_{\pm}^{(l)} = (x', y', (-1)^l z' \pm lL_z).$$

The above ICM representation of Green's function provides a theoretical benchmark for the systems considered here. However, due to the long-range nature of electrostatic interactions, (2.7) is not well suited to large-scale MD simulations of quasi-2D charged systems because of its high computational complexity, especially for strongly confined systems (i.e., when $L_z \ll L_{x,y}$).

Finally, we revisit the idea of the Ewald splitting technique for efficient calculations of the electrostatic interactions in a quasi-2D geometry. For quasi-2D systems *without* dielectric interface conditions, the so-called Ewald2D method [73, 33, 14] has been developed, which decomposes the interaction energy U as

$$(2.9) \quad U = U_s + U_l,$$

where the short-range and long-range components are given by

$$(2.10) \quad \begin{aligned} U_s &= \frac{1}{2} \sum_{i,j=1}^N q_i q_j \sum_{\mathbf{m}}' \frac{\operatorname{erfc}(\sqrt{\alpha} \|\mathbf{r}_i - \mathbf{r}_j + \mathbf{L}_{\mathbf{m}}\|)}{\|\mathbf{r}_i - \mathbf{r}_j + \mathbf{L}_{\mathbf{m}}\|} - \sqrt{\frac{\alpha}{\pi}} \sum_{i=1}^N q_i^2, \\ U_l &= \frac{1}{2} \sum_{i,j=1}^N q_i q_j \sum_{\mathbf{m}} \frac{\operatorname{erf}(\sqrt{\alpha} \|\mathbf{r}_i - \mathbf{r}_j + \mathbf{L}_{\mathbf{m}}\|)}{\|\mathbf{r}_i - \mathbf{r}_j + \mathbf{L}_{\mathbf{m}}\|}, \end{aligned}$$

respectively. Note that $\operatorname{erf}(x)$ is the error function

$$(2.11) \quad \operatorname{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du,$$

and $\operatorname{erfc}(x) := 1 - \operatorname{erf}(x)$, $\alpha > 0$ is the splitting parameter that can be adjusted to maximize performance in MD simulations [20]. The computational efficiency can be enhanced via Ewald decomposition because (a) U_s decays rapidly in real space and is short-ranged, so it can be efficiently evaluated via truncation; and (b) U_l is still long-ranged, but the interaction becomes smooth even when $\mathbf{r}_i \rightarrow \mathbf{r}_j$ and $\mathbf{m} = \mathbf{0}$, so

it converges spectrally in Fourier space. Consequently, based on [22, Lemma 2.4], the potential U_l can be transformed into the following summation form and evaluated in k -space:

$$(2.12) \quad U_l = U_l^0 + \sum_{\mathbf{k} \neq \mathbf{0}} U_l^{\mathbf{k}},$$

where

$$(2.13) \quad U_l^{\mathbf{k}} := \frac{\pi}{2L_x L_y} \sum_{i,j=1}^N q_i q_j \frac{e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}}}{k} [\xi^+(k, z_{ij}) + \xi^-(k, z_{ij})],$$

with $\boldsymbol{\rho}_{ij} := (x_i - x_j, y_i - y_j)$, $z_{ij} := \|z_i - z_j\|$, $k := \|\mathbf{k}\|$, and

$$(2.14) \quad \xi^{\pm}(k, z_{ij}) := e^{\pm k z_{ij}} \operatorname{erfc}\left(\frac{k}{2\sqrt{\alpha}} \pm \sqrt{\alpha} z_{ij}\right),$$

$$(2.15) \quad U_l^0 := -\frac{\pi}{L_x L_y} \sum_{i,j=1}^N q_i q_j \left[z_{ij} \operatorname{erf}(\sqrt{\alpha} z_{ij}) + \frac{e^{-\alpha z_{ij}^2}}{\sqrt{\alpha\pi}} \right].$$

While the Ewald2D summation accelerates numerical computations for the interaction energy U , it has several significant drawbacks: (a) even with an optimal choice of α , computing U for an N -particle system requires a computational complexity of $O(N^2)$, which is still very expensive for large particle numbers; (b) the functions $\xi^{\pm}(k, z_{ij})$ are ill-conditioned, as they grow exponentially with $k z_{ij}$, resulting in catastrophic error cancellation in numerical computations; and (c) the Ewald2D formula is applicable only to homogeneous systems without dielectric interface conditions. These challenges underscore the need to develop novel numerical methods that can simultaneously handle long-range interactions, quasi-2D geometry, and dielectric interface conditions, while ensuring both numerical stability and computational efficiency.

3. The quasi-Ewald splitting for Green's function. In this section, we present the quasi-Ewald splitting, a novel kernel decomposition strategy tailored to quasi-2D geometry.

First, consider a point source located at $\mathbf{r}' = (x', y', z')$. The quasi-Ewald splitting decomposes the Dirac delta function as

$$(3.1) \quad \begin{aligned} \delta(\mathbf{r} - \mathbf{r}') &= \left[\delta(\mathbf{r} - \mathbf{r}') - \left(\frac{\alpha}{\pi}\right) e^{-\alpha \|\boldsymbol{\rho} - \boldsymbol{\rho}'\|^2} \delta(z - z') \right] \\ &\quad + \left(\frac{\alpha}{\pi}\right) e^{-\alpha \|\boldsymbol{\rho} - \boldsymbol{\rho}'\|^2} \delta(z - z'), \end{aligned}$$

where $\mathbf{r} := (\boldsymbol{\rho}, z) := (x, y, z)$, $\boldsymbol{\rho} := (x, y)$, and $\boldsymbol{\rho}' := (x', y')$. A 3D illustration of the quasi-Ewald splitting is shown in Figure 2 for charged particles in a unit simulation cell under quasi-2D confinement. In (3.1), the first term on the right-hand side (RHS) represents a point source *screened* by a Gaussian density centered at $\mathbf{r}'$, spread in the xy plane to align with the quasi-2D cylindrical symmetry. The second term on the RHS compensates for this by adding back the Gaussian contribution to restore the original delta function. We further define the two densities on the RHS as follows:

$$(3.2) \quad \begin{aligned} \sigma_s(\mathbf{r}; \mathbf{r}') &:= \delta(\mathbf{r} - \mathbf{r}') - \left(\frac{\alpha}{\pi}\right) e^{-\alpha \|\boldsymbol{\rho} - \boldsymbol{\rho}'\|^2} \delta(z - z'), \\ \sigma_l(\mathbf{r}; \mathbf{r}') &:= \left(\frac{\alpha}{\pi}\right) e^{-\alpha \|\boldsymbol{\rho} - \boldsymbol{\rho}'\|^2} \delta(z - z'). \end{aligned}$$

Next, we define the following *quasi-2D Fourier transform*, which will be extensively used throughout this paper.

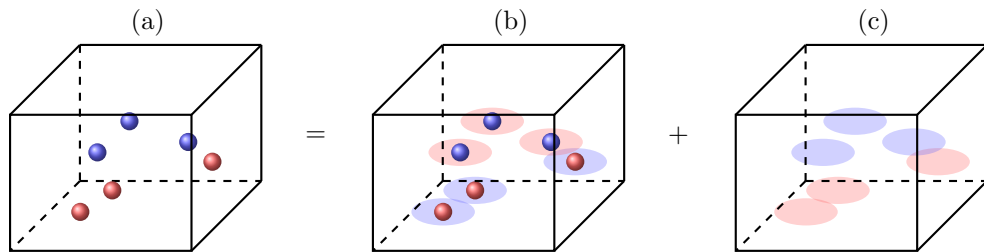


FIG. 2. An illustration of the quasi-Ewald splitting strategy in a unit cell. (a) Charged particles are distributed in the simulation box; cations and anions are represented by red and blue spheres, respectively. Subfigures (b) and (c) show how the quasi-Ewald splitting works. The discs represent 2D Gaussian charge density clouds in the xy planes, which screen the point sources. This splits the original problem into two subproblems: one with charge-neutral particles, so that the interactions are short-ranged, and the other with a smooth charge density that fits the cylindrical symmetry of the quasi-2D geometry and can therefore be solved rapidly in reciprocal space. (Figure in color online.)

DEFINITION 3.1. Given a function $f(\boldsymbol{\rho}, z)$, its quasi-2D Fourier transform is defined by

$$(3.3) \quad \hat{f}(\mathbf{k}, z) := \int_{\mathbb{R}^2} f(\boldsymbol{\rho}, z) e^{-i\mathbf{k} \cdot \boldsymbol{\rho}} d\boldsymbol{\rho}.$$

The function $f(\boldsymbol{\rho}, z)$ can be recovered from $\hat{f}(\mathbf{k}, z)$ by the corresponding inverse quasi-2D Fourier transform

$$(3.4) \quad f(\boldsymbol{\rho}, z) = \frac{1}{4\pi^2} \int_{\mathbb{R}^2} \hat{f}(\mathbf{k}, z) e^{i\mathbf{k} \cdot \boldsymbol{\rho}} d\mathbf{k}.$$

Taking the quasi-2D Fourier transform of σ_s and σ_l in (3.2), we obtain their counterparts $\hat{\sigma}_s$ and $\hat{\sigma}_l$, summarized in the following proposition.

PROPOSITION 3.2. Given a fixed point $\mathbf{r}' = (x', y', z')$ with $\boldsymbol{\rho}' = (x', y')$, the nonzero modes of the 2D Fourier transforms of $\sigma_s(\mathbf{r}; \mathbf{r}')$ and $\sigma_l(\mathbf{r}; \mathbf{r}')$ are, respectively, given by

$$\begin{aligned} \hat{\sigma}_s(\mathbf{k}, z; z') &= \delta(z - z') e^{-i\mathbf{k} \cdot \boldsymbol{\rho}'} \left(1 - e^{-\frac{k^2}{4\alpha}} \right), \\ \hat{\sigma}_l(\mathbf{k}, z; z') &= \delta(z - z') e^{-i\mathbf{k} \cdot \boldsymbol{\rho}'} e^{-\frac{k^2}{4\alpha}}, \end{aligned}$$

where $\mathbf{k} \neq \mathbf{0}$, and the zeroth mode reads

$$\begin{aligned} \hat{\sigma}_s(\mathbf{0}, z; z') &= 0, \\ \hat{\sigma}_l(\mathbf{0}, z; z') &= \delta(z - z'). \end{aligned}$$

Proof. By direct application of Definition 3.1, the integrals can be evaluated analytically; hence, we omit the details. $\square$

Now, given a source point $\mathbf{r}_0 := (\boldsymbol{\rho}_0, z_0) := (x_0, y_0, z_0) \in \Omega_c$, Green's function $G(\mathbf{r}; \mathbf{r}_0)$ (as defined in E (2.5)) can be solved in k -space using Proposition 3.2 and the Dirichlet-to-Neumann map. The resulting expressions are summarized in Theorem 3.3, whose proof can be found in the supplementary materials (sm.pdf [local/web 248KB]).

THEOREM 3.3. Let us define

$$(3.5) \quad \hat{G}(\mathbf{k}, z; z_0) = \int_{\mathbb{R}^2} G(\mathbf{r}; \mathbf{r}_0) e^{-i\mathbf{k} \cdot \boldsymbol{\rho}} d\boldsymbol{\rho},$$

then, for $\mathbf{k} = \mathbf{0}$,

$$(3.6) \quad \hat{G}(\mathbf{0}, z; z_0) = -\frac{|z - z_0|}{2\epsilon_c},$$

and for $\mathbf{k} \neq \mathbf{0}$,

$$(3.7) \quad \hat{G}(\mathbf{k}, z; z_0) = \frac{e^{-i\mathbf{k} \cdot \boldsymbol{\rho}_0}}{2k\epsilon_c(1 - \gamma_u\gamma_d e^{-2kL_z})} \sum_{p=1}^4 \Gamma_p e^{-ka_p(z; z_0)},$$

where

$$\begin{aligned} \Gamma_{1:4} &:= [1, \gamma_d, \gamma_u, \gamma_u\gamma_d], \\ a_{1:4}(z; z_0) &:= [|z - z_0|, z + z_0, 2L_z - z - z_0, 2L_z - |z - z_0|]. \end{aligned}$$

Remark 3.4. (a) The condition $|\gamma_u\gamma_d| < 1$ ensures the uniqueness of the quasi-2D Green's function; (b) all the components in $a_{1:4}(z; z_0)$ have positive values; (c) the overall charge neutrality condition (2.2) is needed so that for $k = 0$, the infinite boundary condition can be met for N -particle systems.

Based on the quasi-Ewald splitting introduced in (3.1)–(3.2) for the delta source, namely, $\delta(\mathbf{r} - \mathbf{r}_0) = \sigma_s(\mathbf{r}; \mathbf{r}_0) + \sigma_l(\mathbf{r}; \mathbf{r}_0)$, we obtain the corresponding decomposition of Green's function:

$$(3.8) \quad G(\mathbf{r}; \mathbf{r}_0) = G_s(\mathbf{r}; \mathbf{r}_0) + G_l(\mathbf{r}; \mathbf{r}_0),$$

where $G_s(\mathbf{r}; \mathbf{r}_0)$ and $G_l(\mathbf{r}; \mathbf{r}_0)$ are the electrostatic potentials generated by the charge densities $\sigma_s(\mathbf{r}; \mathbf{r}_0)$ and $\sigma_l(\mathbf{r}; \mathbf{r}_0)$, respectively. These can be solved analogously by using Proposition 3.2; the resulting expressions are summarized in the following corollary.

COROLLARY 3.5. *Green's function given in Theorem 3.3 admits a quasi-Ewald splitting, namely,*

$$(3.9) \quad G(\mathbf{r}; \mathbf{r}_0) = G_s(\mathbf{r}; \mathbf{r}_0) + G_l(\mathbf{r}; \mathbf{r}_0),$$

where for any $\mathbf{k} \neq \mathbf{0}$,

$$\begin{aligned} \hat{G}_s(\mathbf{k}, z; z_0) &= \hat{G}(\mathbf{k}, z; z_0) \left(1 - e^{-\frac{k^2}{4\alpha}}\right), \\ \hat{G}_l(\mathbf{k}, z; z_0) &= \hat{G}(\mathbf{k}, z; z_0) e^{-\frac{k^2}{4\alpha}}, \end{aligned}$$

and for $\mathbf{k} = \mathbf{0}$,

$$\begin{aligned} \hat{G}_s(\mathbf{0}, z; z_0) &= 0, \\ \hat{G}_l(\mathbf{0}, z; z_0) &= \hat{G}(\mathbf{0}, z; z_0). \end{aligned}$$

Proof. The proof is straightforward: one can solve for $\hat{G}_s$ and $\hat{G}_l$ by replacing the Dirac delta source with σ_s and σ_l , then using Proposition 3.2 and following the same steps as in the proof of Theorem 3.3. We omit the details. $\square$

Finally, one can recover $G_s(\mathbf{r}; \mathbf{r}_0)$ and $G_l(\mathbf{r}; \mathbf{r}_0)$ in real space by using the inverse quasi-2D Fourier transform,

$$\begin{aligned} G_s(\mathbf{r}; \mathbf{r}_0) &= \frac{1}{4\pi^2} \int_{\mathbb{R}^2} \hat{G}_s(\mathbf{k}, z; z_0) e^{i\mathbf{k} \cdot \boldsymbol{\rho}} d\mathbf{k} = \frac{1}{4\pi^2} \int_{\mathbb{R}^2} \hat{G}(\mathbf{k}, z; z_0) \left(1 - e^{-\frac{k^2}{4\alpha}}\right) e^{i\mathbf{k} \cdot \boldsymbol{\rho}} d\mathbf{k}, \\ G_l(\mathbf{r}; \mathbf{r}_0) &= \frac{1}{4\pi^2} \int_{\mathbb{R}^2} \hat{G}_l(\mathbf{k}, z; z_0) e^{i\mathbf{k} \cdot \boldsymbol{\rho}} d\mathbf{k} = \frac{1}{4\pi^2} \int_{\mathbb{R}^2} \hat{G}(\mathbf{k}, z; z_0) e^{-\frac{k^2}{4\alpha}} e^{i\mathbf{k} \cdot \boldsymbol{\rho}} d\mathbf{k}. \end{aligned}$$

Thus the total electrostatic interaction energy U can be expressed as

$$U = U_s + U_l,$$

where

$$(3.10) \quad U_s := \frac{1}{2} \sum_{\mathbf{m}}' \sum_{i,j=1}^N q_i q_j G_s(\mathbf{r}_i; \mathbf{r}_j + \mathbf{L}_m),$$

and

$$(3.11) \quad U_l := \frac{1}{2} \sum_{\mathbf{m}} \sum_{i,j=1}^N q_i q_j G_l(\mathbf{r}_i; \mathbf{r}_j + \mathbf{L}_m).$$

In the following sections, we will present a collection of numerical techniques that enable the evaluation of (3.10)–(3.11) in particle-based simulations with an optimal computational cost of $\mathcal{O}(N)$.

4. Optimal quadrature rules for short-range interactions. We begin by deriving an optimal quadrature rule for the evaluation of the short-range interaction energy U_s . As discussed earlier, G_s is the potential field generated by σ_s , which represents a source point screened by a flattened Gaussian density surrounding it. Due to this fact, the leading order of G_s in the far field behaves as a quadrupole, i.e., the potential decays as $1/r^3$. Note that although the bare pairwise kernel G_s is marginally long-ranged in $\mathbb{R}^3$, the interaction lattice sum (3.10) is fast convergent due to the charge neutrality condition (2.2) within each cell. Specifically, since each local cell satisfies (2.2), so the leading order $1/r^3$ in its multipoles expansion naturally vanishes. Therefore, the lattice sum (3.10) becomes faster convergent under cell neutrality, despite the marginally long-ranged nature of the bare kernel, and can be truncated to a finite sum in real space with an interparticle cutoff distance r_c ,

$$(4.1) \quad U_s \approx U_{s,*} = \frac{1}{2} \sum_{\|\boldsymbol{\rho}_{ij,m}\| \leq r_c}' q_i q_j G_s(\mathbf{r}_i; \mathbf{r}_j + \mathbf{L}_m),$$

where $\boldsymbol{\rho}_{ij,m} := \boldsymbol{\rho}_i - \boldsymbol{\rho}_j + (L_x m_x, L_y m_y)$, indicating that among all possible pairs of particles, only the terms with $\|\boldsymbol{\rho}_{ij,m}\| \leq r_c$ need to be computed. As such, neighbor-list algorithms can be applied to reduce the cost to $\mathcal{O}(N)$ [20] if r_c is a constant that does not vary with the system size.

The main difficulty in computing (4.1) lies in developing efficient and accurate quadrature rules for evaluating G_s , which reads

$$G_s(\mathbf{r}_i; \mathbf{r}_j) = \frac{1}{8\pi^2 \epsilon_c} \int_{\mathbb{R}^2} \frac{e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}}}{k(1 - \gamma_u \gamma_d e^{-2kL_z})} \left(1 - e^{-\frac{k^2}{4\alpha}}\right) \left(\sum_{p=1}^4 \Gamma_p e^{-ka_p(z_i; z_j)}\right) d\mathbf{k},$$

where $\boldsymbol{\rho}_{ij} := \boldsymbol{\rho}_i - \boldsymbol{\rho}_j$. Due to the cylindrical symmetry, G_s can be further reduced to the following one-dimensional (1D) *inverse Hankel transform* form:

$$(4.2) \quad \begin{aligned} G_s(\mathbf{r}_i; \mathbf{r}_j) &= \frac{1}{8\pi^2 \epsilon_c} \int_{\mathbb{R}^2} \frac{e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}}}{k(1 - \gamma_u \gamma_d e^{-2kL_z})} \left(1 - e^{-\frac{k^2}{4\alpha}}\right) \left(\sum_{p=1}^4 \Gamma_p e^{-ka_p(z_i; z_j)}\right) d\mathbf{k}, \\ &= \frac{1}{4\pi \epsilon_c} \int_0^{+\infty} \frac{\sum_{p=1}^4 \Gamma_p e^{-ka_p(z_i; z_j)}}{1 - \gamma_u \gamma_d e^{-2kL_z}} \left(1 - e^{-\frac{k^2}{4\alpha}}\right) \mathcal{J}_0(\rho_{ij} k) dk, \end{aligned}$$

where $\rho_{ij} := \|\boldsymbol{\rho}_{ij}\| = \|\boldsymbol{\rho}_i - \boldsymbol{\rho}_j\|$, and $\mathcal{J}_0(\cdot)$ is the zeroth-order Bessel function of the first kind, whose expression reads $\mathcal{J}_0(r) := \frac{1}{2\pi} \int_0^{2\pi} e^{ir \sin \theta} d\theta$.

Without loss of generality, we develop optimal quadrature rules for evaluating the following integral associated with (4.2):

$$(4.3) \quad \int_0^{+\infty} \frac{e^{-ak}}{1 - \gamma_u \gamma_d e^{-2kL_z}} \left(1 - e^{-\frac{k^2}{4\alpha}}\right) \mathcal{J}_0(\rho k) dk,$$

where $a > 0$ and $\rho > 0$ are constants. First, we split (4.3) into the summation of two terms,

$$\begin{aligned} & \int_0^{+\infty} \frac{e^{-ak}}{1 - \gamma_u \gamma_d e^{-2kL_z}} \left(1 - e^{-\frac{k^2}{4\alpha}}\right) \mathcal{J}_0(\rho k) dk \\ &= \underbrace{\int_0^{+\infty} \frac{1}{1 - \gamma_u \gamma_d e^{-2kL_z}} e^{-ak} \mathcal{J}_0(\rho k) dk}_{\text{Term I}} - \underbrace{\int_0^{+\infty} \frac{1}{1 - \gamma_u \gamma_d e^{-2kL_z}} e^{-\frac{k^2}{4\alpha}} e^{-ak} \mathcal{J}_0(\rho k) dk}_{\text{Term II}}. \end{aligned}$$

Clearly, Term II is numerically more tractable, as its integrand contains the factor $e^{-\frac{k^2}{4\alpha}}$, which decays rapidly with increasing k . For Term I, we further decompose it into two terms:

$$\begin{aligned} & \int_0^{+\infty} \frac{1}{1 - \gamma_u \gamma_d e^{-2kL_z}} e^{-ak} \mathcal{J}_0(\rho k) dk \\ &= \underbrace{\int_0^{+\infty} e^{-ak} \mathcal{J}_0(\rho k) dk}_{\text{Term I(a)}} + \underbrace{\int_0^{+\infty} \frac{\gamma_u \gamma_d}{1 - \gamma_u \gamma_d e^{-2kL_z}} e^{-2kL_z} e^{-ak} \mathcal{J}_0(\rho k) dk}_{\text{Term I(b)}}. \end{aligned}$$

Notice that $\{e^{-ax}, \frac{1}{\sqrt{a^2+1}}\}$ is a Hankel transform pair, namely, $\int_0^{+\infty} e^{-ax} \mathcal{J}_0(x) dx = \frac{1}{\sqrt{a^2+1}}$, thus Term I(a) can be obtained analytically,

$$(4.4) \quad \int_0^{+\infty} e^{-ak} \mathcal{J}_0(\rho k) dk = \frac{1}{\sqrt{a^2 + \rho^2}}.$$

Although $\mathcal{J}_0(r)$ is slowly decaying and oscillatory as $r \rightarrow +\infty$, both Term I(b) and Term II contain rapidly decaying factors, namely e^{-2kL_z} and $e^{-\frac{k^2}{4\alpha}}$, allowing efficient calculations using the optimal quadrature rules proposed by Trefethen in [78]. For a given truncation parameter $M > 0$, the infinite integral can be first approximated by truncation,

$$\int_0^{+\infty} F(k) dk \approx \int_0^M F(k) dk,$$

and then the integral on $[0, M]$ can be efficiently evaluated using Gauss–Legendre quadrature. We further provide truncation error estimates to determine M in practice, which are summarized in the following theorem.

THEOREM 4.1. *We denote the truncation errors of Term I(b) and Term II, respectively, by*

$$\begin{aligned} \Delta \text{I}_b(M) &:= \int_M^{+\infty} \frac{\gamma_u \gamma_d}{1 - \gamma_u \gamma_d e^{-2kL_z}} e^{-2kL_z} e^{-ak} \mathcal{J}_0(\rho k) dk, \\ \Delta \text{II}(M) &:= \int_M^{+\infty} \frac{1}{1 - \gamma_u \gamma_d e^{-2kL_z}} e^{-\frac{k^2}{4\alpha}} e^{-ak} \mathcal{J}_0(\rho k) dk, \end{aligned}$$

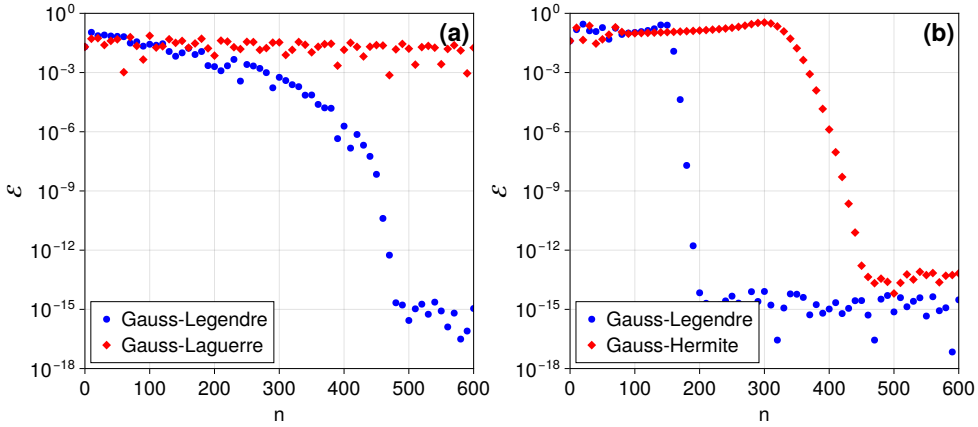


FIG. 3. Absolute error $\mathcal{E}$ in the evaluation of $\int_0^\infty \mathcal{J}_0(50x)e^{-x} dx$ and $\int_{-\infty}^\infty \mathcal{J}_0(50x)e^{-x^2} dx$ using (a) Gauss-Laguerre (half interval), and (b) Gauss-Hermite (full interval) and truncated Gauss-Legendre quadrature on finite intervals $[0, 36]$ and $[-6, 6]$, where n denotes the quadrature order.

whose estimates read

$$(4.5) \quad \|\Delta I_b(M)\| \leq \frac{|\gamma_u \gamma_d|}{1 - \max\{0, \gamma_u \gamma_d\}} \frac{1}{\sqrt{\rho L_z}} \operatorname{erfc}(\sqrt{2L_z M}),$$

$$(4.6) \quad \|\Delta \Pi(M)\| \leq \frac{\sqrt{\pi \alpha}}{1 - \max\{0, \gamma_u \gamma_d\}} \operatorname{erfc}\left(\frac{M}{2\sqrt{\alpha}}\right).$$

Proof. The proof relies on the properties of the special function $\mathcal{J}_0(r)$ [50, 72]; details are omitted here but can be found in the supplementary materials (sm.pdf [local/web 248KB]). Note that $\operatorname{erfc}(\cdot)$ decays exponentially, ensuring fast convergence in M . $\square$

We validate the proposed quadrature rule by testing its convergence on two benchmark integrals involving the zeroth-order Bessel function of the first kind, i.e., $\int_0^\infty \mathcal{J}_0(\rho x)e^{-x} dx$ and $\int_{-\infty}^\infty \mathcal{J}_0(\rho x)e^{-x^2} dx$. Furthermore, we compare our results with standard Gauss-Laguerre and Gauss-Hermite quadratures, which are specifically tailored for integrals of these forms. First, fixing $\rho = 50$, the absolute error $\mathcal{E}$ versus the number of quadrature points n is presented in Figure 3. Our proposed truncated Gauss-Legendre rule converges significantly faster than Gauss-Laguerre and Gauss-Hermite quadrature, consistent with the findings in [78]. Moreover, for varying $\rho \in [0, 10]$, we set the absolute errors $\mathcal{E} = 10^{-4}$, 10^{-8} , and 10^{-12} (by choosing a suitable M according to Theorem 4.1), respectively. We examine the minimal number of quadrature points n required for the proposed quadrature rule to achieve the desired accuracy. As shown in Figure 4, only a few tens of points suffice for both integrals, demonstrating the efficiency of the method.

Remark 4.2. Theorem 4.1 indicates that the cost of evaluating the integral in Eq. (4.3) is independent of the aspect ratios L_x/L_z and L_y/L_z . Therefore, the proposed quadrature rule remains efficient even for systems with large aspect ratios.

5. Fast algorithms for long-range interactions. We now present efficient methods to compute the long-range interaction energy U_l . First, based on the Poisson summation formula, we have

$$(5.1) \quad \sum_{\mathbf{m}} G_l(\mathbf{r}_i; \mathbf{r}_j + \mathbf{L}_m) = \frac{1}{L_x L_y} \sum_{\mathbf{k} \in \mathcal{K}^2} \hat{G}_l(\mathbf{k}, z_i; z_j) e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}},$$

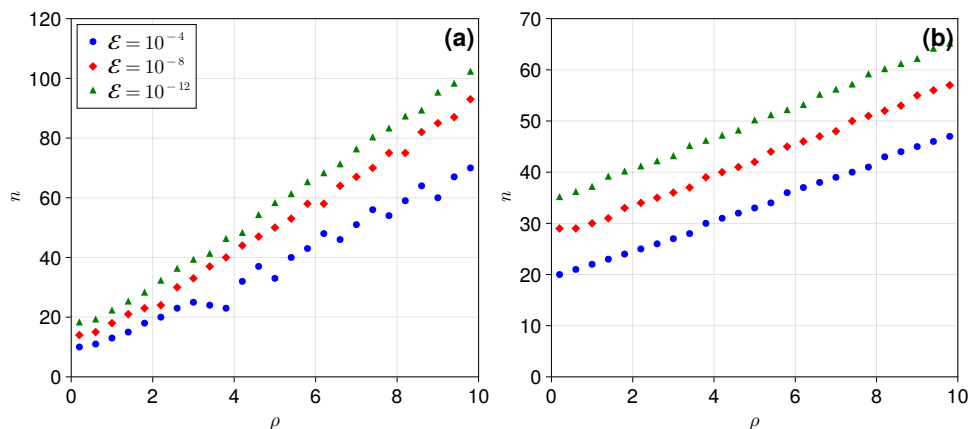


FIG. 4. Required quadrature order n versus oscillation parameter $\rho \in [0, 10]$ for the prescribed accuracy $\mathcal{E}$, using truncated Gauss–Legendre quadrature for (a) $\int_0^\infty J_0(\rho x) e^{-x} dx$ on $[0, k_a]$; and (b) $\int_{-\infty}^\infty J_0(\rho x) e^{-x^2} dx$ on $[-k_b, k_b]$. Here, k_a and k_b are determined based on Theorem 4.1.

where

$$\mathcal{K}^2 := \left\{ \mathbf{k} \in \frac{2\pi}{L_x} \mathbb{Z} \times \frac{2\pi}{L_y} \mathbb{Z} \right\}.$$

We denote the smallest nonzero lattice wavenumber by

$$k_{\min} := \min_{\mathbf{k} \in \mathcal{K}^2, \mathbf{k} \neq \mathbf{0}} \|\mathbf{k}\| = \frac{2\pi}{\max\{L_x, L_y\}}.$$

Substituting $\hat{G}_l(\mathbf{k}, z_i; z_j)$ derived in Corollary 3.5, we obtain the following formula for U_l :

$$\begin{aligned} U_l &= \frac{1}{2} \sum_{\mathbf{m}} \sum_{i,j=1}^N q_i q_j G_l(\mathbf{r}_i, \mathbf{r}_j + \mathbf{L}_m) \\ (5.2) \quad &= \frac{1}{4\epsilon_c L_x L_y} \sum_{i,j=1}^N q_i q_j \left\{ -|z_i - z_j| \right. \\ &\quad \left. + \sum_{\mathbf{k} \in \mathcal{K}^2, \mathbf{k} \neq \mathbf{0}} \frac{e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}}}{k(1 - \gamma_u \gamma_d e^{-2kL_z})} \left(\sum_{p=1}^4 \Gamma_p e^{-k a_p(z_i; z_j)} \right) e^{-\frac{k^2}{4\alpha}} \right\}. \end{aligned}$$

To reduce the computational cost for (5.2) to $\mathcal{O}(N)$, we integrate the random batch sampling method with an efficient pairwise summation technique. The details of our approach will be discussed in the remainder of this section.

5.1. Part one: $\mathcal{O}(N)$ pairwise summation method. First, for simplicity, we define auxiliary functions $h_{1:4}(\mathbf{k})$ as

$$\begin{aligned} h_1(\mathbf{k}) &:= \frac{1}{4\epsilon_c L_x L_y k(1 - \gamma_u \gamma_d e^{-2kL_z})}, \\ h_2(\mathbf{k}) &:= \frac{\gamma_d}{4\epsilon_c L_x L_y k(1 - \gamma_u \gamma_d e^{-2kL_z})}, \\ h_3(\mathbf{k}) &:= \frac{\gamma_u e^{-2kL_z}}{4\epsilon_c L_x L_y k(1 - \gamma_u \gamma_d e^{-2kL_z})}, \\ h_4(\mathbf{k}) &:= \frac{\gamma_u \gamma_d e^{-2kL_z}}{4\epsilon_c L_x L_y k(1 - \gamma_u \gamma_d e^{-2kL_z})}, \end{aligned}$$

and another set of auxiliary quantities S_0 and $S_{1:4}(\mathbf{k})$ by

$$\begin{aligned} S_0 &:= \frac{1}{4\epsilon_c L_x L_y} \sum_{i,j=1}^N q_i q_j |z_i - z_j|, \\ S_1(\mathbf{k}) &:= \sum_{i,j=1}^N q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{-k|z_i - z_j|}, \\ S_2(\mathbf{k}) &:= \sum_{i,j=1}^N q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{-k(z_i + z_j)}, \\ S_3(\mathbf{k}) &:= \sum_{i,j=1}^N q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{k(z_i + z_j)}, \\ S_4(\mathbf{k}) &:= \sum_{i,j=1}^N q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{k|z_i - z_j|}. \end{aligned}$$

Consequently, the long-range interaction energy U_l can be written as

$$(5.3) \quad U_l = S_0 + \sum_{\mathbf{k} \in \mathcal{K}^2, \mathbf{k} \neq \mathbf{0}} e^{-\frac{k^2}{4\alpha}} \left(\sum_{p=1}^4 S_p(\mathbf{k}) h_p(\mathbf{k}) \right).$$

Evaluating $S_{0:4}(\mathbf{k})$ by direct summation would incur an $\mathcal{O}(N^2)$ computational cost. However, the auxiliary functions $S_2(\mathbf{k})$ and $S_3(\mathbf{k})$ are *multiplicatively separable*; that is, they can be expressed as

$$\begin{aligned} S_2(\mathbf{k}) &= \sum_{i,j=1}^N q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{-k(z_i + z_j)} = \left(\sum_{i=1}^N q_i e^{i\mathbf{k} \cdot \boldsymbol{\rho}_i} e^{-kz_i} \right) \left(\sum_{j=1}^N q_j e^{-i\mathbf{k} \cdot \boldsymbol{\rho}_j} e^{-kz_j} \right), \\ S_3(\mathbf{k}) &= \sum_{i,j=1}^N q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{k(z_i + z_j)} = \left(\sum_{i=1}^N q_i e^{i\mathbf{k} \cdot \boldsymbol{\rho}_i} e^{kz_i} \right) \left(\sum_{j=1}^N q_j e^{-i\mathbf{k} \cdot \boldsymbol{\rho}_j} e^{kz_j} \right), \end{aligned}$$

which reduces their computational complexity to $\mathcal{O}(N)$. In contrast, S_0 , $S_1(\mathbf{k})$, and $S_4(\mathbf{k})$ are nonseparable due to the presence of the absolute value term $|z_i - z_j|$, obstructing direct factorization. Consequently, to eliminate the absolute value operation, we first sort all N particles according to their positions along the z -axis, ensuring the order:

$$0 < z_1 < z_2 < \cdots < z_{N-1} < z_N < L_z.$$

Since for all i , $z_i \in (0, L_z)$ is uniformly bounded within the simulation box, strategies such as bucket sorting [11] can be applied, and the computational cost can be of order $\mathcal{O}(N)$. In particle-based simulations, only local corrections are needed between successive time steps. Now, once all N particles are sorted, S_0 can be written as

$$S_0 = \frac{1}{4\epsilon_c L_x L_y} \sum_{i=1}^N q_i \left(\sum_{j=1}^N q_j (z_i - z_j) \right) = \frac{1}{2\epsilon_c L_x L_y} \sum_{i=1}^N q_i \left(z_i \sum_{j=1}^i q_j - \sum_{j=1}^i z_j q_j \right).$$

To efficiently compute this sum, we further introduce two auxiliary sequences $\{T_1(i)\}_{i=1}^N$ and $\{T_2(i)\}_{i=1}^N$, both of which can be iteratively updated as follows:

$$\begin{aligned} T_1(1) &= q_1, & T_1(i+1) &= T_1(i) + q_{i+1}, \\ T_2(1) &= z_1 q_1, & T_2(i+1) &= T_2(i) + z_{i+1} q_{i+1}. \end{aligned}$$

Finally, using these auxiliary sequences, S_0 can be efficiently calculated as

$$S_0 = \frac{1}{2\epsilon_c L_x L_y} \sum_{i=1}^N q_i (z_i T_1(i) - T_2(i)),$$

which requires only $\mathcal{O}(N)$ operations.

A similar strategy [38] can be applied for the evaluation of $S_1(\mathbf{k})$ and $S_4(\mathbf{k})$. For $S_1(\mathbf{k})$, after sorting, we have

$$\begin{aligned} S_1(\mathbf{k}) &= \sum_{i,j=1}^N q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{-k|z_i - z_j|} \\ &= - \sum_{i=1}^N q_i^2 + \sum_{i=1}^N \sum_{j=1}^i q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{-k(z_i - z_j)} + \sum_{i=1}^N \sum_{j=i}^N q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{-k(z_j - z_i)} \\ &= - \sum_{i=1}^N q_i^2 + \sum_{i=1}^N q_i e^{i\mathbf{k} \cdot \boldsymbol{\rho}_i} e^{-kz_i} \sum_{j=1}^i q_j e^{-i\mathbf{k} \cdot \boldsymbol{\rho}_j} e^{kz_j} + \sum_{i=1}^N q_i e^{i\mathbf{k} \cdot \boldsymbol{\rho}_i} e^{kz_i} \sum_{j=i}^N q_j e^{-i\mathbf{k} \cdot \boldsymbol{\rho}_j} e^{-kz_j}. \end{aligned}$$

We introduce two additional auxiliary sequences $\{T_3(i)\}_{i=1}^N$ and $\{T_4(i)\}_{i=1}^N$. Note that $\{T_3(i)\}_{i=1}^N$ is constructed through forward iteration, whereas $\{T_4(i)\}_{i=1}^N$ is generated through backward iteration:

$$\begin{aligned} T_3(1) &= q_1 e^{-i\mathbf{k} \cdot \boldsymbol{\rho}_1} e^{kz_1}, \\ T_3(i+1) &= T_3(i) + q_{i+1} e^{-i\mathbf{k} \cdot \boldsymbol{\rho}_{i+1}} e^{kz_{i+1}}, \\ T_4(N) &= q_N e^{-i\mathbf{k} \cdot \boldsymbol{\rho}_N} e^{-kz_N}, \\ T_4(i-1) &= T_4(i) + q_{i-1} e^{-i\mathbf{k} \cdot \boldsymbol{\rho}_{i-1}} e^{-kz_{i-1}}, \end{aligned}$$

and $S_1(\mathbf{k})$ can be efficiently calculated as

$$S_1(\mathbf{k}) = - \sum_{i=1}^N q_i^2 + \sum_{i=1}^N q_i e^{i\mathbf{k} \cdot \boldsymbol{\rho}_i} [e^{-kz_i} T_3(i) + e^{kz_i} T_4(i)].$$

We observe that the same recurrence scheme can be applied to the calculation of $S_4(\mathbf{k})$, and the details are omitted for brevity.

In summary, for any given $\mathbf{k}$ in (5.3), it now takes only $\mathcal{O}(N)$ operations to evaluate S_0 and $\sum_{p=1}^4 S_p(\mathbf{k}) h_p(\mathbf{k})$. We proceed to introduce the random batch method to efficiently perform the summation over $\mathbf{k}$.

5.2. Part two: Random batch importance sampling in k -space. In this section, we introduce the random batch method [46, 43] for efficient summation over $\mathbf{k}$, so that the overall computational complexity for U_l can be reduced to $\mathcal{O}(N)$. The idea of random minibatch sampling originates from optimization and machine learning, such as the well-known stochastic gradient descent (SGD) method. Jin, Li, and Liu first proposed the random batch method (RBM) for interacting particle systems [43]. This approach was subsequently extended to sampling in k -space using importance sampling for variance reduction. The resulting random batch Ewald (RBE) method [46, 58, 57, 56, 59, 61, 60, 23] has since been successfully applied to various ensembles and systems, demonstrating remarkable superscalability in large-scale simulations.

Here, to further accelerate the computation of the long-range interaction energy U_l , we first define $\phi(\mathbf{k})$ as

$$(5.4) \quad \phi(\mathbf{k}) := \sum_{p=1}^4 S_p(\mathbf{k}) h_p(\mathbf{k}),$$

then (5.3) becomes

$$(5.5) \quad U_l = S_0 + \sum_{\mathbf{k} \in \mathcal{K}^2, \mathbf{k} \neq \mathbf{0}} \phi(\mathbf{k}) e^{-\frac{\mathbf{k}^2}{4\alpha}}.$$

We define

$$(5.6) \quad U_l^{\mathbf{0}} := S_0 \quad \text{and} \quad U_l^{\mathbf{k} \neq \mathbf{0}} := \sum_{\mathbf{k} \in \mathcal{K}^2, \mathbf{k} \neq \mathbf{0}} \phi(\mathbf{k}) e^{-\frac{\mathbf{k}^2}{4\alpha}},$$

then U_l can be written as $U_l = U_l^{\mathbf{0}} + U_l^{\mathbf{k} \neq \mathbf{0}}$. Since $U_l^{\mathbf{0}}$ can be computed with $\mathcal{O}(N)$ cost, we focus on the efficient evaluation of $U_l^{\mathbf{k} \neq \mathbf{0}}$ via the random batch method.

By interpreting the lattice summation over $\mathbf{k}$ as an expectation under the probability measure $\mathcal{P}(\mathbf{k}) \propto e^{-\frac{\mathbf{k}^2}{4\alpha}}$ defined on the lattice $\mathcal{K}^2$, we can build a stochastic approximation for $U_l^{\mathbf{k} \neq \mathbf{0}}$ via importance sampling:

$$(5.7) \quad U_l^{\mathbf{k} \neq \mathbf{0}} \approx U_{l,*}^{\mathbf{k} \neq \mathbf{0}} := \frac{H}{P} \sum_{\eta=1}^P \phi(\mathbf{k}_\eta) = \frac{H}{P} \sum_{\eta=1}^P \sum_{q=1}^4 S_q(\mathbf{k}_\eta) h_q(\mathbf{k}_\eta),$$

where $\{\mathbf{k}_\eta\}_{\eta=1}^P$ is a minibatch of frequencies sampled from $\mathcal{P}(\mathbf{k})$ using the Metropolis algorithm, and P is the batch size [69]. We denote by

$$H := \sum_{\mathbf{k} \in \mathcal{K}^2, \mathbf{k} \neq \mathbf{0}} e^{-\frac{\mathbf{k}^2}{4\alpha}}$$

the normalization constant for $\mathcal{P}$. Then the corresponding stochastic estimator of forces in Fourier space can also be obtained as

$$(5.8) \quad \mathbf{F}_{l,i} \approx \mathbf{F}_{l,i}^* = -\nabla_{\mathbf{r}_i} U_l^{\mathbf{0}} - \nabla_{\mathbf{r}_i} U_{l,*}^{\mathbf{k} \neq \mathbf{0}}.$$

In what follows, we present a theoretical analysis of the random batch approximation, emphasizing its convergence rate. We demonstrate that the batch size P is independent of the particle number N , which ensures that the summation over $\mathbf{k}$ does not affect the overall linear scaling. Let us begin by considering the fluctuations, i.e., the stochastic error introduced by the importance sampling at each time step. The fluctuations of the force acting on the i th particle due to the random batch approximation, denoted as χ_i , are defined as follows:

$$(5.9) \quad \chi_i := \mathbf{F}_{l,i}^* - \mathbf{F}_{l,i} = -\nabla_{\mathbf{r}_i} U_{l,*}^{\mathbf{k} \neq \mathbf{0}} + \nabla_{\mathbf{r}_i} U_l^{\mathbf{k} \neq \mathbf{0}}.$$

The unbiasedness of the random batch approximation is summarized in the following proposition.

PROPOSITION 5.1. $\mathbf{F}_{l,i}^*$ is an unbiased estimator, i.e., $\mathbb{E}\chi_i = \mathbf{0}$, and its variance can be expressed as

$$\mathbb{E} \|\chi_i\|^2 = \frac{H}{P} \sum_{\mathbf{k} \in \mathcal{K}^2, \mathbf{k} \neq \mathbf{0}} e^{-\frac{\|\mathbf{k}\|^2}{4\alpha}} \left\| \nabla_{\mathbf{r}_i} \phi(\mathbf{k}) - \frac{1}{H} \sum_{\mathbf{k}' \in \mathcal{K}^2, \mathbf{k}' \neq \mathbf{0}} \nabla_{\mathbf{r}_i} \phi(\mathbf{k}') e^{-\frac{\|\mathbf{k}'\|^2}{4\alpha}} \right\|^2.$$

Furthermore, under the Debye–Hückel (DH) approximation [51], we have Lemma 5.2, whose proof can be found in the supplementary materials (sm.pdf [local/web 248KB]).

LEMMA 5.2. *Under the assumption of the DH theory, given a function of the form*

$$(5.10) \quad \mathcal{G}(\mathbf{r}_i) = \sum_{j \neq i} q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} f(z_{ij}),$$

where $|f(z_{ij})|$ is bounded by a constant C_f independent of z_{ij} , the magnitude of $\mathcal{G}(\mathbf{r}_i)$ is bounded above by

$$(5.11) \quad |\mathcal{G}(\mathbf{r}_i)| \leq q_i C_f \lambda_D^2,$$

where λ_D represents the Debye length.

Finally, we introduce Theorem 5.3 for the boundedness and convergence of the fluctuations originating from the random batch approximation.

THEOREM 5.3. *Under the assumption of the DH theory, the variance of the force estimators has the following upper bound:*

$$(5.12) \quad \mathbb{E} \|\boldsymbol{\chi}_i\|^2 \leq \frac{H^2 q_i^2 \lambda_D^4}{2P \epsilon_c^2 L_x^2 L_y^2} \left(\frac{1 + |\gamma_u| + |\gamma_d| + |\gamma_u \gamma_d|}{1 - \max\{0, \gamma_u \gamma_d e^{-2k_{\min} L_z}\}} \right)^2,$$

where λ_D represents the Debye length.

In particular, for any fixed simulation box the denominator above is strictly positive, so the variance bound remains finite even in the symmetric conductor-like limit $\gamma_u = \gamma_d \rightarrow -1$.

Proof. We observe that

$$\nabla_{\mathbf{r}_i} \phi(\mathbf{k}) = \sum_{q=1}^4 \nabla_{\mathbf{r}_i} \{S_q(\mathbf{k})\} h_q(\mathbf{k}),$$

thus, we have

$$\begin{aligned} \nabla_{\mathbf{r}_i} S_1(\mathbf{k}) &= \sum_{j, j \neq i} q_i q_j \begin{pmatrix} i\mathbf{k} \\ \pm k \end{pmatrix} e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{-k|z_i - z_j|}, \\ \nabla_{\mathbf{r}_i} S_2(\mathbf{k}) &= \sum_{j, j \neq i} q_i q_j \begin{pmatrix} i\mathbf{k} \\ -k \end{pmatrix} e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{-k(z_i + z_j)}, \\ \nabla_{\mathbf{r}_i} S_3(\mathbf{k}) &= \sum_{j, j \neq i} q_i q_j \begin{pmatrix} i\mathbf{k} \\ k \end{pmatrix} e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{k(z_i + z_j)}, \\ \nabla_{\mathbf{r}_i} S_4(\mathbf{k}) &= \sum_{j, j \neq i} q_i q_j \begin{pmatrix} i\mathbf{k} \\ \pm k \end{pmatrix} e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} e^{k|z_i - z_j|}, \end{aligned}$$

and the choice of $+$ or $-$ depends on the particle considered. Consequently, $\nabla_{\mathbf{r}_i} \phi(\mathbf{k})$ takes the form

$$\nabla_{\mathbf{r}_i} \phi(\mathbf{k}) = \sum_{j, j \neq i} q_i q_j e^{i\mathbf{k} \cdot \boldsymbol{\rho}_{ij}} \begin{pmatrix} i\mathbf{k} \\ \pm k \end{pmatrix} g(z_{ij}),$$

Since the random batch estimator in (5.7) samples only modes with $\mathbf{k} \neq \mathbf{0}$, every sampled mode satisfies $k \geq k_{\min}$. Therefore,

$$1 - \gamma_u \gamma_d e^{-2k L_z} \geq 1 - \max\{0, \gamma_u \gamma_d e^{-2k_{\min} L_z}\},$$

and the estimate for $g(z_{ij})$ reads

$$|g(z_{ij})| \leq \frac{1 + |\gamma_u| + |\gamma_d| + |\gamma_u \gamma_d|}{4\epsilon_c L_x L_y k (1 - \max\{0, \gamma_u \gamma_d e^{-2k_{\min} L_z}\})}.$$

By Lemma 5.2, an upper bound for $\|\nabla_{\mathbf{r}_i} \phi(\mathbf{k})\|$ can be estimated as follows:

$$(5.13) \quad \|\nabla_{\mathbf{r}_i} \phi(\mathbf{k})\| \leq \frac{q_i \lambda_D^2}{2\epsilon_c L_x L_y} \frac{1 + |\gamma_u| + |\gamma_d| + |\gamma_u \gamma_d|}{1 - \max\{0, \gamma_u \gamma_d e^{-2k_{\min} L_z}\}}.$$

Finally, the variance of the force on the i th particle is bounded above by

$$\begin{aligned} \mathbb{E} \|\chi_i\|^2 &\leq \frac{2H}{P} \sum_{\mathbf{k} \in \mathcal{K}^2, \mathbf{k} \neq \mathbf{0}} e^{-\frac{\|\mathbf{k}\|^2}{4\alpha}} \|\nabla_{\mathbf{r}_i} \phi(\mathbf{k})\|^2 \\ &\leq \frac{2H^2}{P} \left(\frac{q_i \lambda_D^2}{2\epsilon_c L_x L_y} \frac{1 + |\gamma_u| + |\gamma_d| + |\gamma_u \gamma_d|}{1 - \max\{0, \gamma_u \gamma_d e^{-2k_{\min} L_z}\}} \right)^2 \\ &= \frac{H^2 q_i^2 \lambda_D^4}{2P \epsilon_c^2 L_x^2 L_y^2} \left(\frac{1 + |\gamma_u| + |\gamma_d| + |\gamma_u \gamma_d|}{1 - \max\{0, \gamma_u \gamma_d e^{-2k_{\min} L_z}\}} \right)^2. \quad \square \end{aligned}$$

We note that $H \sim L_x L_y$ and $\mathbb{E} \|\chi_i\|^2 = \mathcal{O}(\frac{1}{P})$, which is *independent* of the particle number N . Next, we demonstrate that such a random batch approximation for forces can capture the finite time dynamics of the Langevin thermostat, i.e., (2.3). Specifically, consider a numerical integration of (2.3) with discretized time step Δt , where $\mathbf{r}_i$, m_i , and $\mathbf{p}_i$ denote the position, mass, and momentum of the i th particle, respectively. We have the following strong convergence result.

THEOREM 5.4 (strong convergence). *Let $(\mathbf{r}_i, \mathbf{v}_i)$ be the solutions to*

$$\begin{aligned} d\mathbf{r}_i &= \mathbf{v}_i dt, \\ m_i d\mathbf{v}_i &= [\mathbf{F}_i - \gamma \mathbf{v}_i] dt + \sqrt{\frac{2\gamma}{\beta}} d\mathbf{W}_i, \end{aligned}$$

where $\{\mathbf{W}_i\}_{i=1}^N$ are i.i.d. Wiener processes. Let $(\tilde{\mathbf{r}}_i, \tilde{\mathbf{v}}_i)$ be the solutions to

$$\begin{aligned} d\tilde{\mathbf{r}}_i &= \tilde{\mathbf{v}}_i dt, \\ m_i d\tilde{\mathbf{v}}_i &= [\mathbf{F}_i + \chi_i - \gamma \tilde{\mathbf{v}}_i] dt + \sqrt{\frac{2\gamma}{\beta}} d\mathbf{W}_i, \end{aligned}$$

with the same initial values as $(\mathbf{r}_i, \mathbf{v}_i)$. Suppose that the masses m_i are bounded uniformly from above and below. If the forces $\mathbf{F}_i$ are bounded and Lipschitz and $\mathbb{E}\chi_i = 0$, then for any $T > 0$, there exists $C(T) > 0$ such that

$$\mathbb{E} \left[\frac{1}{N} \sum_i (\|\mathbf{r}_i - \tilde{\mathbf{r}}_i\|^2 + \|\mathbf{v}_i - \tilde{\mathbf{v}}_i\|^2) \right] \leq C(T) \sqrt{\Lambda \Delta t},$$

where Λ is an upper bound for $\max_i \mathbb{E} \|\chi_i\|^2$ and is independent of N .

Similar proofs can be found in [54, 44, 87], so we omit the proof here. It is important to note, however, that in practical molecular dynamics (MD) simulations, both electrostatic and Lennard–Jones interactions can violate the required Lipschitz continuity and boundedness conditions as $r \rightarrow 0$. Consequently, rigorously justifying convergence with singular interactions is challenging and remains an open question. Nonetheless, we contend that Theorem 5.4 should still hold in practice for two reasons: (1) the Lennard–Jones (LJ) potential, which is employed in MD simulations to represent the finite size of particles, provides strong short-range repulsion, preventing particles from approaching the singularity; and (2) the substantial variance reduction achieved through the importance sampling technique mitigates stability issues. Numerical results presented in the next section will further validate the effectiveness of the random batch method in capturing finite-time structure and dynamic properties, consistent with the conclusions of Theorem 5.4.

6. Numerical results. In this section, we evaluate the accuracy and efficiency of the proposed QEM method using representative charged systems under confinement. These examples highlight characteristic multiscale phenomena, including dielectric boundary effects, anisotropic diffusion, and electrical double layer (EDL) structures under charge-asymmetric conditions. Simulations were performed on a single core of an AMD Ryzen Threadripper PRO 3995WX @ 2.2 GHz workstation. The software implementation [21] relies on Julia [7] and *CellListMap.jl* [65], with visualizations generated via *Makie.jl* [12].

6.1. Convergence validation on static configurations. We first validate the convergence of our method by calculating electrostatic energy and force fields for static particle configurations under quasi-2D confinement. Figure 5 compares the electrostatic fields in the x and z directions for a pair of oppositely charged particles under different dielectric confinements against reference values from the Image Charge Method (ICM). The simulation box is $(100, 100, 50)$. A charge $q_1 = +1$ is fixed at $(50, 50, 1)$, while a second charge $q_2 = -1$ moves along either the x - or z -axis. For QEM, parameters are $\alpha = 1.0$ and $n = 50$. For the ICM benchmark, we use (2.7) with $(200, 200)$ periodic images in xy and 40 reflections in z (totaling 16,000 image charges per source) to guarantee high accuracy. The results in Figure 5 show excellent agreement between QEM and the ICM benchmarks. Specifically, Figure 5(a) reveals that confinement by conductor-like materials ($\gamma = -0.95$) weakens the Coulomb attraction between opposite charges, whereas insulator-like confinement ($\gamma = 0.95$) enhances it. Furthermore, Figure 5(b) shows that the dielectric boundary exerts an attraction or repulsion on particles near the wall, arising from self-interaction with image charges. These results confirm that QEM accurately captures dielectric boundary effects under doubly periodic conditions.

We further validate QEM convergence by calculating the electrostatic interaction energy for a system of 100 randomly distributed particles, comparing against the standard Ewald2D method combined with ICM. Figure 6(a) plots the relative energy error as a function of the reflection factor γ and the error control parameter E . Here, E is chosen according to Theorem 4.1 such that the truncation errors satisfy

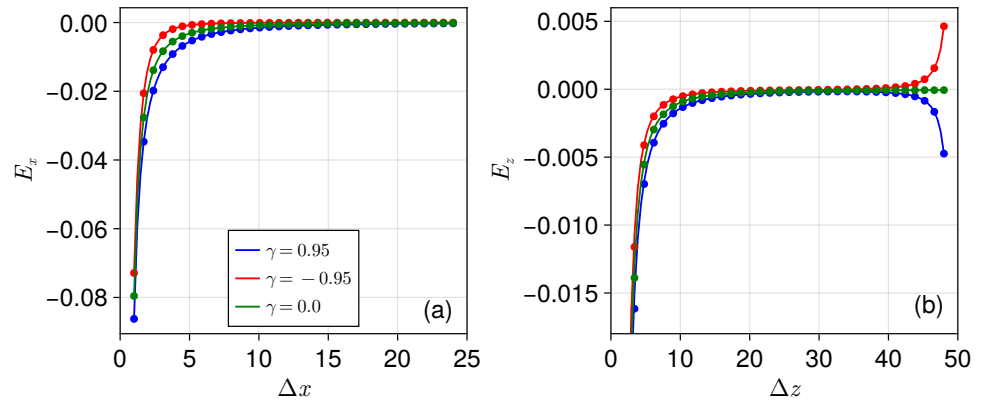


FIG. 5. Electrostatic fields in the (a) x and (b) z directions for a pair of oppositely charged particles confined in a box of size $(100, 100, 50)$. The positive particle is fixed at $(50, 50, 1)$, while the negative charge moves along (a) $(50 + \Delta x, 50, 1)$ and (b) $(50, 50, \Delta z)$, respectively. The solid lines are results obtained using QEM, and the dots represent benchmark values from ICM with a direct lattice sum of 16,000 image charges per particle.

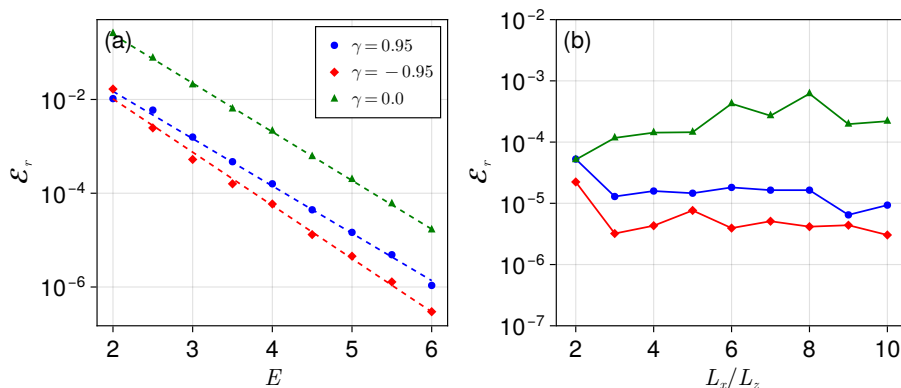


FIG. 6. Relative error of the electrostatic interaction energy of QEM compared to the Ewald2D method with ICM. The reflection factor γ is chosen as ± 0.95 or 0. (a) One hundred charged particles randomly distributed in a box of size $(100, 100, 50)$, as a function of the error control parameter E obtained from the truncation error analysis in Theorem 4.1. (b) Systems with $L_z = 10\tau_0$ and varying $L_x = L_y$ from $20\tau_0$ to $100\tau_0$, with a fixed particle density $\rho = 0.01$ and error control parameter $E = 4$. Each data point is averaged over 10 independent random configurations.

$\|\Delta I_b(M)\| \leq 10^{-E}$ and $\|\Delta \Pi(M)\| \leq 10^{-E}$. The results confirm that the relative error decreases as E increases, consistent with our theoretical analysis.

We also validate the convergence of QEM for systems with high aspect ratios, where we fix the thickness of the system in z to be $10\tau_0$, and vary the size of the system in x and y from $20\tau_0$ to $100\tau_0$ with a fixed particle density $\rho = 0.01$. In all cases, we fix the error control parameter E to be 4, with the other parameters chosen according to Theorem 4.1. As shown in Figure 6(b), the relative error remains stable across all aspect ratios, demonstrating the robustness of QEM performance, even under high aspect ratios.

6.2. Applications in MD simulations. To demonstrate the practical utility of QEM for MD simulations, we study prototypical ionic systems confined between two dielectric interfaces. The simulation box has dimensions $(100\tau_0, 100\tau_0, L_z)$ and contains 436 charged particles in a continuum solvent with Bjerrum length $\ell_B = e_0^2/(4\pi\epsilon_c k_B T) = 3.5\tau_0$. Ions are modeled as soft spheres of diameter τ_0 with excluded-volume interactions given by a purely repulsive shifted-truncated LJ potential with energy scale $\varepsilon_{LJ} = k_B T$. Confinement is enforced by purely repulsive shifted-truncated LJ walls ($\varepsilon_{\text{ion-wall}} = k_B T$; $\tau_{\text{ion-wall}} = 0.5\tau_0$) at $z = 0$ and $z = L_z$. We use a time step of $0.001t_0$, where $t_0 = \tau_0\sqrt{m_0/k_B T}$ is the time unit (with ion mass $m_0 = 1$), and control temperature via a Nosé–Hoover thermostat. QEM parameters are set to $E = 4$, $n = 40$, and batch size $P = 30$. Systems are equilibrated for 2×10^6 steps, followed by a production run of 3×10^6 steps. Sampling is performed every 100 steps, yielding 3×10^4 sampled configurations for statistical analysis.

6.2.1. MD simulations of symmetric systems. We first investigate symmetric systems with identical top and bottom reflection factors $\gamma = 0.95$ or -0.95 and a channel height $L_z = 50\tau_0$. The system comprises 218 cations and 218 anions with symmetric charges $\pm e_0$. To validate our QEM results, we compare the ion density profiles with benchmark data from the Harmonic Surface Mapping Algorithm (HSMA) [62]. Figure 7 shows excellent agreement between QEM and HSMA. Consistent with the static analysis in Figure 5(b), we observe ion accumulation near conductor-like

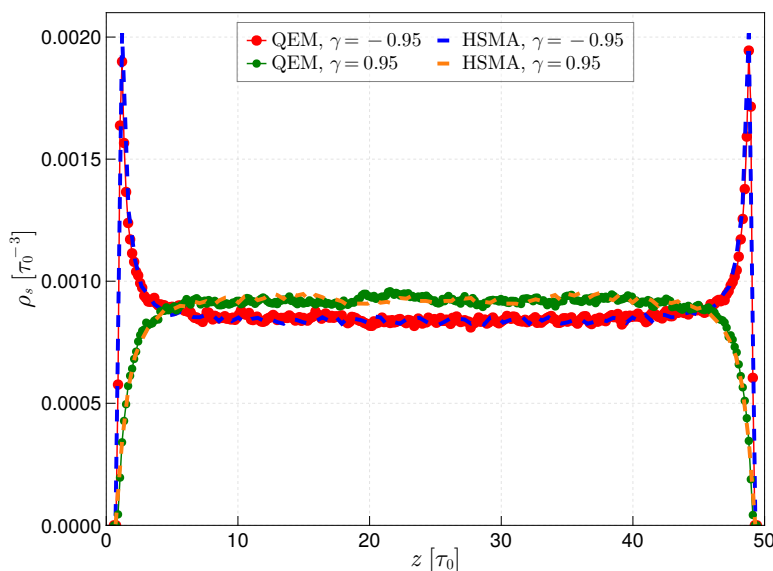


FIG. 7. Equilibrium distributions of ion densities in z for symmetric electrolytes. The simulation box contains 218 cations and 218 anions, with reflection factors $\gamma_u = \gamma_d = \pm 0.95$ at $z = 0$ and $50\tau_0$, respectively. The solid lines indicate results obtained by QEM, and dashed lines are benchmark values using the HSMA method.

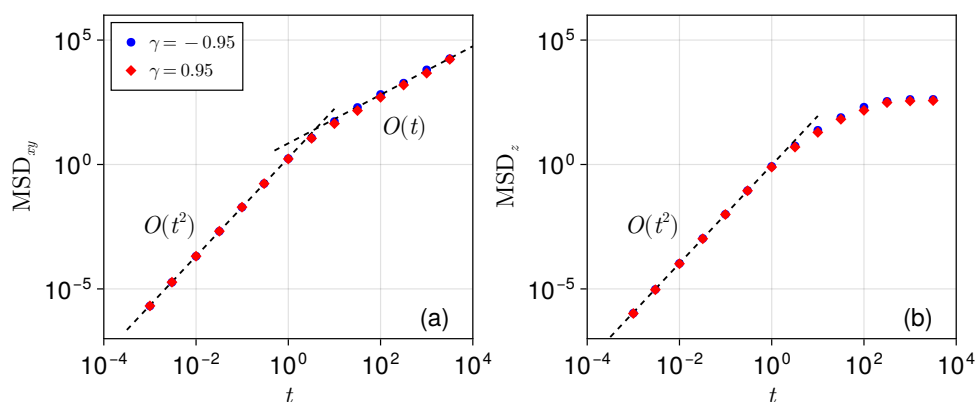


FIG. 8. The mean square displacements (MSD) of the confined particles in the (a) xy directions and (b) z direction, respectively, as a function of timescale t . Two reflection factor values, $\gamma = 0.95$ and -0.95 , are considered.

interfaces and depletion near insulator-like interfaces. We also compute the mean square displacements (MSD) in the xy plane and z direction. As shown in Figure 8(a), MSD_{xy} exhibits standard bulk-like behavior: a ballistic regime ($\sim t^2$) for $t < 1$ and a diffusive regime ($\sim t$) for $t > 1$. In contrast, Figure 8(b) shows that MSD_z saturates at large timescales. This anisotropic diffusion is a direct consequence of confinement.

The CPU time required by QEM to evaluate the interactions among N confined particles is shown in Figure 9, where the cost of the Ewald2D method is also plotted as a reference. We fix the thickness of the system in z to be $50\tau_0$, and vary the number of charged particles from 10^2 to 10^5 while keeping the ionic density fixed. Since we choose $E = 4$ in QEM, the Ewald2D parameters are also chosen to guarantee 4-digit

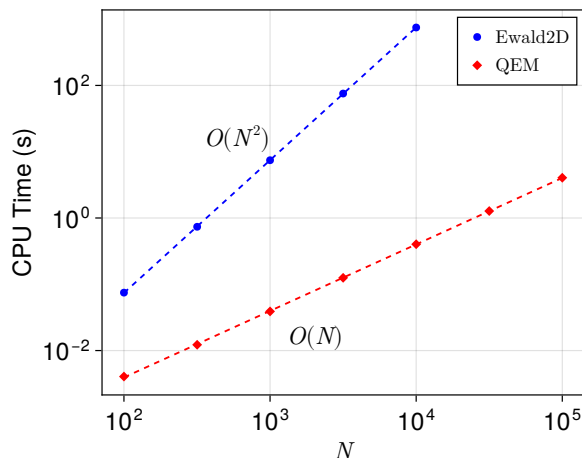


FIG. 9. CPU times for computing the electrostatic interactions between N particles. Blue and red dots indicate the CPU times of the Ewald2D method and QEM, respectively. Dashed lines are fitted scaling curves of $\mathcal{O}(N^2)$ and $\mathcal{O}(N)$. (Figure in color online.)

accuracy for a fair comparison. The CPU time results shown in Figure 9 indicate that the computational complexity of QEM is $\mathcal{O}(N)$, which allows the interactions among more than 10^4 particles to be computed within 1 s on a single core.

6.2.2. MD simulations of asymmetric systems. We now consider quasi-2D systems with asymmetry. Specifically, we consider two asymmetric scenarios: scenario I, asymmetry in the dielectric mismatches; and scenario II, charge asymmetry between cations and anions. In both scenarios, the thickness of the system is set as $L_z = 10\tau_0$, so that $L_{x/y}/L_z = 10$.

Scenario I: Effect of dielectric asymmetry. In this scenario, we investigate how asymmetric dielectric mismatches affect equilibrium ionic density distributions. We set $\gamma_d = -0.95$ and $\gamma_u = 0.95$ for a system containing 218 cations ($+e_0$) and 218 anions ($-e_0$). Figure 10 shows the resulting z -density profiles. Both cations and anions are attracted to the conductor-like lower interface and repelled by the insulator-like upper interface, creating a strongly biased ionic distribution.

Scenario II: Effect of charge asymmetry. Next, we examine the effect of charge asymmetry using a 3 : 1 salt solution. We set $\gamma_u = \gamma_d$ to 0.95 or -0.95 and simulate a system with 109 trivalent cations and 327 monovalent anions (maintaining 436 total particles). For conductor-like interfaces ($\gamma = -0.95$, Figure 11(a)), both species are attracted to the walls. However, the multivalent cations experience a stronger attraction, leading to a higher concentration near the interface. This accumulation effectively renders the neutral interface positively charged from a far-field perspective—a manifestation of “charge renormalization” [79]. Consequently, a secondary peak in the anion density appears at approximately $1.5\tau_0$, indicating charge stratification. This effect is known to be amplified near strongly charged surfaces or with larger ions [52]. Conversely, for insulator-like interfaces ($\gamma = 0.95$, Figure 11(b)), both ion types are repelled from the walls and concentrate in the channel center. Due to stronger repulsion forces, the multivalent cations are confined more strongly to the channel center, creating an effectively positive central layer surrounded by a diffuse cloud of anions. This results in the formation of an electrical double layer (EDL) at the channel center, driven by the interplay between dielectric boundary effects and many-body electrostatic interactions.

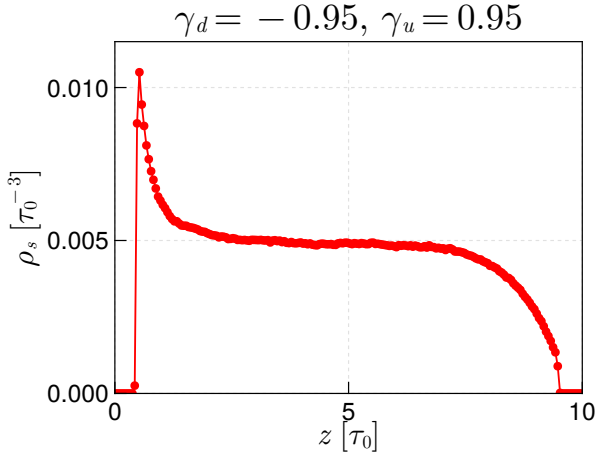


FIG. 10. Ionic density in z for symmetric electrolytes containing 218 cations and 218 anions, confined by neutral dielectric interfaces with $\gamma_u = 0.95$ and $\gamma_d = -0.95$ at $z = 0$ and $10\tau_0$, respectively. Due to the charge symmetry of the cations and anions, only the cation density is shown.

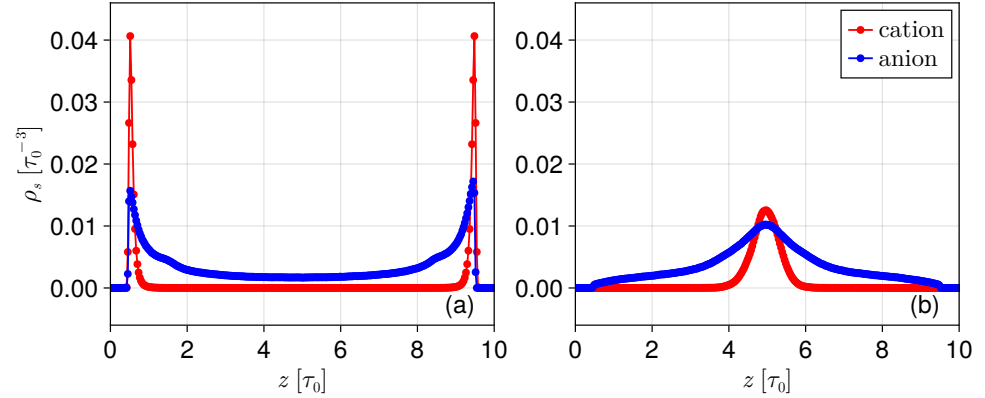


FIG. 11. Cation and anion densities in z for a 3 : 1 salt with 109 trivalent cations and 327 monovalent anions confined by neutral dielectric substrates with $\gamma_u = \gamma_d$ set to (a) -0.95 and (b) 0.95 . Here, red and blue lines indicate the densities of cations and anions, respectively. (Figure in color online.)

7. Conclusion. In summary, we have developed the quasi-Ewald method (QEM) for fast computation of quasi-2D nanoconfined electrostatics. Our method has been shown to be efficient and accurate, and it can be used to investigate various dielectric confinement effects in quasi-2D charged many-body systems. In the future, we will consider extending QEM to quasi-2D systems confined by metamaterials, where the dielectric contrast γ can be extended to the whole complex plane except for countably many poles [91]. Notably, ICM diverges in such scenarios, but we expect QEM to still work since it does not rely on ICM. Furthermore, we plan to apply QEM to practical applications, such as simulations of biomembranes and battery-electrolyte systems, where confinement effects can significantly influence material properties. Another interesting direction is to extend the current method to nonplanar geometries, such as confinement by undulating interfaces, which are commonly encountered in biological and energy storage systems. We anticipate that a boundary integral formulation

can be incorporated in such scenarios—where the quasi-Ewald splitting strategy may still be applied on the source charges to accelerate the numerical computations. We finally note that the variance bound proven in Theorem 5.3 is based on the DH theory, which becomes inaccurate for strongly correlated ionic systems [18, 3]; obtaining a tight variance bound for such challenging scenarios is reserved for future investigation.

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