Passing from Discrete to Continuum Models of Electrostatic Energy

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Abstract

We analyze the passage from discrete (i.e., point) charges and the corresponding discrete electrostatic energies to a continuum charge density and the corresponding continuum electrostatic energy in the limit of a large number of point charges. Given a continuous function on a bounded region that represents a continuum charge density, we construct a sequence of point charges and prove that the corresponding discrete electrostatic energies converge to the continuum counterpart. In a more general setting, we consider a given, compactly supported, signed Radon measure in the three-dimensional space representing the distribution of charges. We construct a sequence of point charges that converge to the given signed Radon measure and show that the corresponding discrete energies converge to the continuum one defined by the signed Radon measure. Conversely, for any sequence of point charges that satisfy certain reasonable assumptions on local geometry and excluded volumes, we prove that there exists a subsequence converging to a signed Radon measure and that the corresponding discrete energies converge to the continuum one defined by the limiting signed Radon measure. Tools used in our analysis include the explicit constructions of point charges from a given signed Radon measure as well as approximation properties of signed Radon measures. Finally, we apply our discrete-to-continuum analysis to the minimization of electrostatic energy related to the classical balayage problem in the potential theory. Such minimization can be potentially applied to the modeling of charged molecular systems with heterogeneously distributed charges embedded in a continuum solvent.

Keywords: Electrostatic energy, discrete-to-continuum passage, signed Radon measures, convergence, energy minimization.

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1 Introduction

The continuum electrostatic energy is defined to be [15, 19, 21, 25]

$$\int_{\mathbb{R}^3} \frac{1}{2}\rho\psi \, dx,$$

where the dielectric coefficient is taken to be unity in certain units. Here, $\rho : \mathbb{R}^3 \to \mathbb{R}$ is a given function representing a continuum charge density and $\psi : \mathbb{R}^3 \to \mathbb{R}$ is the electrostatic potential determined uniquely by Poisson's equation together with boundary conditions

$$\Delta\psi = -\rho \quad \text{in } \mathbb{R}^3 \qquad \text{and} \qquad \phi(\infty) = 0.$$

With some assumptions, the potential ψ can be expressed as (cf. p.23 in [12] and Section 1.7 in [21])

$$\psi(x) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{\rho(y)}{|x-y|} \, dy \qquad \forall x \in \mathbb{R}^3,$$

and the corresponding electrostatic energy can be expressed as

$$\int_{\mathbb{R}^3} \frac{1}{2}\rho\psi \, dx = \frac{1}{8\pi} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} \, dxdy. \tag{1.1}$$

In contrast, given a set of point charges $Q_i \in \mathbb{R}^3$ located at $x_i \in \mathbb{R}^3$ $(i = 1, \ldots, N)$, which determine a discrete charge density

$$\mu = \sum_{i=1}^{N} Q_i \delta_{x_i},$$

where δ_a is the Dirac measure concentrated at $a \in \mathbb{R}^3$, the discrete electrostatic energy, the Coulomb energy, is given by [15, 19, 21, 25]

$$\frac{1}{8\pi} \sum_{1\le i,j\le N, i\ne j} \frac{Q_i Q_j}{|x_i - x_j|}. \tag{1.2}$$

Both the continuum and discrete descriptions of electric charges and electrostatic energies are widely used in many areas of science and engineering, such as molecular biology, colloidal science, and chemical engineering. The discrete description of electrostatics is a main part of an interaction potential (i.e., forcefield) for a macromolecular system in molecular dynamics and Monte Carlo simulations that have been extensively developed in recent decades [10, 17, 20, 22, 23, 31, 35]. In implicit-solvent models for biological molecules, both discrete and continuum descriptions of charge densities are used [8, 34, 36, 39, 40].

Intuitively, the passage from the discrete to continuum description is clear: if the number of point charges is large enough, then the discrete charge density and the discrete electrostatic energy should be close to the continuum charge density and the continuum electrostatic energy, respectively. This is indeed true, as we justify here such a statement in several settings.

Our main results are as follows:

(1) Assume Ω is a bounded region in $\mathbb{R}^3$ and $\rho \in C(\overline{\Omega})$. We can decompose the region Ω into the union of many small regions ω^i and define charges $Q_i = \rho(x^i)|\omega^i|$ with x^i and $|\omega^i|$ a point in ω^i and the volume of ω^i, respectively. Then as the number of charges increases to infinity and the volume of each small region decreases to zero, the discrete electrostatic energies (cf. (1.2)) converge to the continuum one (cf. (1.1)); cf. Theorem 2.1;

(2) Given a compactly supported signed Radon measure μ on $\mathbb{R}^3$, we construct a sequence of point charges

$$\mu_n = \frac{1}{N_n} \sum_{i=1}^{N_n} Q_n^i \delta_{x_n^i} \tag{1.3}$$

that converge in a weak sense to the signed Radon measure μ and that the corresponding discrete energies converge to the energy defined by the given signed Radon measure; cf. Theorem 3.1; and

(3) Conversely, given a sequence of point charges as in (1.3) such that their locations are nearly evenly distributed in a bounded region in $\mathbb{R}^3$ and that their values are uniformly bounded (i.e., $\sup_{n,i} |Q_n^i| < \infty$), we show that there exists a subsequence that converges to a limiting signed Radon measure, and the corresponding discrete energies converge to the continuum one; cf. Theorem 4.1. We also give an example to show the nonuniqueness of such a subsequence.

In addition, we apply our analysis to an electrostatic energy minimization problem related to the classical balayage problem in the potential theory; cf. Theorem 5.1. Such an application can potentially be developed into a model for the charged molecules embedded in a continuum solvent, where the charge distributions are often heterogeneous [7,8,39,41].

Let us make several remarks on our results. First, our result on the discrete-to-continuum passage with a given continuous and bounded function representing a charge density (cf. Part (1) above) is a special case with a given signed Radon measure (cf. Part (2) above), as any continuous and bounded function defines uniquely such a measure. However, with a continuous function, the construction of discrete charges is explicit, and the proof of the discrete-to-continuum passage is also more intuitive, allowing us to better understand such a passage. Second, our results are not complete and there are still some open questions. One of them is whether or not the results in Part (3) above can be generalized to the case where the sequence of discrete charges are not quite evenly distributed in the entire region but are rather concentrated only on a measurable subset that may be very irregular. Another related question is to identify conditions under which the density of a limiting measure is continuous or even differentiable. Third and finally, we only prove the discrete-to-continuum convergence of charge densities and electrostatic energies, but provide no quantitative convergence rates. In particular, since we do not consider effects of charge sizes, correlations, and fluctuations, our analysis does not justify the use of continuum electrostatics in certain circumstances where the discreteness is strong.

The mathematical analysis of the discrete-to-continuum passage is a common task in understanding an underlying physical system. Often, one begins with a pairwise inter-

action potential, augmented by some external potential, defined on lattices, and derives a continuum energy in the limit of vanishing lattice size. For instance, in recent studies on problems arising from solid mechanics and materials, the interaction potential can be the Lennard-Jones potential or some potential modeling material defects (e.g., dislocations), and the techniques of analysis include homogenization and Γ-convergence; cf. e.g., [1–3, 5, 18, 30].

Relevant to our work are the studies presented in [6,11,32,37,38] (cf. also the references therein). In [6], the authors considered the discrete electrostatic energy of the interaction of N (-1)-charges and between these "electrons" and M positively charged "atomic nuclei" with a hard core and a total charge Z. They show the Γ-convergence as $N, Z \to \infty$ with M fixed and N/Z asymptotically equal to a constant λ of these discrete energy functionals to a continuum energy functional I defined on all the Radon measures μ on $\mathbb{R}^3$ given by

$$I(\mu) = \frac{1}{2} \iint_{(\mathbb{R}^3\setminus\Omega)\times(\mathbb{R}^3\setminus\Omega)} \frac{d\mu(x)d\mu(y)}{|x-y|} + \int_{\mathbb{R}^3\setminus\Omega} V(x)\, d\mu(x),$$

if the total mass of μ is bounded above by λ and $I(\mu) = +\infty$ otherwise, where V describes the Coulomb interaction between the nuclei and electrons through their limiting distributions and where Ω is the hardcore region of all the nuclei. The large-N analysis further shows charge screening. Some parts of the analysis in [32, 37, 38] (cf. also the references therein) obtain a similar Γ-convergence for a sequence of discrete energies as the number of charges tends to infinity. Each energy results from the interaction among finitely many $(+1)$-charges together with an external potential on each of these charges. A growth assumption on the external potential is made to show that the infimum of the Γ-limit is finite and the convergence of the discrete minimizers and minimum values to their continuum counterparts.

In contrast, we consider charges of different signs and different values (partial charges) confined in an arbitrary bounded region (with some regularities), and our results are for any sequence of discrete charge configurations not necessary energy-minimizing ones. We also consider a general question on the construction of discrete quantities from a given continuum one and obtain the discrete-to-continuum passage, not just inequalities as in the Γ-convergence analysis. In addition, our renewed result on the classical balayage problem (cf. section 5) may possibly be applied to the study of charged macromolecules that often have heterogenous charge distributions.

Our analysis relies on several techniques. One of them is the construction of point charges from a given signed Radon measure. Such constructions have been initially developed in [6]; cf. also [37]. The other is to construct a family of diffeomorphisms to "flow" the charges on the boundary of an underlying bounded open set into the interior of such an open set so that various smoothing and approximating methods can be used to define the point charges that are supported inside the open set. This technique may be used to smooth out surface charges. In studying the continuum limit of a sequence of discrete charges, we identify geometrical conditions that imply the existence of an L^∞-density.

The rest of the paper is organized as follows. In section 2, we are given a continuous

function on a bounded region and define discrete charges from such a function. We then prove the convergence of the corresponding discrete energies to the continuum one. In section 3, we consider the general case in which a compactly supported signed Radon measure is given to represent a distribution of charges. We construct discrete charges and show that they converge to the signed Radon measure and that the corresponding discrete energies converge to the continuum one defined by the signed Radon measure. In section 4, we prove the converse: given a sequence of point charges satisfying certain geometrical conditions, there exists a subsequence of such charges that converges to a signed Radon measure. Moreover, the corresponding energies also converge to the one defined by the limiting signed Radon measure. Finally, in section 5, we prove the existence and uniqueness of the minimizer of the electrostatic energy functional defined on signed Radon measures with an external field, and also prove that the minimizer can be approximated by point charges that are supported in a small neighborhood of the boundary of the underlying bounded region.

2 Convergence of Discrete Energies with a Given Continuous Function of Charge Density

In this section, we construct a sequence of discrete charges from a given continuum charge density. We prove that the corresponding sequence of discrete energies converge to the continuum energy defined by the given charge density.

Let Ω be a nonempty, bounded, open subset of $\mathbb{R}^3$ with a Lipschitz-continuous boundary $\partial\Omega$. Let $\rho \in C(\overline{\Omega})$ represent a charge density. The corresponding (continuum) electrostatic energy is given by [21]

$$\frac{1}{8\pi}\iint_{\Omega\times\Omega}\frac{\rho(x)\rho(y)}{|x-y|}\,dxdy, \tag{2.1}$$

where the dielectric coefficient is taken to be unity in certain units.

We now define a sequence of discrete charges from the density ρ. We call a class of finitely many subsets of $\overline{\Omega}$ a *partition* of $\overline{\Omega}$, if each of these subsets is a domain in $\mathbb{R}^3$ with a Lipschitz-continuous boundary, these subsets are pairwise disjoint, and the union of the closures of these subsets is $\overline{\Omega}$. We call these subsets *cells* of the partition. A sequence of partitions, $\{\mathcal{P}_n\}_{n=1}^{\infty}$, of $\overline{\Omega}$ is *admissible* if there exist natural numbers $N_n \nearrow +\infty$ and real numbers $r_n \searrow 0$ such that each $\mathcal{P}_n$ consists of two parts: ω_n^i $(i = 1, \ldots, N_n)$ (called *regular cells*) and the remaining cells, if any (called *irregular cells*), that satisfy the following two conditions:

- *The uniform size condition:* There exists a constant $\gamma \in (0, 1)$, and for each $n \geq 1$ and each i $(1 \leq i \leq N_n)$, there exists $x_n^i \in \omega_n^i$ (a point of charge) such that

$$B(x_n^i, r_n) \subseteq \omega_n^i \subseteq B\left(x_n^i, \frac{r_n}{\gamma}\right); \tag{2.2}$$

- *The almost covering condition:*

$$\lim_{n\to\infty}\left|\overline{\Omega}\setminus\left(\bigcup_{i=1}^{N_n}\overline{\omega_n^i}\right)\right|=0. \tag{2.3}$$

Here and below, we denote by $|A|$ the Lebesgue measure of a Lebesgue-measurable set A. Since $r_n \searrow 0$, the uniform size condition implies that

$$\|\mathcal{P}_n\|_{\text{reg}} := \max_{1\le i\le N_n} \operatorname{diam}(\overline{\omega_n^i}) \le \frac{2r_n}{\gamma} \to 0 \qquad \text{as } n\to\infty. \tag{2.4}$$

A typical example of an admissible sequence of partitions $\mathcal{P}_n$ $(n = 1, 2, \dots)$ of Ω is as follows: all the regular cells of $\mathcal{P}_n$ consist of all the cubes that are subsets of $\overline{\Omega}$ and that have their sides 2^{-n} and faces on coordinate planes with values $j + k2^{-n}$, where j and k are integers and $0 \le k \le 2^n - 1$. We have $r_n = 2^{-n-1}$. The points x_n^i are the centers of the regular cells. The uniform size condition is satisfied with $\gamma = 2/\sqrt{3}$. Since the boundary $\partial\Omega$ is Lipschitz-continuous,

$$\lim_{\eta\to 0}|\{x\in\Omega : \operatorname{dist}(x,\partial\Omega)\le\eta\}| = 0;$$

cf. e.g., [27]. Therefore, the almost covering condition (2.3) is satisfied.

Given an admissible sequence of partitions $\{\mathcal{P}_n\}_{n=1}^{\infty}$ of $\overline{\Omega}$ as above, we define the sequence of discrete charges $\{Q_n^i\delta_{x_n^i}\}_{i=1}^{N_n}$ $(n = 1, 2, \dots)$ (i.e., we place the charge Q_n^i at point x_n^i) corresponding to the given charge density ρ by

$$Q_n^i = \rho(x_n^i)|\omega_n^i|, \qquad i = 1,\dots,N_n;\ n = 1,2,\dots \tag{2.5}$$

This means that the discrete charge density for each n is

$$\mu_n = \sum_{i=1}^{N_n} Q_n^i\delta_{x_n^i} = \frac{1}{N_n}\sum_{i=1}^{N_n}\hat{Q}_n^i\delta_{x_n^i},$$

where $\hat{Q}_n^i = N_nQ_n^i$. By (2.2) and (2.3), we see that $\hat{Q}_n^i$ and $\rho(x_n^i)$ are of the same order, i.e., the ratio $\hat{Q}_n^i/\rho(x_n^i)$ (if $\rho(x_n^i)\neq 0$) is bounded above and below by two positive constants that are independent of i and n, if n is large enough. Note in particular that the total charge in the limit of large number of charges is

$$\lim_{n\to\infty}\sum_{i=1}^{N_n} Q_n^i = \int_\Omega \rho(x)\,dx.$$

By Coulomb's law [21], the corresponding discrete electrostatic energy for each n is given by

$$\frac{1}{8\pi}\sum_{i,j=1,i\neq j}^{N_n}\frac{Q_n^iQ_n^j}{|x_n^i - x_n^j|}. \tag{2.6}$$

The main result of this section is Theorem 2.1 below. It states that the discrete electrostatic energies converge to the continuum one given by (2.1). This is a special case of Lemma 3.2 in terms of the discrete-to-continuum passage. But the construction of nearly evenly distributed discrete charges here is natural and explicit, and is a stronger result.

Theorem 2.1. *Let $\Omega \subset \mathbb{R}^3$ be nonempty, bounded, and open with a Lipschitz-continuous boundary $\partial\Omega$. Let $\rho \in C(\overline{\Omega})$. Let $\{\mathcal{P}_n\}_{n=1}^{\infty}$ be a sequence of admissible partitions of Ω with regular cells ω_n^i and charges Q_n^i at points $x_n^i \in \omega_n^i$ $(i = 1, \dots, N_n; n = 1, 2, \dots)$, all as defined above. We have*

$$\lim_{n\to\infty} \sum_{i,j=1, i\neq j}^{N_n} \frac{Q_n^i Q_n^j}{\left|x_n^i - x_n^j\right|} = \iint_{\Omega\times\Omega} \frac{\rho(x)\rho(y)}{|x-y|}\, dxdy. \tag{2.7}$$

We need the following lemma to prove the theorem: (This lemma will also be used in proving Lemma 3.2.)

Lemma 2.1. *If x_0, $y_0 \in \mathbb{R}^3$ and R, $S > 0$ satisfy $B(x_0, R) \cap B(y_0, S) = \emptyset$, then*

$$\frac{1}{|x_0 - y_0|} = \frac{1}{|B(x_0, R)|\,|B(y_0, S)|} \int_{B(x_0,R)} \int_{B(y_0,S)} \frac{1}{|x-y|}\, dydx$$

Proof. Note that $1/|z|$ is a harmonic function for $z \in \mathbb{R}^3 \setminus \{0\}$. Note also that $x \notin B(y_0, S)$ if $x \in B(x_0, R)$. Thus it follows from the (volumetric) mean-value theorem for a harmonic function that

$$\begin{aligned}
\frac{1}{|x_0 - y_0|} &= \frac{1}{|B(x_0, R)|} \int_{B(x_0,R)} \frac{1}{|x - y_0|}\, dx \\
&= \frac{1}{|B(x_0, R)|} \int_{B(x_0,R)} \left[\frac{1}{|B(y_0, S)|} \int_{B(y_0,S)} \frac{1}{|x-y|}\, dy \right] dx \\
&= \frac{1}{|B(x_0, R)|\,|B(y_0, S)|} \int_{B(x_0,R)} \int_{B(y_0,S)} \frac{1}{|x-y|}\, dydx,
\end{aligned}$$

The proof is complete. □

Proof of Theorem 2.1. We denote

$$f(x, y) = \frac{\rho(x)\rho(y)}{|x-y|} \qquad \forall x, y \in \Omega.$$

Clearly, $f \in L^1(\Omega \times \Omega)$. We also denote

$$E = \iint_{\Omega\times\Omega} f(x, y)\, dxdy \qquad \text{and} \qquad E_n = \sum_{i,j=1, i\neq j}^{N_n} \frac{Q_n^i Q_n^j}{\left|x_n^i - x_n^j\right|}.$$

We need to prove $\lim_{n\to\infty} E_n = E$, and we divide our proof into three steps.

Step 1. Treatment of irregular cells. For each $n \geq 1$, let us denote by R_n and I_n the class of all regular cells and irregular cells of the partition $\mathcal{P}_n$, and by $\cup R_n$ and $\cup I_n$ their unions, respectively. Since $f(x,y) = f(y,x)$, for each n we have by (2.1) that

$$\begin{aligned}
E &= \iint_{\Omega\times\Omega} f(x,y)\,dxdy \\
&= \left(\int_{\cup R_n} + \int_{\cup I_n}\right)\left[\left(\int_{\cup R_n} + \int_{\cup I_n}\right) f(x,y)\,dx\right] dy \\
&= \int_{\cup R_n}\int_{\cup R_n} f(x,y)\,dxdy + \int_{\cup I_n}\int_{\cup I_n} f(x,y)\,dxdy + 2\int_{\cup I_n}\int_{\cup R_n} f(x,y)\,dxdy \\
&= \iint_{(\cup R_n)\times(\cup R_n)} f(x,y)\,dxdy + \iint_{(\cup I_n)\times(\cup I_n)} f(x,y)\,dxdy + 2\iint_{(\cup I_n)\times(\cup R_n)} f(x,y)\,dxdy.
\end{aligned}$$

It then follows from the almost covering condition (2.3) that $\lim_{n\to\infty} |\cup I_n| = 0$, which implies that $\lim_{n\to\infty} |(\cup I_n)\times(\cup I_n)| = 0$ and $\lim_{n\to\infty} |(\cup I_n)\times(\cup R_n)| = 0$. Hence,

$$E = \lim_{n\to\infty} \iint_{(\cup R_n)\times(\cup R_n)} f(x,y)\,dxdy.$$

It therefore suffices to show that, for any $\varepsilon > 0$, there exists a natural number N such that

$$\left|\iint_{(\cup R_n)\times(\cup R_n)} f(x,y)\,dxdy - E_n\right| < \varepsilon \qquad \forall n \geq N. \tag{2.8}$$

Step 2. Treatment of pairs of regular cells in a small neighborhood of the diagonal region $D := \{(x,y) \in \overline{\Omega}\times\overline{\Omega} : x = y\}$. By the integrability of $f(x,y)$ and that of $1/|x-y|$ on $\Omega\times\Omega$, there exists $\delta > 0$ such that for any measurable subset $A \subseteq \Omega\times\Omega$

$$\iint_A |f(x,y)|\,dxdy < \frac{\varepsilon}{3} \quad \text{and} \quad \iint_A \frac{dxdy}{|x-y|} < \frac{\varepsilon\gamma^6}{3(\|\rho\|_\infty^2 + 1)} \qquad \text{if } |A| < \delta, \tag{2.9}$$

where γ is the same as in (2.2). Denote

$$D_\alpha = \{(x,y) \in \Omega\times\Omega : \operatorname{dist}((x,y), D) < \alpha\}$$

for any $\alpha > 0$. Since Ω is bounded, $|D_\alpha| \to 0$ as $\alpha \to 0$. Thus, there exists $\eta > 0$ such that

$$|D_{2\eta}| < \delta. \tag{2.10}$$

For each $n \geq 1$, let us denote

$$\begin{aligned}
T_{n,\eta} &= \{\omega_n^i \times \omega_n^j : 1 \leq i,j \leq n, (\omega_n^i \times \omega_n^j) \cap D_\eta \neq \emptyset\}, \\
S_{n,\eta} &= \{\omega_n^i \times \omega_n^j : 1 \leq i,j \leq n, (\omega_n^i \times \omega_n^j) \cap D_\eta = \emptyset\}.
\end{aligned}$$

Note that $S_{n,\eta}$ and $T_{n,\eta}$ are disjoint. Moreover,

$$(\cup R_n) \times (\cup R_n) = (\cup S_{n,\eta}) \cup (\cup T_{n,\eta}). \tag{2.11}$$

By (2.4), there exists $\tilde{N}$ such that

$$\cup T_{n,\eta} \subseteq D_{2\eta} \qquad \text{if } n \geq \tilde{N}. \tag{2.12}$$

This, together with (2.10) and (2.9), implies that

$$\iint_{\cup T_{n,\eta}} |f(x,y)|\, dxdy < \frac{\varepsilon}{3} \quad \text{and} \quad \iint_{\cup T_{n,\eta}} \frac{dxdy}{|x-y|} < \frac{\varepsilon\gamma^6}{3(\|\rho\|_\infty^2+1)} \quad \text{if } n \geq \tilde{N}. \tag{2.13}$$

Now, let $\omega_n^i \times \omega_n^j \in T_{n,\eta}$ with $i \neq j$. It follows from the definition of Q_n^i and Q_n^j (cf. (2.5)), Lemma 2.1, and the uniform size condition (cf. (2.2)) that

$$\begin{aligned}
\frac{|Q_n^i Q_n^j|}{|x_n^i - x_n^j|} &\leq \frac{\|\rho\|_\infty^2 |\omega_n^i|\, |\omega_n^j|}{|x_n^i - x_n^j|} \\
&= \frac{\|\rho\|_\infty^2 |\omega_n^i|\, |\omega_n^j|}{|B(x_n^i, r_n)|\, |B(x_n^j, r_n)|} \iint_{B(x_n^i,r_n)\times B(x_n^j,r_n)} \frac{dxdy}{|x-y|} \\
&\leq \frac{\|\rho\|_\infty^2}{\gamma^6} \iint_{\omega_n^i\times\omega_n^j} \frac{dxdy}{|x-y|} \qquad \text{if } n \geq \tilde{N}.
\end{aligned}$$

This and (2.13) then imply that

$$\left| \sum_{\omega_n^i\times\omega_n^j \in T_{n,\eta}, i\neq j} \frac{Q_n^i Q_n^j}{|x_n^i - x_n^j|} \right| \leq \frac{\|\rho\|_\infty^2}{\gamma^6} \int_{\cup T_{n,\eta}} \frac{dxdy}{|x-y|} < \frac{\varepsilon}{3} \qquad \text{if } n \geq \tilde{N}. \tag{2.14}$$

Step 3. Treatment of pairs of regular cells away from the diagonal region D. The uniform continuity of f on $\overline{\Omega\times\Omega} \setminus D_\eta$ implies the existence of $\sigma > 0$ such that

$$|f(x,y) - f(x',y')| < \frac{\varepsilon}{3|\Omega\times\Omega|} \qquad \text{if } |(x,y)-(x',y')| < \sigma. \tag{2.15}$$

By (2.4), there exists a natural number $\hat{N}$ such that $\|\mathcal{P}_n\|_{\text{reg}} < \sigma$ if $n \geq \hat{N}$. Note that if $\omega_n^i \times \omega_n^j \in S_{n,\eta}$, then we must have $i \neq j$. Therefore, it follows from (2.5) and (2.15) that

$$\begin{aligned}
&\left| \iint_{\cup S_{n,\eta}} f(x,y)\, dxdy - \sum_{\omega_n^i\times\omega_n^j \in S_{n,\eta}} \frac{Q_n^i Q_n^j}{|x_n^i - x_n^j|} \right| \\
&\qquad \leq \sum_{\omega_n^i\times\omega_n^j \in S_{n,\eta}} \iint_{\omega_n^i\times\omega_n^j} \left| f(x,y) - f(x_n^i, x_n^j) \right| dxdy
\end{aligned}$$

$$< \frac{\varepsilon}{3} \qquad \text{if } n \geq \hat{N}. \tag{2.16}$$

Finally, let $N = \max\{\tilde{N}, \hat{N}\}$. We have by (2.11), (2.13), (2.14), and (2.16) that

$$\begin{aligned}
&\left| \iint_{(\cup R_n)\times(\cup R_n)} f(x,y)\,dxdy - E_n \right| \\
&\quad \leq \iint_{\cup T_{n,\eta}} |f(x,y)|\,dxdy + \left| \sum_{\omega_n^i \times \omega_n^j \in T_{n,\eta}, i\neq j} \frac{Q_n^i Q_n^j}{|x_n^i - x_n^j|} \right| \\
&\qquad + \left| \iint_{\cup S_{n,\eta}} f(x,y)\,dxdy - \sum_{\omega_n^i \times \omega_n^j \in S_{n,\eta}} \frac{Q_n^i Q_n^j}{|x_n^i - x_n^j|} \right| \\
&\quad < \varepsilon \qquad \text{if } n \geq N,
\end{aligned}$$

leading to (2.8). □

3 Convergence of Discrete Energies with a Given Signed Radon Measure of Charge Density

In this section, we consider a given charge density represented by a compactly supported signed Radon measure on $\mathbb{R}^3$. We construct a sequence of discrete charges such that they converge to the given signed Radon measure and that the corresponding discrete energies converge to the continuum energy defined by the given signed Radon measure.

We first recall some definition and notation. For any nonnegative Radon measures α and β on $\mathbb{R}^3$, we set

$$E[\alpha,\beta] := \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{d(\alpha\times\beta)(x,y)}{|x-y|} = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{d\alpha(x)d\beta(y)}{|x-y|} = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{d\beta(y)d\alpha(x)}{|x-y|}.$$

The second and third equalities follow from the Fubini–Tonelli Theorem. In general $E[\alpha,\beta] \in [0,\infty]$. For any signed Radon measure μ on $\mathbb{R}^3$, let $\mu = \mu^+ - \mu^-$ be the unique Jordan decomposition of μ into nonnegative Radon measures μ^+ and μ^- on $\mathbb{R}^3$, respectively. If $E[\mu^+,\mu^-] < \infty$, then we define

$$E[\mu] = E[\mu^+,\mu^+] + E[\mu^-,\mu^-] - 2E[\mu^+,\mu^-].$$

If μ is a positive Radon measure on $\mathbb{R}^3$, then $E[\mu] = E[\mu,\mu]$.

For any nonempty, bounded, open set $\Omega \subseteq \mathbb{R}^3$, we denote

$$\mathcal{M}(\overline{\Omega}) = \{\text{all signed Radon measures } \mu \text{ on } \mathbb{R}^3 \text{ such that } \operatorname{supp}(\mu) \subseteq \overline{\Omega}\}. \tag{3.1}$$

If $\mu \in \mathcal{M}(\overline{\Omega})$ then the total variation of μ is $\|\mu\| = |\mu|(\mathbb{R}^3) = |\mu|(\overline{\Omega}) < \infty$. We also denote

$$\mathcal{A}(\overline{\Omega}) = \left\{ \frac{1}{N} \sum_{i=1}^{N} Q_i \delta_{x_i} : Q_i \in \mathbb{R}, x_i \in \overline{\Omega}, \text{ and } x_i \neq x_j \text{ if } i \neq j, N = 1, 2, \dots \right\}. \tag{3.2}$$

For any $\lambda > 0$, we denote

$$\mathcal{M}_\lambda(\overline{\Omega}) = \{\mu \in \mathcal{M}(\overline{\Omega}) : \|\mu\| \leq \lambda\}, \tag{3.3}$$

$$\mathcal{A}_\lambda(\overline{\Omega}) = \left\{ \frac{1}{N} \sum_{i=1}^{N} Q_i \delta_{x_i} : |Q_i| \leq \lambda, x_i \in \overline{\Omega}, \text{ and } x_i \neq x_j \text{ if } i \neq j, N = 1, 2, \dots \right\}, \tag{3.4}$$

We define the discrete energy

$$E_{\mathrm{d}}[\mu] = \frac{1}{N^2} \sum_{1 \leq i,j \leq N, i \neq j} \frac{Q_i Q_j}{|x_i - x_j|} \qquad \text{if } \mu = \frac{1}{N} \sum_{i=1}^{N} Q_i \delta_{x_i}, \tag{3.5}$$

where $Q_i \in \mathbb{R}$ and $x_i \in \mathbb{R}^3$ with $x_i \neq x_j$ if $i \neq j$. Since $\delta_a \times \delta_b = \delta_{(a,b)}$ for any $a, b \in \mathbb{R}^3$ we have

$$E_{\mathrm{d}}[\mu] = \iint_{\{(x,y) \in \mathbb{R}^3 \times \mathbb{R}^3 : x \neq y\}} \frac{d(\mu \times \mu)(x, y)}{|x - y|}. \tag{3.6}$$

Note that we drop the factor $1/2$ in our definition of $E[\alpha, \beta]$, $E[\mu]$, and $E_{\mathrm{d}}[\mu]$.

For any signed Radon measure μ on $\mathbb{R}^3$ and any $g \in C_0(\mathbb{R}^3)$, we denote

$$\langle \mu, g \rangle = \int_{\mathbb{R}^3} g \, d\mu.$$

When no confusion arises, we also use $\langle \cdot, \cdot \rangle$ to denote the $L^2(\mathbb{R}^3)$-inner product. If μ_n, μ $(n = 1, 2, \dots)$ are all signed Radon measures on $\mathbb{R}^3$, then the vague convergence (i.e., the weak-$*$ convergence) of μ_n to μ, denoted $\mu_n \overset{*}{\rightharpoonup} \mu$, is defined by $\langle \mu_n, g \rangle \to \langle \mu, g \rangle$ for any $g \in C_0(\mathbb{R}^3)$.

Our main result of this section is the following:

Theorem 3.1. *Let $\Omega \subset \mathbb{R}^3$ be a nonempty, bounded, open subset with a C^2 boundary. Let $\lambda > 0$. Assume $\mu \in \mathcal{M}_\lambda(\overline{\Omega})$ with $E[|\mu|] < \infty$. Then there exist $\mu_n \in \mathcal{A}_\lambda(\overline{\Omega})$ $(n = 1, 2, \dots)$ such that*

$$\mu_n \overset{*}{\rightharpoonup} \mu \qquad \textit{and} \qquad E_{\mathrm{d}}[\mu_n] \to E[\mu] \qquad \textit{as } n \to \infty.$$

Moreover, if $\operatorname{supp}(\mu) \subseteq \partial\Omega$ *and $\varepsilon > 0$, then the measures μ_n can be constructed so that*

$$\operatorname{supp}(\mu_n) \subseteq \{x \in \overline{\Omega} : \operatorname{dist}(x, \partial\Omega) < \varepsilon\} \qquad (n = 1, 2, \dots).$$

To prove the theorem, we need two lemmas. The first lemma states that the charge distribution represented by a signed Radon measure that is compactly supported in $\overline{\Omega}$ can be approximated by those with C^∞-densities (with respect to the Lebesgue measure)

that are compactly supported inside Ω. The approximation is carried out by a family of diffeomorphisms that "flow" the support of the given measure into the interior of Ω, providing space for smoothing. Such diffeomorphisms are vector fields (cf. Chapter 9 of [9]), and are determined here locally by the gradient of signed distance to the boundary $\partial\Omega$.

Lemma 3.1. *Let Ω, λ, and μ be the same as in Theorem 3.1. There exist $\nu_n \in \mathcal{M}_\lambda(\overline{\Omega})$ $(n = 1, 2 \dots)$ that satisfy the following:*

(1) *For each n, ν_n is absolutely continuous with respect to the Lebesgue measure with a C^∞-density, and supp $(\nu_n) \subset \Omega$. Moreover, if* $\operatorname{supp}(\mu) \subseteq \partial\Omega$ *and $\varepsilon > 0$, then the measures ν_n can be constructed so that*

$$\operatorname{supp}(\nu_n) \subseteq \{x \in \overline{\Omega} : \operatorname{dist}(x, \partial\Omega) < \varepsilon\} \qquad (n = 1, 2, \dots);$$

(2) *$\nu_n \overset{*}{\rightharpoonup} \mu$ and $E[\nu_n] \to E[\mu]$ as $n \to \infty$.*

Proof. We divide our proof into four steps. In Step 1, we use the gradient of the signed distance function (with the distance to the boundary $\partial\Omega$) to construct a family of diffeomorphisms that can flow the points on the boundary $\partial\Omega$ into the interior of Ω. In Step 2, we use the diffeomorphisms to construct the corresponding push-forward measures that are compactly supported inside Ω and prove the desired convergence properties. In Step 3, we mollify those push-forward measures to construct signed Radon measures supported inside Ω with C^∞-densities. Finally, in Step 4, we construct the desired sequence of signed Radon measures $\{\nu_n\}_{n=1}^\infty$ and prove the related convergence properties.

Step 1. Construction of a family of diffeomorphisms. We define the signed distance function

$$d(x) = \begin{cases} \operatorname{dist}(x, \partial\Omega) & \text{if } x \in \overline{\Omega}, \\ -\operatorname{dist}(x, \partial\Omega) & \text{if } x \in \mathbb{R}^3 \setminus \overline{\Omega}, \end{cases} \tag{3.7}$$

For $r > 0$, set $T_r := \{x \in \mathbb{R}^3 : |d(x)| < r\}$. Since $\partial\Omega$ is C^2, there exists $\delta > 0$ such that

$$d \in C^2(T_\delta) \qquad \text{and} \qquad |\nabla d| = 1 \quad \text{in } T_\delta. \tag{3.8}$$

Moreover, for every $x \in T_\delta$ there exists a unique $x' \in \partial\Omega$ such that $|x - x'| = \operatorname{dist}(x, \partial\Omega)$ (cf. Theorem 3 in [24]). Since $\partial\Omega = \{x \in \mathbb{R}^3 : d(x) = 0\}$, at each point on $\partial\Omega$, ∇d is the unit normal to $\partial\Omega$, and is oriented toward the interior of Ω. Let $\xi \in C_c^\infty(\mathbb{R}^3)$ be such that $\xi = 1$ on $T_{\delta/2}$ and $\operatorname{supp}(\xi) \subset T_\delta$. Define

$$\tilde{d}(x) = d(x)\xi(x) \qquad \forall x \in \mathbb{R}^3. \tag{3.9}$$

Note that $\tilde{d} \in C_c^2(\mathbb{R}^3)$, $\operatorname{supp}(\tilde{d}) \subset T_\delta$, and $\tilde{d} = d$ on $T_{\delta/2}$. The vector field $\nabla\tilde{d} : \mathbb{R}^3 \to \mathbb{R}^3$ is Lipschitz-continuous with the Lipschitz constant

$$L = \sup_{x,y \in \mathbb{R}^3, x \neq y} \frac{|\nabla\tilde{d}(x) - \nabla\tilde{d}(y)|}{|x - y|} < \infty. \tag{3.10}$$

The global Lipschitz continuity of $\nabla\tilde{d}$ ensures the existence of a unique family of diffeomorphisims $\Phi_t : \mathbb{R}^3 \to \mathbb{R}^3$ defined by

$$\frac{d}{dt}\Phi_t(x) = \nabla\tilde{d}(\Phi_t(x)) \quad \text{and} \quad \Phi_0(x) = x. \tag{3.11}$$

We have the following properties:

- The family of transformations $\{\Phi_t\}_{t\in\mathbb{R}}$ form a group of diffeomorphisms with $\Phi_t \circ \Phi_s = \Phi_{t+s}$ for any $t, s \in \mathbb{R}$, and in particular, $\Phi_t \circ \Phi_{-t} = \Phi_0 = id$, where $id : \mathbb{R}^3 \to \mathbb{R}^3$ is the identity map. These follow from the definition (3.11);
- Since $\tilde{d} \in C^2_{\mathrm{c}}(\mathbb{R}^3)$ and Ω is bounded, there exists $R > 0$ such that

$$\overline{\Omega} \subseteq \overline{B(0,R)} \quad \text{and} \quad \Phi_t(x) = x \quad \forall x \in \mathbb{R}^3 \setminus \overline{B(0,R)} \text{ and } \forall t \in \mathbb{R}; \tag{3.12}$$

- We have

$$e^{-L|t|}|x-y| \le |\Phi_t(x) - \Phi_t(y)| \le e^{L|t|}|x-y| \qquad \forall x, y \in \mathbb{R}^3 \text{ and } \forall t \in \mathbb{R}. \tag{3.13}$$

To show (3.13), let us first consider $t \ge 0$. By (3.11) and (3.10), we have

$$\begin{aligned}
|\Phi_t(x) - \Phi_t(y)| &= \left| x - y + \int_0^t \left[\nabla\tilde{d}(\Phi_s(x)) - \nabla\tilde{d}(\Phi_s(y))\right] ds \right| \\
&\le |x-y| + \int_0^t \left|\nabla\tilde{d}(\Phi_s(x)) - \nabla\tilde{d}(\Phi_s(y))\right| ds \\
&\le |x-y| + \int_0^t L\,|\Phi_s(x) - \Phi_s(y)|\, ds.
\end{aligned}$$

Gronwall's inequality then leads to the second inequality in (3.13) for $t \ge 0$. Similarly,

$$|\Phi_{-t}(x) - \Phi_{-t}(y)| \le e^{Lt}|x-y|.$$

Note that $\Phi_{-t}(\Phi_t(x)) = x$ for any t and x. So, replacing x and y above by $\Phi_t(x)$ and $\Phi_t(y)$, respectively, we obtain

$$|x-y| \le e^{Lt}|\Phi_t(x) - \Phi_t(y)|,$$

which leads to the first inequality in (3.13) for $t \ge 0$. If $t < 0$, then we can replace x and y in (3.13) for $t > 0$ by $\Phi_{-t}(x)$ and $\Phi_{-t}(y)$, respectively, to obtain the inequalities in (3.13) for $t < 0$. We have thus proved (3.13).

Step 2. Construction of signed Radon measures supported inside Ω with the desired convergence properties. For the given $\mu \in \mathcal{M}_\lambda(\overline{\Omega})$ in the lemma, we consider the family of push-forward measures $\{\mu \circ \Phi_t^{-1}\}_{t\in\mathbb{R}}$, where $(\mu \circ \Phi_t^{-1})(A) = \mu(\Phi_t^{-1}(A))$ for any Borel set $A \subseteq \mathbb{R}^3$. We claim:

(2.1) For any $t \in \mathbb{R}$, $\mu \circ \Phi_t^{-1}$ is a signed Radon measure on $\mathbb{R}^3$ with $\|\mu \circ \Phi_t^{-1}\| = \|\mu\|$ and

$$\operatorname{supp}(\mu \circ \Phi_t^{-1}) \subseteq \Phi_t(\operatorname{supp}(\mu)) \subseteq \Phi_t(\overline{\Omega}) \subseteq \overline{B(0,R)},$$

where R is the same as in (3.12);

(2.2) As $t \to 0$, $\mu \circ \Phi_t^{-1} \overset{*}{\rightharpoonup} \mu$ and $E[\mu \circ \Phi_t^{-1}] \to E[\mu]$; and

(2.3) If $t > 0$, then $\operatorname{supp}(\mu \circ \Phi_t^{-1}) \subset \Omega$ and $\mu \circ \Phi_t^{-1} \in \mathcal{M}_\lambda(\overline{\Omega})$. Moreover, if $\operatorname{supp}(\mu) \subseteq \partial\Omega$ and $\varepsilon > 0$ then there exists $t_\varepsilon > 0$ such that

$$\operatorname{supp}(\mu \circ \Phi_t^{-1}) \subset \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) < \varepsilon/2\}, \quad \text{provided that } 0 < t \le t_\varepsilon.$$

Proof of Claim (2.1). Fix $t \in \mathbb{R}$. Since $\Phi_t : \mathbb{R}^3 \to \mathbb{R}^3$ is a homeomorphism, $\mathbb{R}^3 = P \cup N$ is a Hahn decomposition for μ (i.e., P and N are disjoint Borel subsets of $\mathbb{R}^3$, and they are positive and negative sets for μ, respectively) if and only if $\mathbb{R}^3 = \Phi_t(P) \cup \Phi_t(N)$ is a Hahn decomposition for $\mu \circ \Phi_t^{-1}$. Consequently,

$$\begin{aligned}\left\|\mu \circ \Phi_t^{-1}\right\| &= \left|\mu \circ \Phi_t^{-1}\right|(\mathbb{R}^3) = \left(\mu \circ \Phi_t^{-1}\right)(\Phi_t(P)) - \left(\mu \circ \Phi_t^{-1}\right)(\Phi_t(N)) \\ &= \mu(P) - \mu(N) = |\mu|(\mathbb{R}^3) = \|\mu\|.\end{aligned}$$

Thus, $\mu \circ \Phi_t^{-1}$ is a signed Radon measure on $\mathbb{R}^3$ with $\|\mu \circ \Phi_t^{-1}\| = \|\mu\| \le \lambda$. Let A be a Borel subset of $\mathbb{R}^3$. If $A \cap \Phi_t(\operatorname{supp}(\mu)) = \emptyset$, then $\Phi_t^{-1}(A) \cap \operatorname{supp}(\mu) = \emptyset$ and hence $(\mu \circ \Phi_t^{-1})(A) = \mu(\Phi_t^{-1}(A)) = 0$. Thus, $\operatorname{supp}(\mu \circ \Phi_t^{-1}) \subseteq \Phi_t(\operatorname{supp}(\mu)) \subseteq \Phi_t(\overline{\Omega})$. If $x \in \overline{B(0,R)}$ but $\Phi_t(x) \in \mathbb{R}^3 \setminus \overline{B(0,R)}$ for some t, then by (3.12) $x = \Phi_{-t}(\Phi_t(x)) \in \mathbb{R}^3 \setminus \overline{B(0,R)}$, a contradiction. Thus, $\Phi_t(\overline{B(0,R)}) \subseteq \overline{B(0,R)}$. Hence $\Phi_t(\overline{\Omega}) \subseteq \Phi_t(\overline{B(0,R)}) \subseteq \overline{B(0,R)}$. The proof of Claim (2.1) is complete.

Proof of Claim (2.2). Let $g \in C_c(\mathbb{R}^3)$. Let $R > 0$ be the same as in (3.12). Choose $\tilde{R} > R$ so that $\operatorname{supp}(g) \subseteq B(0,\tilde{R})$. If $x \in \mathbb{R}^3$ and $|x| > \tilde{R}$, then $g(\Phi_t(x)) = g(x) = 0$ for all $t \in \mathbb{R}$. Thus, $|g \circ \Phi_t| \le \|g\|_\infty \chi_{B(0,\tilde{R})}$ on $\mathbb{R}^3$ for all $t \in \mathbb{R}$. Since each $\Phi_t : \mathbb{R}^3 \to \mathbb{R}^3$ is a homeomorphism and $\|\mu\| \le \lambda$, we have by the change of variables (cf. Theorem 3.6.1 in [4]), the Dominated Convergence Theorem, and the fact that $\Phi_0(x) = x$ for all $x \in \mathbb{R}^3$ that

$$\lim_{t\to 0} \int_{\mathbb{R}^3} g \, d\left(\mu \circ \Phi_t^{-1}\right) = \lim_{t\to 0} \int_{\mathbb{R}^3} g \circ \Phi_t \, d\mu = \int_{\mathbb{R}^3} \lim_{t\to 0} g \circ \Phi_t \, d\mu = \int_{\mathbb{R}^3} g \, d\mu.$$

Thus, $\mu \circ \Phi_t^{-1} \overset{*}{\rightharpoonup} \mu$ as $t \to 0$.

Now let $\mu = \mu^+ - \mu^-$ be the Jordan decomposition of μ corresponding to the Hahn decomposition $\mathbb{R}^3 = P \cup N$, where P and N are disjoint Borel subsets of $\mathbb{R}^3$, positive and negative for μ, respectively. We have $\mu^+(A) = \mu(A \cap P)$ and $\mu^-(A) = -\mu(A \cap N)$ for any Borel subset $A \subseteq \mathbb{R}^3$. Thus, for each $t \in \mathbb{R}$, $\mathbb{R}^3 = \Phi_t(P) \cup \Phi_t(N)$ is a Hahn decomposition for $\mu \circ \Phi_t^{-1}$, and $\mu \circ \Phi_t^{-1} = \mu^+ \circ \Phi_t^{-1} - \mu^- \circ \Phi_t^{-1}$ is the Jordan decomposition for μ, i.e., $(\mu \circ \Phi_t^{-1})^+ = \mu^+ \circ \Phi_t^{-1}$ and $(\mu \circ \Phi_t^{-1})^- = \mu^- \circ \Phi_t^{-1}$. If $h \in C(\mathbb{R}^3 \times \mathbb{R}^3)$ is nonnegative and bounded, then by the fact that $\|(\mu \circ \Phi_t)^+\| \le \|\mu \circ \Phi_t\| = \|\mu\| \le \lambda$ and $\|(\mu \circ \Phi_t)^-\| \le \|\mu \circ \Phi_t\| = \|\mu\| \le \lambda$, the change of variables, and Fubini's Theorem, we have

$$\begin{aligned}&\iint_{\mathbb{R}^3 \times \mathbb{R}^3} h(x,y) \, d((\mu \circ \Phi_t^{-1})^+ \times (\mu \circ \Phi_t^{-1})^-)(x,y) \\ &\quad = \int_{\mathbb{R}^3} \left[\int_{\mathbb{R}^3} h(x,y) \, d(\mu^+ \circ \Phi_t^{-1})(x)\right] d(\mu^- \circ \Phi_t^{-1})(y)\end{aligned}$$

$$
\begin{aligned}
&= \int_{\mathbb{R}^3} \left[\int_{\mathbb{R}^3} h(\Phi_t(x), y)\, d\mu^+(x) \right] d(\mu^- \circ \Phi_t^{-1})(y) \\
&= \int_{\mathbb{R}^3} \left[\int_{\mathbb{R}^3} h(\Phi_t(x), \Phi_t(y))\, d\mu^+(x) \right] d\mu^-(y) \\
&= \iint_{\mathbb{R}^3 \times \mathbb{R}^3} h(\Phi_t(x), \Phi_t(y))\, d(\mu^+ \times \mu^-)(x, y).
\end{aligned}
$$

Define $h_n(x, y) = \min(1/|x - y|, n)$ $(n = 1, 2, \dots)$. Then each $h_n \in C(\mathbb{R}^3 \times \mathbb{R}^3)$ is nonnegative and bounded, and $h_n \le h_{n+1}$ $(n = 1, 2, \dots)$. Replacing h above with h_n and applying the Monotone Convergence Theorem, we obtain that

$$
\begin{aligned}
&E[(\mu \circ \Phi_t^{-1})^+, (\mu \circ \Phi_t^{-1})^-] \\
&\quad = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{d((\mu \circ \Phi_t^{-1})^+ \times (\mu \circ \Phi_t^{-1})^-)(x, y)}{|x - y|} \\
&\quad = \lim_{n \to \infty} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} h_n(x, y)\, d((\mu \circ \Phi_t^{-1})^+ \times (\mu \circ \Phi_t^{-1})^-)(x, y) \\
&\quad = \lim_{n \to \infty} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} h_n(\Phi_t(x), \Phi_t(y))\, d(\mu^+ \times \mu^-)(x, y) \\
&\quad = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{d(\mu^+ \times \mu^-)(x, y)}{|\Phi_t(x) - \Phi_t(y)|}.
\end{aligned} \tag{3.14}
$$

It follows from (3.13) that

$$
\frac{e^{-L|t|}}{|x - y|} \le \frac{1}{|\Phi_t(x) - \Phi_t(y)|} \le \frac{e^{L|t|}}{|x - y|} \qquad \forall t \in \mathbb{R}. \tag{3.15}
$$

We can replace $|t|$ in the exponent by some $T > 0$ so that the inequalities hold true for all $t \in [-T, T]$. Since $E[|\mu|] < \infty$, the function $1/|x - y|$, and hence $1/|\Phi_t(x) - \Phi_t(y)|$ for each t, is integrable against the product measure $\mu^+ \times \mu^-$. Therefore, by (3.14) and the Dominated Convergence Theorem,

$$
\lim_{t \to 0} E[(\mu \circ \Phi_t^{-1})^+, (\mu \circ \Phi_t^{-1})^-] = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{d(\mu^+ \times \mu^-)(x, y)}{|x - y|} = E[\mu^+, \mu^-].
$$

Similarly,

$$
E[(\mu \circ \Phi_t^{-1})^+] \to E[\mu^+] \qquad \text{and} \qquad E[(\mu^- \circ \Phi_t^{-1})^-] \to E[\mu^-] \qquad \text{as } t \to 0.
$$

The proof of Claim (2.2) is complete.

Proof of Claim (2.3). We first show that there exists $t_0 > 0$ such that

$$
d(x) < d(\Phi_t(x)) < \frac{\delta}{2} \quad \text{if } 0 \le d(x) \le \frac{\delta}{4} \text{ and } 0 < t \le t_0, \tag{3.16}
$$

where $\delta > 0$ is the same as in (3.8). Let $x \in \mathbb{R}^3$ and assume $0 \le d(x) \le \delta/4$. (This implies that $x \in \overline{\Omega}$.) Recall from (3.9) that $\tilde{d} \in C^2(\mathbb{R}^3)$, $\operatorname{supp}(\tilde{d}) \subset T_\delta$, and $\tilde{d} = d$ on $T_{\delta/2}$. Taylor expanding $\Phi_t(x)$ at $t = 0$, we have by (3.8) and (3.11) that

$$\begin{aligned}\Phi_t(x) &= \Phi_0(x) + t\frac{d}{dt}\Phi_t(x)\bigg|_{t=0} + \frac{t^2}{2}\frac{d^2}{dt^2}\left(\Phi_t(x)\right)\bigg|_{t=\tau} \\ &= x + t\nabla d(x) + \frac{t^2}{2}\nabla^2\tilde{d}(\Phi_\tau(x))\nabla\tilde{d}(\Phi_\tau(x)) \qquad \forall t > 0, \end{aligned} \tag{3.17}$$

where $\tau = \tau(x,t) \in [0,t]$ and $\nabla^2\tilde{d}$ denotes the Hessian matrix of $\tilde{d}$. Thus, since $|\nabla d(x)| = 1$,

$$|\Phi_t(x) - x| \le t + \frac{t^2}{2}\|\nabla^2\tilde{d}\|_\infty\|\nabla\tilde{d}\|_\infty.$$

Consequently, since $0 \le d(x) \le \delta/4$, the distance function is Lipschitz-continuous with the Lipschitz constant 1 (cf. the proof of Lemma 3.2.34 in [14] and Section 1.1 of [42]), which implies that

$$d(\Phi_t(x)) \le d(x) + |\Phi_t(x) - x| \le \frac{\delta}{4} + |\Phi_t(x) - x|,$$

and $\Phi_t(x)$ is continuous in t, there exists $t_1 > 0$ such that $d(\Phi_t(x)) < \delta/2$ if $0 < t \le t_1$. Now, denoting

$$w(x,t) = (1/2)\nabla^2\tilde{d}(\Phi_\tau(x))\nabla\tilde{d}(\Phi_\tau(x)),$$

Taylor expanding $d(\Phi_t(x))$ with $\Phi_t(x)$ given in (3.17), and noting that $d = \tilde{d}$ on $T_{\delta/2}$, we obtain

$$\begin{aligned} d(\Phi_t(x)) &= \tilde{d}(\Phi_t(x)) \\ &= \tilde{d}\left(x + t\nabla d(x) + t^2 w(x,t)\right) \\ &= \tilde{d}(x) + \nabla\tilde{d}(x)\cdot\left[t\nabla d(x) + t^2 w(x,t)\right] \\ &\qquad + \frac{1}{2}\nabla^2\tilde{d}(\hat{x}_t)\left[t\nabla d(x) + t^2 w(x,t)\right]\cdot\left[t\nabla d(x) + t^2 w(x,t)\right] \\ &= d(x) + t + u(x,t), \end{aligned}$$

where $\hat{x}_t \in \mathbb{R}^3$ lies on the line segment connecting x and $\Phi_t(x)$ and

$$|u(x,t)| \le C\left(t^2 + t^3 + t^4\right)$$

with $C = C(\|\nabla^2\tilde{d}\|_\infty, \|\nabla\tilde{d}\|_\infty) > 0$ a constant independent on x and t. Therefore, there exists $t_0 \in (0, t_1]$ such that (3.16) is true.

We now claim:

(2.3.1) $d(\Phi_t(x)) > d(x)$ for any $x \in \overline{\Omega}$ with $0 \le d(x) \le \delta/8$ and any $t > 0$; and

(2.3.2) $d(\Phi_t(x)) \ge \delta/8$ for any $x \in \overline{\Omega}$ with $d(x) > \delta/8$ and for any $t > 0$.

If these are proved, then $\Phi_t(\overline{\Omega}) \subset \Omega$ for any $t > 0$. By Claim (2.1), we have for any $t > 0$ that $\operatorname{supp}(\mu \circ \Phi_t^{-1}) \subseteq \Phi_t(\operatorname{supp}(\mu)) \subseteq \Phi_t(\overline{\Omega})$. This, together with Claim (2.1) again, implies that $\mu \circ \Phi_t^{-1} \in \mathcal{M}_\lambda(\overline{\Omega})$. Moreover, assume $\operatorname{supp}(\mu) \subseteq \partial\Omega$ and $\varepsilon > 0$. Then, replacing $\delta > 0$ in (3.16) by ε and setting $t_\varepsilon = t_0$ there, we have by Claim (2.1) and (3.16) that

$$\operatorname{supp}(\mu \circ \Phi_t^{-1}) \subseteq \Phi_t(\operatorname{supp}(\mu)) \subseteq \Phi_t(\partial\Omega) \subset \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) < \varepsilon/2\},$$

provided that $0 < t < t_\varepsilon$. Claim (2.3) will then be true.

To prove Claim (2.3.1), we assume on the contrary that there existed some x with $0 \le d(x) \le \delta/8$ and some $t' > 0$ such that $d(\Phi_{t'}(x)) \le d(x)$. By (3.16), $t' > t_0$ and $d(x) < d(\Phi_{t_0}(x)) < \delta/2$. Let $d_{\mathrm{c}} = \min(d(\Phi_{t_0}(x)), \delta/4)$. Since $d(\Phi_t(x))$ is continuous in t, $d(\Phi_{t_0}(x)) \ge d_{\mathrm{c}}$, and $d(\Phi_{t'}(x)) \le d(x) < d_{\mathrm{c}}$, the set $\{t \in [t_0, t'] : d(\Phi_t(x)) = d_{\mathrm{c}}\}$ is nonempty and compact, and hence has a maximum value $t_{\mathrm{m}} \in [t_0, t')$. It satisfies $d(\Phi_{t_{\mathrm{m}}}(x)) = d_{\mathrm{c}} \le \delta/4$ and

$$d(\Phi_t(x)) < d_{\mathrm{c}} \quad \text{if } t_{\mathrm{m}} < t \le t'. \tag{3.18}$$

Now, let $t'' \in (0, t_0]$ be such that $t_{\mathrm{m}} + t'' \le t'$. Then, we have by (3.16) with $\Phi_{t_{\mathrm{m}}}(x)$ replacing x that $d(\Phi_{t_{\mathrm{m}}+t''}(x)) = d(\Phi_{t''}(\Phi_{t_{\mathrm{m}}}(x))) > d(\Phi_{t_{\mathrm{m}}}(x)) = d_{\mathrm{c}}$. This contradicts (3.18). Thus, Claim (2.3.1) is true. Claim (2.3.2) can be proved similarly: If $d(x) > \delta/8$ but $d(\Phi_t(x)) < \delta/8$ for some $t > 0$, then there would exist $t'_{\mathrm{m}} \in (0, t)$ such that $d(\Phi_s(x)) \ge \delta/8$ for all $s \in [0, t'_{\mathrm{m}}]$ but $d(\Phi_s(x)) < \delta/8$ if $s \in (t'_{\mathrm{m}}, t)$. Again by (3.16) with $\Phi_{t'_{\mathrm{m}}}(x)$ replacing x, it would lead to a contradiction. The proof of Claim (2.3) is complete.

Step 3. Construction of signed Radon measures supported inside Ω with C^∞-densities and the desired convergence properties. Let $\varphi \in C_{\mathrm{c}}^\infty(\mathbb{R}^3)$ be nonnegative and radially symmetric with $\operatorname{supp}(\varphi) \subset \overline{B(0,1)}$ and

$$\int_{\mathbb{R}^3} \varphi \, dx = \int_{B(0,1)} \varphi \, dx = 1. \tag{3.19}$$

Define

$$\varphi_\alpha(x) = \alpha^{-3} \varphi\left(\frac{x}{\alpha}\right) \qquad \forall \alpha > 0 \ \forall x \in \mathbb{R}^3.$$

For any $t \in \mathbb{R}$ and any $\alpha > 0$, we consider the function $\varphi_\alpha * (\mu \circ \Phi_t^{-1}) : \mathbb{R}^3 \to \mathbb{R}$. Since $\mu \circ \Phi_t^{-1}$ is a signed Radon measure with $\|\mu \circ \Phi_t^{-1}\| = \|\mu\| \le \lambda$ (cf. Claim (2.1) in Step 2), by the definition of partial derivatives and the Dominated Convergence Theorem, we have $\varphi_\alpha * (\mu \circ \Phi_t^{-1}) \in C^\infty(\mathbb{R}^3)$. Moreover, since

$$\operatorname{supp}(\varphi_\alpha * (\mu \circ \Phi_t^{-1})) \subseteq \operatorname{supp}(\varphi_\alpha) + \operatorname{supp}(\mu \circ \Phi_t^{-1}) \subseteq \overline{B(0,\alpha)} + \overline{B(0,R)}, \tag{3.20}$$

where R is the same as in (3.12), the function $\varphi_\alpha * (\mu \circ \Phi_t^{-1})$ is compactly supported. Hence, $\varphi_\alpha * (\mu \circ \Phi_t^{-1}) \in C_{\mathrm{c}}^\infty(\mathbb{R}^3)$.

For any $\alpha > 0$ and any $t \in \mathbb{R}$, we define the signed measure $\nu_{\alpha,t}$ on the Borel subsets of $\mathbb{R}^3$ by $d\nu_{\alpha,t} = \varphi_\alpha * (\mu \circ \Phi_t^{-1}) \, dx$, i.e.,

$$\nu_{\alpha,t}(A) = \int_A \varphi_\alpha * (\mu \circ \Phi_t^{-1}) \, dx \qquad \text{for any Borel set } A \subseteq \mathbb{R}^3.$$

We claim:

(3.1) For any $t \in \mathbb{R}$ and any $\alpha > 0$, $\nu_{\alpha,t}$ is a signed Radon measure with a compact support and a C_c^∞-density (with respect to the Lebesgue measure), and $\|\nu_{\alpha,t}\| \le \|\mu\| \le \lambda$;

(3.2) For each $t \in \mathbb{R}$,

$$\nu_{\alpha,t} \overset{*}{\rightharpoonup} \mu \circ \Phi_t^{-1} \qquad \text{and} \qquad E[\nu_{\alpha,t}] \to E[\mu \circ \Phi_t^{-1}] \qquad \text{as } \alpha \to 0^+;$$

(3.3) For any $t > 0$, there exists $\alpha_t > 0$ such that $\nu_{\alpha,t} \in \mathcal{M}_\lambda(\overline{\Omega})$ with $\operatorname{supp}(\nu_{\alpha,t}) \subset \Omega$ for all $\alpha \in (0, \alpha_t]$. If $\operatorname{supp}(\mu) \subseteq \partial\Omega$ and $\varepsilon > 0$, then there exists $\alpha_\varepsilon > 0$ such that

$$\operatorname{supp}(\nu_{\alpha,t}) \subset \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) < \varepsilon\} \qquad \forall \alpha \in (0, \alpha_\varepsilon]\ \forall t \in (0, t_\varepsilon]. \tag{3.21}$$

where $t_\varepsilon > 0$ is the same as that in Claim (2.3) in Step 2.

Proof of Claim (3.1). Since the density $\varphi_\alpha * (\mu \circ \Phi_t^{-1}) \in C_c^\infty(\mathbb{R}^3)$, the measure $\nu_{\alpha,t}$ has a compact support and also a C_c^∞-density. Noting that $d|\nu_{\alpha,t}| = |\varphi_\alpha * (\mu \circ \Phi_t^{-1})|\, dx$, we have by Fubini's Theorem that

$$\begin{aligned}
\|\nu_{\alpha,t}\| &= \int_{\mathbb{R}^3} |\varphi_\alpha * (\mu \circ \Phi_t^{-1})|\, dx \\
&= \int_{\mathbb{R}^3} \left| \int_{\mathbb{R}^3} \varphi_\alpha(x-y)\, d(\mu \circ \Phi_t^{-1})(y) \right| dx \\
&\le \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \varphi_\alpha(x-y)\, d|\mu \circ \Phi_t^{-1}|(y)\, dx \\
&= \int_{\mathbb{R}^3} \left[\int_{\mathbb{R}^3} \varphi_\alpha(x-y)\, dx \right] d|\mu \circ \Phi_t^{-1}|(y) \\
&= \int_{\mathbb{R}^3} d|\mu \circ \Phi_t^{-1}|(y) \\
&= \|\mu \circ \Phi_t^{-1}\|.
\end{aligned}$$

Thus, $\|\nu_{\alpha,t}\| \le \|\mu\| \le \lambda$ (cf. Claim (2.1) in Step 2). The proof of Claim (3.1) is complete.

Proof of Claim (3.2). Fix $t \in \mathbb{R}$ and $g \in C_0(\mathbb{R}^3)$. Note that $\varphi_\alpha * g \to g$ uniformly on $\mathbb{R}^3$ as $\alpha \to 0^+$. We have by Fubini's Theorem that

$$\begin{aligned}
\int_{\mathbb{R}^3} g(x)\, d\nu_{\alpha,t}(x) &= \int_{\mathbb{R}^3} g(x) \left[\int_{\mathbb{R}^3} \varphi_\alpha(y-x)\, d(\mu \circ \Phi_t^{-1})(y) \right] dx \\
&= \int_{\mathbb{R}^3} (\varphi_\alpha * g)(y)\, d(\mu \circ \Phi_t^{-1})(y) \\
&\to \int_{\mathbb{R}^3} g(y)\, d(\mu \circ \Phi_t^{-1})(y) \qquad \text{as } \alpha \to 0^+.
\end{aligned}$$

Hence, $\nu_{\alpha,t} \overset{*}{\rightharpoonup} \mu \circ \Phi_t^{-1}$ as $\alpha \to 0^+$.

Since $E[|\mu|] < \infty$, it follows from (3.14) and (3.15) that $E[(\mu \circ \Phi_t^{-1})^+, (\mu \circ \Phi_t^{-1})^-] < \infty$. Similarly, $E[(\mu \circ \Phi_t^{-1})^+, (\mu \circ \Phi_t^{-1})^+] < \infty$ and $E[(\mu \circ \Phi_t^{-1})^-, (\mu \circ \Phi_t^{-1})^-] < \infty$. Hence, $E[|\mu \circ \Phi_t^{-1}|] < \infty$. Consequently, by the definition of $\nu_{\alpha,t}$ for $\alpha > 0$ and Lemma A1 in [6]

(cf. also Step 2.3 in the proof of Theorem 4.1), $E[\nu_{\alpha,t}] \to E[\mu \circ \Phi_t^{-1}]$ as $\alpha \to 0^+$. The proof of Claim (3.2) is complete.

Proof of Claim (3.3). Let $t > 0$ and $K_t = \mathrm{supp}\,(\mu \circ \Phi_t^{-1})$. By the Claim (2.3) in Step 2, K_t is a compact subset of Ω. Let $\alpha_t = \mathrm{dist}(K_t, \partial\Omega)/4 > 0$. Then, for any $\alpha \in (0, \alpha_t]$, we have by the first inclusion in (3.20) that

$$\mathrm{supp}\,(\varphi_\alpha * (\mu \circ \Phi_t^{-1})) \subseteq \overline{B(0,\alpha)} + K_t = \bigcup_{x \in K_t} \overline{B(x,\alpha)} \subset \Omega.$$

This, together with the definition of $\nu_{\alpha,t}$ and Claim (3.1), implies that $\nu_{\alpha,t} \in \mathcal{M}_\lambda(\overline{\Omega})$ with $\mathrm{supp}\,(\nu_{\lambda,t}) \subset \Omega$ for all $\alpha \in (0, \alpha_t]$. Assume $\mathrm{supp}\,(\mu) \subseteq \partial\Omega$ and $\varepsilon > 0$. Let $t_\varepsilon > 0$ be the same as in Claim (2.3) of Step 2. Then $K_t \subset \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) < \varepsilon/2\}$ if $t \in (0, t_\varepsilon]$. By choosing $\alpha_\varepsilon \in (0, \varepsilon/2)$, we obtain (3.21) by the same argument and the definition of $\nu_{\alpha,t}$. The proof of Claim (3.3) is complete.

Step 4. Construction of the desired sequence $\{\nu_n\}_{n=1}^\infty$ of signed Radon measures and proof of the related convergence properties. Since $C(\overline{\Omega})$ is a separable Banach space, the closed unit ball of the dual space $[C(\overline{\Omega})]^*$ is metrizable with respect to the vague (i.e., weak-star) topology (cf. Lemma 3.101 in [13]). But $[C(\overline{\Omega})]^*$ is isometrically isomorphic to the space of signed Radon measures on $\overline{\Omega}$ (cf. e.g., Theorem 7.18 in [16]). By identifying measures on $\overline{\Omega}$ with their zero extensions to $\mathbb{R}^3$, we find the closed unit ball of the set of signed Radon measures on $\overline{\Omega}$ to be isometrically isomorphic to $\mathcal{M}_1(\overline{\Omega})$. Therefore, $\mathcal{M}_1(\overline{\Omega})$, and hence $\mathcal{M}_\lambda(\overline{\Omega})$, is metrizable with respect to the vague topology. Let us denote this metric by $D_\lambda : \mathcal{M}_\lambda(\overline{\Omega}) \times \mathcal{M}_\lambda(\overline{\Omega}) \to \mathbb{R}$. If $\xi, \xi_n \in \mathcal{M}_\lambda(\overline{\Omega})$ $(n = 1, 2, \dots)$, then $\xi_n \overset{*}{\rightharpoonup} \xi$ if and only if $D_\lambda(\xi_n, \xi) \to 0$.

Let $\hat{\nu}_n = \mu \circ \Phi_{1/n}^{-1}$ $(n = 1, 2, \dots)$. By Step 2 (cf. Claims (2.2) and (2.3)), each $\hat{\nu}_n \in \mathcal{M}_\lambda(\overline{\Omega})$ and $\mathrm{supp}\,(\hat{\nu}_n) \subset \Omega$, and

$$D_\lambda(\hat{\nu}_n, \mu) \to 0 \qquad \text{and} \qquad E[\hat{\nu}_n] \to E[\mu] \qquad \text{as } n \to \infty.$$

Now, by Step 3 (cf. Claims (3.1)–(3.3)), for each n, there exists $\alpha(n) > 0$ such that $\nu_n := \nu_{\alpha(n),1/n} = \varphi_{\alpha(n)} * \hat{\nu}_n \in \mathcal{M}_\lambda(\overline{\Omega})$, ν_n is absolutely continuous with respect to the Lebesgue measure with a $C_c^\infty(\mathbb{R}^3)$-density, $\mathrm{supp}\,(\nu_n) \subset \Omega$,

$$D_\lambda(\nu_n, \hat{\nu}_n) \le 1/n \qquad \text{and} \qquad |E[\nu_n] - E[\hat{\nu}_n]| \le 1/n \qquad (n = 1, 2, \dots).$$

In the case that $\mathrm{supp}\,(\mu) \subseteq \partial\Omega$ and $\varepsilon > 0$, set $\hat{\nu}_n = \mu \circ \Phi_{t_\varepsilon/n}^{-1}$ $(n = 1, 2, \dots)$, where t_ε is given in Claim (2.3) of Step 2. Then, similarly, for each n, $\hat{\nu}_n \in \mathcal{M}_\lambda(\overline{\Omega})$ and

$$\mathrm{supp}\,(\hat{\nu}_n) \subset \{x \in \Omega : \mathrm{dist}\,(x, \partial\Omega) < \varepsilon/2\}.$$

Moreover,

$$D_\lambda(\hat{\nu}_n, \mu) \to 0 \qquad \text{and} \qquad E[\hat{\nu}_n] \to E[\mu] \qquad \text{as } n \to \infty.$$

Now, by Step 3 (cf. Claims (3.1)–(3.3)), for each n, there exists $\alpha(n) \in (0, \alpha_\varepsilon)$, where α_ε is given in (3.21), such that $\nu_n := \nu_{\alpha(n), t_\varepsilon/n} = \varphi_{\alpha(n)} * \hat{\nu}_n \in \mathcal{M}_\lambda(\overline{\Omega})$, ν_n is absolutely continuous with respect to the Lebesgue measure with a $C_{\mathrm{c}}^\infty(\mathbb{R}^3)$-density, and

$$\operatorname{supp}(\nu_n) \subset \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) < \varepsilon\}.$$

Moreover,

$$D_\lambda(\nu_n, \hat{\nu}_n) \le 1/n, \qquad \text{and} \qquad |E[\nu_n] - E[\hat{\nu}_n]| \le 1/n \qquad (n = 1, 2, \dots).$$

In both cases, we have

$$\begin{aligned} D_\lambda(\nu_n, \mu) &\le D_\lambda(\nu_n, \hat{\nu}_n) + D_\lambda(\hat{\nu}_n, \mu) \le \frac{1}{n} + D_\lambda(\hat{\nu}_n, \mu) \to 0, \\ |E[\nu_n] - E[\mu]| &\le |E[\nu_n] - E[\hat{\nu}_n]| + |E[\hat{\nu}_n] - E[\mu]| \le \frac{1}{n} + |E[\hat{\nu}_n] - E[\mu]| \to 0, \end{aligned}$$

as $n \to \infty$. This concludes the proof of Lemma 3.1. □

The second lemma states that the result of Theorem 3.1 holds true if the given signed Radon measure has an $L^\infty(\Omega)$-density with respect to the Lebesgue measure. Note that the smoothness of the boundary $\partial\Omega$ is relaxed here. In proving the lemma, we apply the method in [6] (with some modifications) to construct the sequence of discrete charges. For any $\rho \in L^\infty(\Omega)$, we denote

$$E_{\mathrm{c}}[\rho] = \iint_{\Omega\times\Omega} \frac{\rho(x)\rho(y)}{|x-y|}\, dxdy. \tag{3.22}$$

Lemma 3.2. *Let $\Omega \subset \mathbb{R}^3$ be a nonempty, bounded, open set with a Lipschitz-continuous boundary $\partial\Omega$. Let $\rho \in L^\infty(\Omega)$ with $\lambda := \|\rho\|_{L^1(\Omega)} > 0$. Set $\rho = 0$ on $\mathbb{R}^3 \setminus \Omega$. There exist $\mu_n \in \mathcal{A}_\lambda(\overline{\Omega})$ $(n = 1, 2, \dots)$ such that*

$$\lim_{n\to\infty} \langle \mu_n, g\rangle = \langle \rho, g\rangle \quad \forall g \in C_0(\mathbb{R}^3) \qquad \textit{and} \qquad \lim_{n\to\infty} E_{\mathrm{d}}[\mu_n] = E_{\mathrm{c}}[\rho].$$

Moreover, if $\varepsilon > 0$ and $\rho = 0$ on $\{x \in \Omega : \operatorname{dist}(x, \partial\Omega) > \varepsilon\}$, then μ_n can be constructed so that

$$\operatorname{supp}(\mu_n) \subset \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) < 2\varepsilon\} \qquad (n = 1, 2, \dots).$$

Proof. For convenience, let us denote by μ the signed Radon measure on $\mathbb{R}^3$ with the density ρ, i.e., $d\mu = \rho\, dx$. Thus, for any Borel set $A \subseteq \mathbb{R}^3$,

$$\mu(A) = \int_A \rho(x)\, dx, \quad |\mu|(A) = \int_A |\rho|(x)\, dx, \quad \text{and} \quad E[\mu] = E_{\mathrm{c}}[\rho].$$

Note that $\operatorname{supp}(\mu) \subseteq \overline{\Omega}$ and $\|\mu\| = |\mu|(\mathbb{R}^3) = |\mu|(\Omega) = \lambda$. So, $\mu \in \mathcal{M}_\lambda(\overline{\Omega})$.

We now proceed in three steps.

Step 1. Construction of discrete densities. Since Ω is bounded in $\mathbb{R}^3$, there exists a natural number $L_0 > 0$ such that $\overline{\Omega} \subseteq [-L_0, L_0]^3$. We divide the cube $[-L_0, L_0]^3$ into $(2L_0)^3$ (open) cubes of side 1 and vertices (k_1, k_2, k_3) with each k_j an integer and $-L_0 \le k_j \le L_0$. Bisecting sides of those cubes to divide each of them into 8 small cubes, we obtain a new collection of small cubes of side 2^{-1}. Continuing this process, we obtain a sequence of collections of open cubes. All cubes in the same nth collection have the same side 2^{-n}; and each of such cubes is one of those 8 cubes composed of a cube of side 2^{-n+1} in the preceding collection. Since Ω is open, there exists a smallest integer $n_0 \ge 0$ such that at least one of those cubes of side $h_0 := 2^{-n_0}$ is contained in Ω. In the case that $\rho = 0$ on $\{x \in \Omega : \mathrm{dist}\,(x, \partial\Omega) > \varepsilon\}$, we choose n_0 to be large enough so that $\sqrt{3}h_0 < \varepsilon/2$.

For each integer $n \ge 1$, we denote by $\mathcal{C}_n$ the sub-collection of cubes in $\mathbb{R}^3$ of side $h_0 2^{-n}$ that are completely contained in $\overline{\Omega}$. We denote by m_n the total number of cubes in the collection $\mathcal{C}_n$, and enumerate these cubes as $\mathcal{C}_n = \{\omega_{n,1}, \ldots, \omega_{n,m_n}\}$. Since $\partial\Omega$ is Lipschitz-continuous, we have $m_n \to \infty$ as $n \to \infty$ and

$$\lim_{n\to\infty} \left| \overline{\Omega} \setminus \left(\bigcup_{i=1}^{m_n} \omega_{n,i} \right) \right| = 0. \tag{3.23}$$

Let $\{p_n\}_{n=1}^{\infty}$ be an increasing sequence of natural numbers such that $p_n \to \infty$ as $n \to \infty$. For each integer $n \ge 1$, we set $\hat{N}_n = m_n p_n$. Fix n and $i \in \{1, \ldots, m_n\}$. Since $|\mu|(\omega_{n,i})/|\mu|(\Omega) \in [0, 1]$, there exists a unique integer $N_{n,i} \in [0, \hat{N}_n]$ such that

$$0 \le \frac{N_{n,i}}{\hat{N}_n} - \frac{|\mu|(\omega_{n,i})}{|\mu|(\Omega)} < \frac{1}{\hat{N}_n}. \tag{3.24}$$

Note that $N_{n,i} = 0$ if and only $|\mu|(\omega_{n,i}) = 0$. Assume $i \in \{1, \ldots, m_n\}$ and $|\mu|(\omega_{n,i}) > 0$. Let $l_{n,i} \ge 1$ be the smallest integer that is greater than or equal to $[1 + \hat{N}_n |\mu|(\omega_{n,i})/|\mu|(\Omega)]^{1/3}$. We divide each side of the cube $\omega_{n,i}$ which has the length $h_0 2^{-n}$ into $l_{n,i}$ small intervals each of which has the length $a_{n,i} := h_0 2^{-n}/l_{n,i}$. We have thus decomposed $\omega_{n,i}$ into a collection of disjoined small cubes with side $a_{n,i}$. The total number of such small cubes is $l_{n,i}^3$, which is larger than $N_{n,i}$ by (3.24). We choose $N_{n,i}$ such small cubes and denote their centers by $x_{n,i}^j$ $(j = 1, \ldots, N_{n,i})$. At each of these points, which are all inside $\omega_{n,i}$ and have the spacing $a_{n,i}$, we place a charge of the value $Q_{n,i}$ defined to be

$$Q_{n,i} = \frac{\mu(\omega_{n,i})|\mu|(\Omega)}{|\mu|(\omega_{n,i})}. \tag{3.25}$$

For convenience, we set $Q_{n,i} = 0$ if $|\mu|(\omega_{n,i}) = 0$ (i.e., if $N_{n,i} = 0$). Setting $N_n = \sum_{i=1}^{m_n} N_{n,i}$, we define

$$\mu_n = \frac{1}{N_n} \sum_{i=1, N_{n,i} \ge 1}^{m_n} \sum_{j=1}^{N_{n,i}} Q_{n,i} \delta_{x_{n,i}^j}. \tag{3.26}$$

Clearly, $\mu_n \in \mathcal{A}_\lambda(\overline{\Omega})$ (where $\lambda = \|\rho\|_{L^1(\Omega)}$). In the case $\rho = 0$ on $\{x \in \Omega : \mathrm{dist}\,(x, \partial\Omega) > \varepsilon\}$, we have $\sqrt{3}h_0 < \varepsilon/2$. Thus, each μ_n is supported in $\{x \in \overline{\Omega} : \mathrm{dist}\,(x, \partial\Omega) < 2\varepsilon\}$.

Summing over $i \in \{1, \dots, m_n\}$ in (3.24), we obtain

$$0 \le \frac{N_n}{\hat{N}_n} - \frac{|\mu|(\cup_{i=1}^{m_n} \omega_{n,i})}{|\mu|(\Omega)} < \frac{1}{p_n}.$$

This and (3.23) lead to

$$\lim_{n\to\infty} \frac{N_n}{\hat{N}_n} = 1. \tag{3.27}$$

Noting that $(a+b)^p \le 2^p(a^p + b^p)$ for any $a, b > 0$ and $p \in [1, \infty)$, we have from our definition of $l_{n,i}$ and the fact that $|\mu|(\omega_{n,i} \le \|\rho\|_{L^\infty(\Omega)} |\omega_{n,i}|$ that

$$\begin{aligned} l_{n,i}^3 &\le \left[\left(\frac{1 + \hat{N}_n |\mu|(\omega_{n,i})}{|\mu|(\Omega)} \right)^{1/3} + 1 \right]^3 \\ &\le 8 \left[\frac{1 + \hat{N}_n |\mu|(\omega_{n,i})}{|\mu|(\Omega)} + 1 \right] \\ &\le 8 \left[\frac{1 + \|\rho\|_{L^\infty(\Omega)} \hat{N}_n |\omega_{n,i}|}{|\mu|(\Omega)} + 1 \right]. \end{aligned}$$

This, together with (3.23) and (3.27), leads to

$$\limsup_{n\to\infty} \max_{1\le i\le m_n} l_{n,i}^3 \le 8 \left(1 + \|\rho\|_{L^\infty(\Omega)} + \frac{1}{|\mu|(\Omega)} \right). \tag{3.28}$$

Step 2. Prove the convergence $\langle \mu_n, g \rangle \to \langle \rho, g \rangle = \langle \mu, g \rangle$ for any $g \in C_0(\mathbb{R}^3)$, i.e., $\mu_n \overset{*}{\rightharpoonup} \mu$. Fix $g \in C_0(\mathbb{R}^3)$. For each n and $i \in \{1, \dots, m_n\}$, we denote by $c_{n,i}$ the center of the cube $\omega_{n,i}$. We have by the definition of μ_n, $Q_{n,i}$, and $x_{n,i}^j$ $(j = 1, \dots, N_{n,i})$ above that

$$\begin{aligned} \langle \mu_n, g \rangle - \langle \rho, g \rangle = &\sum_{i=1, N_{n,i}\ge 1}^{m_n} \frac{Q_{n,i}}{N_n} \sum_{j=1}^{N_{n,i}} \left[g\left(x_{n,i}^j\right) - g(c_{n,i}) \right] \\ &+ \sum_{i=1, N_{n,i}\ge 1}^{m_n} \left[\frac{N_{n,i} Q_{n,i}}{N_n} g(c_{n,i}) - g(c_{n,i}) \int_{\omega_{n,i}} \rho(x)\, dx \right] \\ &+ \sum_{i=1, N_{n,i}\ge 1}^{m_n} \int_{\omega_{n,i}} \left[g(c_{n,i}) - g(x) \right] \rho(x)\, dx \\ &- \int_{\Omega \setminus (\cup_{i=1}^{m_n} \omega_{n,i})} g(x) \rho(x)\, dx \\ = &\, I_n + J_n + K_n - \varepsilon_n, \end{aligned} \tag{3.29}$$

where we used the fact that $N_{n,i} = 0$ if and only if $|\mu|(\omega_{n,i}) = 0$.

Denoting for any $\sigma > 0$

$$\omega_g(\sigma) = \sup\{|g(x) - g(y)| : x, y \in \overline{\Omega} \text{ and } |x - y| \le \sigma\},$$

the modulus of continuity for g on $\overline{\Omega}$, we have $\omega_g(\sigma) \to 0$ as $\sigma \to 0^+$ since $g \in C(\overline{\Omega})$. Noting that $N_n = \sum_{i=1}^{m_n} N_{n,i}$, $\operatorname{diam}(\omega_{n,i}) = \sqrt{3}h_0 2^{-n}$, and $|Q_{n,i}| \le \|\rho\|_{L^1(\Omega)}$ by (3.25), we have

$$|I_n| = \left| \sum_{i=1, N_{n,i} \ge 1}^{m_n} \frac{Q_{n,i}}{N_n} \sum_{j=1}^{N_{n,i}} \left[g\left(x_{n,i}^j\right) - g(c_{n,i}) \right] \right| \le \omega_g \left(\frac{\sqrt{3}h_0}{2^n} \right) \|\rho\|_{L^1(\Omega)} \to 0 \tag{3.30}$$

as $n \to \infty$. Similarly,

$$|K_n| = \left| \sum_{i=1, N_{n,i} \ge 1}^{m_n} \int_{\omega_{n,i}} [g(c_{n,i}) - g(x)]\, \rho(x)\, dx \right| \le \omega_g \left(\frac{\sqrt{3}h_0}{2^n} \right) \|\rho\|_{L^1(\Omega)} \to 0 \tag{3.31}$$

as $n \to \infty$. It follows from (3.23) and the fact that $g\rho \in L^1(\Omega)$ that

$$|\varepsilon_n| = \left| \int_{\Omega \setminus (\cup_{i=1}^{m_n} \omega_{n,i})} g(x)\rho(x)\, dx \right| \to 0 \qquad \text{as } n \to \infty. \tag{3.32}$$

By the definition of $Q_{n,i}$ (cf. (3.25)), we have

$$\begin{aligned}
|J_n| &= \left| \sum_{i=1, N_{n,i} \ge 1}^{m_n} \left[\frac{N_{n,i} Q_{n,i}}{N_n} g(c_{n,i}) - g(c_{n,i}) \int_{\omega_{n,i}} \rho(x)\, dx \right] \right| \\
&\le \|g\|_\infty \sum_{i=1, N_{n,i} \ge 1}^{m_n} \left| \frac{N_{n,i} \mu(\omega_{n,i}) |\mu|(\Omega)}{N_n |\mu|(\omega_{n,i})} - \mu(\omega_{n,i}) \right| \\
&\le \|g\|_\infty |\mu|(\Omega) \sum_{i=1, N_{n,i} \ge 1}^{m_n} \frac{|\mu(\omega_{n,i})|}{|\mu|(\omega_{n,i})} \left| \frac{N_{n,i}}{N_n} - \frac{|\mu|(\omega_{n,i})}{|\mu|(\Omega)} \right| \\
&\le \|g\|_\infty |\mu|(\Omega) \sum_{i=1}^{m_n} \left| \frac{N_{n,i}}{N_n} - \frac{|\mu|(\omega_{n,i})}{|\mu|(\Omega)} \right| \\
&\le \|g\|_\infty |\mu|(\Omega) \left[\sum_{i=1}^{m_n} \left| \frac{N_{n,i}}{N_n} - \frac{\hat{N}_n |\mu|(\omega_{n,i})}{N_n |\mu|(\Omega)} \right| + \sum_{i=1}^{m_n} \left| \frac{\hat{N}_n}{N_n} - 1 \right| \frac{|\mu|(\omega_{n,i})}{|\mu|(\Omega)} \right] \\
&\overset{(3.24)}{=} \|g\|_\infty |\mu|(\Omega) \left[\frac{1}{N_n} \sum_{i=1}^{m_n} \left(N_{n,i} - \frac{\hat{N}_n |\mu|(\omega_{n,i})}{|\mu|(\Omega)} \right) + \left| \frac{\hat{N}_n}{N_n} - 1 \right| \frac{|\mu|(\cup_{i=1}^{m_n} \omega_{n,i})}{|\mu|(\Omega)} \right] \\
&= \|g\|_\infty |\mu|(\Omega) \left(1 - \frac{\hat{N}_n}{N_n} \frac{|\mu|(\cup_{i=1}^{m_n} \omega_{n,i})}{|\mu|(\Omega)} + \left| \frac{\hat{N}_n}{N_n} - 1 \right| \frac{|\mu|(\cup_{i=1}^{m_n} \omega_{n,i})}{|\mu|(\Omega)} \right)
\end{aligned}$$

$$\to 0 \qquad \text{as } n \to \infty, \tag{3.33}$$

where the last step follows from (3.23) and (3.27).

Combining all (3.29)–(3.33), we obtain the desired convergence.

Step 3. Prove the convergence $E_{\mathrm{d}}[\mu_n] \to E[\mu]$. Denote the Coulomb potential $v(x) = 1/|x|$. For $\alpha > 0$, define the α-cutoff Coulomb potential

$$v_\alpha(x) = \begin{cases} 1/|x| & \text{if } |x| \geq \alpha, \\ 1/\alpha & \text{if } |x| < \alpha. \end{cases}$$

Denoting

$$D = \{(x, y) \in \overline{\Omega} \times \overline{\Omega} : x = y\}$$

and noting that all μ_n and μ are supported in $\overline{\Omega}$, we then have by (3.5) and (3.6) that for any $\alpha > 0$

$$\begin{aligned}
E_{\mathrm{d}}[\mu_n] - E[\mu] &= \iint_{(\overline{\Omega}\times\overline{\Omega})\setminus D} v(x-y)\, d(\mu_n \times \mu_n)(x,y) - \iint_{\overline{\Omega}\times\overline{\Omega}} v(x-y)\, d(\mu \times \mu)(x,y) \\
&= \iint_{(\overline{\Omega}\times\overline{\Omega})\setminus D} [v(x-y) - v_\alpha(x-y)]\; d(\mu_n \times \mu_n)(x,y) \\
&\quad + \iint_{\overline{\Omega}\times\overline{\Omega}} v_\alpha(x-y)\, d(\mu_n \times \mu_n)(x,y) - \iint_{\overline{\Omega}\times\overline{\Omega}} v_\alpha(x-y)\, d(\mu \times \mu)(x,y) \\
&\quad - \iint_D v_\alpha(x-y)\, d(\mu_n \times \mu_n)(x,y) \\
&\quad - \iint_{\overline{\Omega}\times\overline{\Omega}} [v(x-y) - v_\alpha(x-y)]\; d(\mu \times \mu)(x,y) \\
&= A_n(\alpha) + B_n(\alpha) - C_n(\alpha) - D(\alpha).
\end{aligned}$$

We estimate the terms $D(\alpha)$, $C_n(\alpha)$, $B_n(\alpha)$, and finally $A_n(\alpha)$. Let $\varepsilon > 0$. Denote

$$S_\alpha = \{(x, y) \in \overline{\Omega} \times \overline{\Omega} : |x - y| < \alpha\}.$$

Then the $\mathbb{R}^3 \times \mathbb{R}^3$-Lebesgue measure of S_α tends to 0 as $\alpha \to 0$. Since $d\mu = \rho\, dx$, we have

$$d|\mu \times \mu|(x,y) = d|\mu| \times |\mu|(x,y) = |\rho(x)|\, |\rho(y)|\, dxdy.$$

Note that $\rho = 0$ outside $\overline{\Omega}$. We thus have

$$\begin{aligned}
|D(\alpha)| &= \left| \iint_{\overline{\Omega}\times\overline{\Omega}} [v(x-y) - v_\alpha(x-y)]\; d(\mu \times \mu)(x,y) \right| \\
&\leq \iint_{\overline{\Omega}\times\overline{\Omega}} |v(x-y) - v_\alpha(x-y)|\; |\rho(x)|\, |\rho(y)|\, dxdy \\
&= \iint_{S_\alpha} [v(x-y) - v_\alpha(x-y)]\; |\rho(x)|\, |\rho(y)|\, dxdy
\end{aligned}$$

$$
\begin{aligned}
&\leq \iint_{S_\alpha} \frac{|\rho(x)|\,|\rho(y)|}{|x-y|}\,dxdy \\
&\to 0 \qquad \text{as } \alpha \to 0.
\end{aligned}
$$

Thus, there exists $\alpha_D > 0$ such that $|D(\alpha)| < \varepsilon$ if $0 < \alpha \leq \alpha_D$.

For any fixed $\alpha > 0$, we have by (3.25) and the fact that $N_n = \sum_{i=1}^{m_n} N_{n,i}$ that

$$
\begin{aligned}
|C_n(\alpha)| &= \left| \iint_D v_\alpha(x-y)\,d(\mu_n \times \mu_n)(x,y) \right| \\
&= \frac{1}{\alpha N_n^2} \sum_{i=1}^{m_n} \sum_{j=1}^{N_{n,i}} (Q_{n,j})^2 \\
&\leq \frac{\|\rho\|_{L^1(\Omega)}^2}{\alpha N_n} \\
&\to 0 \qquad \text{as } n \to \infty.
\end{aligned}
$$

From Step 2, we have $\mu_n \overset{*}{\rightharpoonup} \mu$. Thus, $\mu_n \times \mu_n \overset{*}{\rightharpoonup} \mu \times \mu$. Since v_α is continuous, we can modify its values outside a large ball containing $\overline{\Omega}$ so that the modified function is in $C_0(\mathbb{R}^3)$. Thus, we have for any fixed $\alpha > 0$ that

$$
\begin{aligned}
B_n(\alpha) &= \iint_{\overline{\Omega}\times\overline{\Omega}} v_\alpha(x-y)\,d(\mu_n \times \mu_n)(x,y) - \iint_{\overline{\Omega}\times\overline{\Omega}} v_\alpha(x-y)\,d(\mu \times \mu)(x,y) \\
&\to 0 \qquad \text{as } n \to \infty.
\end{aligned}
$$

We now estimate $A_n(\alpha)$ for any $\alpha > 0$. By (3.26), we have

$$
|\mu_n| = \frac{1}{N_n} \sum_{i=1, N_{n,i}\geq 1}^{m_n} \sum_{j=1}^{N_{n,i}} |Q_{n,i}| \delta_{x_{n,i}^j}.
$$

It then follows from Lemma 2.1 that

$$
\begin{aligned}
|A_n(\alpha)| &= \left| \iint_{(\overline{\Omega}\times\overline{\Omega})\setminus D} [v(x-y) - v_\alpha(x-y)]\ d(\mu_n \times \mu_n)(x,y) \right| \\
&\leq \iint_{(\overline{\Omega}\times\overline{\Omega})\setminus D} |v(x-y) - v_\alpha(x-y)|\ d(|\mu_n| \times |\mu_n|)(x,y) \\
&= \iint_{\{x\in\overline{\Omega}\times\overline{\Omega}: 0<|x-y|<\alpha\}} [v(x-y) - v_\alpha(x-y)]\ d(|\mu_n| \times |\mu_n|)(x,y) \\
&\leq \iint_{\{x\in\overline{\Omega}\times\overline{\Omega}: 0<|x-y|<\alpha\}} v(x-y)\,d(|\mu_n| \times |\mu_n|)(x,y) \\
&= \frac{1}{N_n^2} \sum_{i=1, N_{n,i}\geq 1}^{m_n} \sum_{j=1, N_{n,j}\geq 1}^{m_n} \sum_{1\leq k\leq N_{n,i}, 1\leq l\leq N_{n,j}, 0<|x_{n,i}^k - x_{n,j}^l|<\alpha} \frac{|Q_{n,i}|\,|Q_{n,j}|}{|x_{n,i}^k - x_{n,j}^l|}
\end{aligned}
$$

$$= \frac{1}{N_n^2} \sum_{i=1,N_{n,i}\geq 1}^{m_n} \sum_{j=1,N_{n,j}\geq 1}^{m_n} \sum_{1\leq k\leq N_{n,i}, 1\leq l\leq N_{n,j}, 0<|x_{n,i}^k - x_{n,j}^l|<\alpha} \frac{|Q_{n,i}|\,|Q_{n,j}|}{|B(0,a_{n,i}/2)|\,|B(0,a_{n,j}/2)|}$$
$$\cdot \int_{B(x_{n,i}^k, a_{n,i}/2)} \int_{B(x_{n,j}^l, a_{n,j}/2)} \frac{dxdy}{|x-y|}.$$

Denoting $a_n = \max_{i=1}^{m_n} a_{n,i}$ and $l_n = \max_{i=1}^{m_n} l_{n,i}$, and noting that $1/|B(0,a_{n,i}/2)| = 6l_{n,i}^3/(\pi|\omega_{n,i}|)$ and that $\omega_n := \omega_{n,i}$ is independent of $i = 1,\dots,m_n$, we continue to have by (3.25) that

$$|A_n(\alpha)| \leq \frac{36\|\rho\|_{L^1(\Omega)}^2 l_n^6}{\pi^2 N_n^2 \omega_n^2}$$
$$\cdot \sum_{i=1,N_{n,i}\geq 1}^{m_n} \sum_{j=1,N_{n,j}\geq 1}^{m_n} \sum_{1\leq k\leq N_{n,i}, 1\leq l\leq N_{n,j}, 0<|x_{n,i}^k - x_{n,j}^l|<\alpha} \int_{B(x_{n,i}^k, a_{n,i}/2)} \int_{B(x_{n,j}^l, a_{n,j}/2)} \frac{dxdy}{|x-y|}$$
$$\leq \frac{36\|\rho\|_{L^1(\Omega)}^2 l_n^6}{\pi^2 N_n^2 \omega_n^2} \iint_{\{(x,y)\in\overline{\Omega}\times\overline{\Omega}: 0<|x-y|<\alpha+a_n\}} \frac{dxdy}{|x-y|}.$$

For the given $\varepsilon > 0$, by the integrability of $1/|x-y|$, there exists $\alpha_A > 0$ such that

$$\iint_{\{(x,y)\in\overline{\Omega}\times\overline{\Omega}: 0<|x-y|<2\alpha\}} \frac{dxdy}{|x-y|} < \varepsilon \qquad \text{if } 0 < \alpha < \alpha_A.$$

Consequently, by (3.28) and (3.23), we have

$$\limsup_{n\to\infty} |A_n(\alpha)| \leq C_0\varepsilon \qquad \text{if } 0 < \alpha < \alpha_A,$$

where C_0 is a constant given by

$$C_0 = \frac{36\cdot 8^6 \|\rho\|_{L^1(\Omega)}^2 \left[1 + \|\rho\|_{L^\infty(\Omega)} + 1/|\mu|(\Omega)\right]^6}{\pi^2|\Omega|^2}.$$

Finally, by choosing $\alpha \in (0, \min(\alpha_D, \alpha_A))$, we have

$$\limsup_{n\to\infty} |E_{\mathrm{d}}[\mu_n] - E[\mu]| \leq \limsup_{n\to\infty} |A_n(\alpha) + B_n(\alpha) - C_n(\alpha) - D(\alpha)|$$
$$\leq (1 + C_0)\varepsilon.$$

Thus, $E_{\mathrm{d}}[\mu_n] \to E[\mu]$. □

We are now ready to prove Theorem 3.1.

Proof of Theorem 3.1. Let $\mu \in \mathcal{M}_\lambda(\overline{\Omega})$ with $E[|\mu|] < \infty$. By Lemma 3.1, there exist $\nu_k \in \mathcal{M}_\lambda(\overline{\Omega})$ $(k = 1, 2, \dots)$ such that each ν_k has a $C_{\mathrm{c}}^\infty(\Omega)$-density and $\operatorname{supp}(\nu_k) \subseteq \Omega$, and

$$\nu_k \overset{*}{\rightharpoonup} \mu \qquad \text{and} \qquad E_{\mathrm{d}}[\nu_k] \to E[\mu] \qquad \text{as } k \to \infty.$$

By Lemma 3.2, for each k, there exist $\nu_{k,n} \in \mathcal{A}_\lambda(\overline{\Omega})$ $(n = 1, 2, \dots)$ such that

$$\nu_{k,n} \overset{*}{\rightharpoonup} \nu_k \qquad \text{and} \qquad E_{\mathrm{d}}[\nu_{k,n}] \to E[\nu_k] \qquad \text{as } n \to \infty.$$

Note that the weak-$*$ topology of $\mathcal{M}_\lambda(\overline{\Omega})$ is metrizable; cf. Step 4 in the proof of Lemma 3.1. Denote this metric by D_λ. By induction, we can choose a sequence of increasing integers $n_k \geq 1$ such that

$$D_\lambda(\nu_{k,n_k}, \nu_k) < 1/k \qquad \text{and} \qquad |E_{\mathrm{d}}[\nu_{k,n_k}] - E[\nu_k]| < 1/k \qquad \text{for all } k = 1, 2, \dots$$

Therefore, setting $\mu_k = \nu_{k,n_k} \in \mathcal{A}_\lambda(\overline{\Omega})$ $(k = 1, 2, \dots)$, we have

$$\begin{aligned} &D_\lambda(\mu_k, \mu) \leq D_\lambda(\nu_{k,n_k}, \nu_k) + D_\lambda(\nu_k, \mu) \to 0, \\ &|E_{\mathrm{d}}[\mu_k] - E[\mu]| \leq |E_{\mathrm{d}}[\mu_{k,n_k}] - E[\nu_k]| + |E[\nu_k] - E[\mu]| \to 0, \end{aligned}$$

as $k \to \infty$. Hence, $\mu_k \overset{*}{\rightharpoonup} \mu$ and $E_{\mathrm{d}}[\mu_k] \to E[\mu]$ as $k \to \infty$.

If $\mathrm{supp}(\mu) \subseteq \partial\Omega$ and $\varepsilon > 0$, then by Lemma 3.1, the measures ν_k above can be constructed so that

$$\mathrm{supp}\,(\nu_k) \subseteq \{x \in \overline{\Omega} : \mathrm{dist}(x, \partial\Omega) < \varepsilon/2\} \qquad (k = 1, 2, \dots).$$

By Lemma 3.2, the measures $\nu_{k,n}$ above can be constructed so that

$$\mathrm{supp}\,(\nu_{k,n}) \subseteq \{x \in \overline{\Omega} : \mathrm{dist}(x, \partial\Omega) < \varepsilon\} \qquad (k, n = 1, 2, \dots).$$

Thus, since $\mu_k = \nu_{k,n_k}$, we have

$$\mathrm{supp}\,(\mu_k) \subseteq \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) < \varepsilon\} \qquad (k = 1, 2, \dots).$$

The proof is complete. □

4 Continuum Limit of a Given Sequence of Discrete Charges

We now study the continuum limit of a given sequence of sets of point charges and the corresponding limit of electrostatic energies. Let N_n be an increasing sequence of natural numbers such that $N_n \to \infty$ as $n \to \infty$. For each $n \in \{1, 2, \dots\}$, let $x_n^1, \dots, x_n^{N_n}$ be N_n distinct points in Ω and let $Q_n^1, \dots, Q_n^{N_n} \in [-1, 1]$. (The particular bound 1 of all the charges Q_n^i is not essential; we can replace 1 by any given positive number.) Define $\mu_n \in \mathcal{A}_1(\overline{\Omega})$ (cf. (3.4)) by

$$\mu_n = \frac{1}{N_n} \sum_{i=1}^{N_n} Q_n^i \delta_{x_n^i}. \tag{4.1}$$

Recall that the corresponding discrete energies $E_{\mathrm{d}}[\mu_n]$ are defined in (3.5). We consider the following *geometric conditions:* For each $n = 1, 2, \dots$ there exists a radius $r_n > 0$ such that

- $B(x_n^i, r_n) \subset \Omega$ for all $i = 1, \dots, N_n$;
- $B(x_n^i, r_n) \cap B(x_n^j, r_n) = \emptyset$ for all $i, j = 1, \dots, N_n$ with $j \neq i$; and
- $\tau := \inf_{n \geq 1} N_n |B_{r_n}| > 0$, where B_λ denotes an open ball of radius $\lambda > 0$.

Since Ω is bounded, a consequence of these conditions is that $r_n \to 0$ as $n \to \infty$.

Theorem 4.1. *Let $\Omega \subset \mathbb{R}^3$ be a nonempty, bounded, open set with a Lipschitz-continuous boundary $\partial\Omega$. For each natural number $n \geq 1$, let $\mu_n \in \mathcal{A}_1(\overline{\Omega})$ be given in (4.1) with distinct $x_n^i \in \Omega$ and $Q_n^i \in [-1, 1]$ $(i = 1, \dots, N_n; n = 1, 2, \dots)$. Assume the geometrical conditions hold true. Then, there is a subsequence of $\{\mu_n\}$, not relabeled, such that $\mu_n \overset{*}{\rightharpoonup} \mu$ on $\mathbb{R}^3$ for some Radon measure μ, given by $d\mu = \rho\, dx$ for some $\rho \in L^\infty(\mathbb{R}^3)$ with $\rho = 0$ a.e. on $\overline{\Omega}^c$. Moreover, $E[|\mu|] < \infty$, and*

$$\lim_{n \to \infty} E_{\mathrm{d}}[\mu_n] = E[\mu]. \tag{4.2}$$

We remark that the geometrical conditions imply that the discrete charges are nearly evenly distributed in the entire region. A limit measure (if exists) may not have an $L^\infty(\Omega)$-density if the geometrical conditions are not satisfied. A simple example is $\Omega = (0, 1)^3$, $N_n = n$, $x_n^i = (i/n, 0, 0)$, and $Q_n^i = 1$. The geometrical conditions with respect to Ω are violated. The limit measure is the Dirac measure concentrated on $[0, 1] \times 0 \times 0 \subset \overline{\Omega}$, which does not have a density (with respect to the Lebesgue measure). We also remark that there may exist different subsequences of $\{\mu_n\}_{n=1}^\infty$ that converge vaguely to different limits, and the corresponding subsequences of rescaled discrete energies converge to different limits. We shall give an example to show such nonuniqueness at the end of this section.

We need two lemmas to prove our theorem. The first lemma below is a variation of Newton's Theorem. The second lemma is similar to a known result (cf. e.g., the proof of Proposition 2.1 in [6]). For $R \in (0, \infty]$, we say that a function $\phi : \overline{B(0, R)} \to \mathbb{R}$ is radially symmetric if there exists a function $\phi_0 : [0, R] \to \mathbb{R}$ such that $\phi(x) = \phi_0(|x|)$ for all $x \in \mathbb{R}^3$ with $|x| \leq R$.

Lemma 4.1. *Let $R > 0$. If $\phi \in C(\overline{B(0, R)})$ is radially symmetric, then*

$$\int_{B(0,R)} \frac{\phi(x)}{|y - x|}\, dx = \frac{1}{|y|} \int_{B(0,R)} \phi(x)\, dx \qquad \forall y \in \mathbb{R}^3 \text{ with } |y| > R.$$

Proof. With abuse of notation, $\phi(|y|) = \phi(y)$, using the spherical coordinates, and by the mean-value property for a harmonic function, we have

$$\begin{aligned}
\int_{B(0,R)} \frac{\phi(x)}{|y - x|}\, dx &= \int_0^R \phi(r) \int_{\partial B(0,r)} \frac{dS_\omega}{|y - \omega|}\, dr \\
&= \int_0^R \phi(r) \frac{4\pi r^2}{|y|}\, dr \\
&= \frac{1}{|y|} \int_{B(0,R)} \phi(x)\, dx,
\end{aligned}$$

completing the proof. □

Lemma 4.2. *If $\phi \in C(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ is radially symmetric, then*

$$\int_{\mathbb{R}^3} \frac{\phi(x)}{|x-y|}\,dx = \int_{\mathbb{R}^3} \min\left(\frac{1}{|x|}, \frac{1}{|y|}\right)\phi(x)\,dx \qquad \forall y \in \mathbb{R}^3.$$

Proof. If $y = 0$, then the two integrals are the same. Assume $y \in \mathbb{R}^3$ and $y \neq 0$. By the Dominated Convergence Theorem and Part (1) of Lemma 4.1, we have

$$\begin{aligned}\int_{B(0,|y|)} \frac{\phi(x)}{|x-y|}\,dx &= \lim_{\varepsilon\to 0^+} \int_{B(0,|y|-\varepsilon)} \frac{\phi(x)}{|x-y|}\,dx \\ &= \lim_{\varepsilon\to 0^+} \int_{B(0,|y|-\varepsilon)} \frac{\phi(x)}{|y|}\,dx \\ &= \int_{B(0,|y|)} \frac{\phi(x)}{|y|}\,dx.\end{aligned}$$

Define

$$h(z) = \int_{\mathbb{R}^3\setminus B(0,|y|)} \frac{\phi(x)}{|x-z|}\,dx \qquad \forall z \in \mathbb{R}^3.$$

Since ϕ is radially symmetric and the Lebesgue measure is rotationally invariant, $h(z) = h(y)$ for any $z \in \partial B(0,|y|)$. Moreover, h is harmonic in the region $|z| \leq |y|$ (see, e.g., Theorem 1.4 in [26]). Therefore, by the mean-value property for a harmonic function, the integral of h over the sphere $\partial B(0,|y|)$ divided by the area of that sphere is just $h(0)$. Hence $h(y) = h(0)$. Therefore,

$$\begin{aligned}\int_{\mathbb{R}^3} \frac{\phi(x)}{|x-y|}\,dx &= \int_{B(0,|y|)} \frac{\phi(x)}{|x-y|}\,dx + \int_{\mathbb{R}^3\setminus B(0,R)} \frac{\phi(x)}{|x-y|}\,dx \\ &= \int_{B(0,|y|)} \frac{\phi(x)}{|y|}\,dx + \int_{\mathbb{R}^3\setminus B(0,|y|)} \frac{\phi(x)}{|x|}\,dx \\ &= \int_{\mathbb{R}^3} \min\left(\frac{1}{|x|}, \frac{1}{|y|}\right)\phi(x)\,dx.\end{aligned}$$

The proof is complete. □

Proof of Theorem 4.1. We divide the proof into two steps.

Step 1. We prove the existence of a subsequence of $\{\mu_n\}_{n=1}^\infty$ that converges vaguely to some Radon measure μ with an $L^\infty(\mathbb{R}^3)$ density vanishing a.e. on $\overline{\Omega}^c$ and $E[|\mu|] < \infty$. It suffices to consider the case that all $Q_n^i \geq 0$, since in general we have the Jordan decomposition $\mu_n = \mu_n^+ - \mu_n^-$ with

$$\mu_n^+ = \frac{1}{N_n}\sum_{i=1}^{N_n} \max(Q_n^i, 0)\delta_{x_n^i} \qquad \text{and} \qquad \mu_n^- = \frac{1}{N_n}\sum_{i=1}^{N_n} \max(-Q_n^i, 0)\delta_{x_n^i},$$

and we can first extract a vaguely convergent subsequence from $\{\mu_n^+\}_{n=1}^\infty$ and then a further vaguely convergent subsequence from $\{\mu_n^-\}_{n=1}^\infty$, with the limiting Radon measures having $L^\infty(\mathbb{R}^3)$ densities vanishing a.e. on $\overline{\Omega}^c$.

Since $0 \le Q_n^i \le 1$ for all i and n, we have $\|\mu_n\| \le 1$ for all $n \ge 1$. Thus, it follows from the Banach–Alaoglu Theorem that there exists a subsequence of $\{\mu_n\}_{n=1}^\infty$, not relabeled, such that $\mu_n \overset{*}{\rightharpoonup} \mu$ for some nonnegative Radon measure μ on $\mathbb{R}^3$.

For any open ball B_λ of radius $\lambda > 0$, we have

$$\mu_n(B_\lambda) \le \frac{1}{N_n}\mathrm{Card}\,(\{i : x_n^i \in B_\lambda\}), \tag{4.3}$$

where Card (A) denotes the cardinality of a set A, For each natural number n, we denote by $B_{\lambda+r_n}$ the ball of radius $\lambda+r_n$ that is concentric with the ball B_λ. Since $B(x_n^i, r_n) \subset B_{\lambda+r_n}$ if $x_n^i \in B_\lambda$ and $B(x_n^i, r_n) \cap B(x_n^j, r_n) = \emptyset$ if $i \ne j$, we have from volume considerations that

$$\mathrm{Card}(\{i : x_n^i \in B_\lambda\}) \le \mathrm{Card}(\{i : B(x_n^i, r_n) \subset B_{\lambda+r_n}\}) \le \frac{|B_{\lambda+r_n}|}{|B_{r_n}|}.$$

This, together with (4.3) and the definition of τ in the geometrical conditions, implies that

$$\mu_n(B_\lambda) \le \frac{|B_{\lambda+r_n}|}{N_n|B_{r_n}|} \le \frac{1}{\tau}|B_{\lambda+r_n}| \to \frac{1}{\tau}|B_\lambda| \qquad \text{as } n \to \infty,$$

since $r_n \to 0$. Consequently, for any open ball $B \subset \mathbb{R}^3$, we have

$$\liminf_{n\to\infty} \mu_n(B) \le \frac{1}{\tau}|B|. \tag{4.4}$$

Suppose $A \subset \mathbb{R}^3$ is bounded with $|A| = 0$ and $\varepsilon > 0$. It follows from Vitali's covering lemma that there exist countably many open balls B_i covering A with $\sum_i |B_i| < \varepsilon$. Since $\mu_n \overset{*}{\rightharpoonup} \mu$, we have

$$\mu(U) \le \liminf_{n\to\infty} \mu_n(U) \tag{4.5}$$

for any open set $U \subseteq \mathbb{R}^3$; cf. Theorem 1.24 in [29]. This and (4.4) imply that

$$\mu(A) \le \mu\left(\bigcup_i B_i\right) \le \sum_i \mu(B_i) \le \frac{1}{\gamma}\sum_i |B_i| < \frac{1}{\gamma}\varepsilon.$$

Hence, it follows from the Radon–Nikodym Theorem that $d\mu = \rho\, dx$ for some $\rho \in L^1(\mathbb{R}^3)$. Since all $\mu_n \ge 0$, we have $\mu \ge 0$, and hence $\rho \ge 0$ a.e. in $\mathbb{R}^3$. The Lebesgue Differentiation Theorem now gives that

$$\rho(x) = \lim_{r\to 0^+} \frac{1}{|B(x,r)|}\int_{B(x,r)} \rho(y)\, dy \qquad \text{a.e. } x \in \mathbb{R}^3.$$

But it follows from (4.4) and (4.5) that

$$\frac{1}{|B(x,r)|}\int_{B(x,r)} \rho(y)\, dy = \frac{1}{|B(x,r)|}\mu(B(x,r))$$

$$
\begin{aligned}
&\le \frac{1}{|B(x,r)|} \liminf_{n\to\infty} |\mu_n|(B(x,r)) \\
&\le \frac{1}{\tau}.
\end{aligned}
$$

Hence, $0 \le \rho(x) \le 1/\tau$ for a.e. $x \in \mathbb{R}^3$; hence $\rho \in L^\infty(\mathbb{R}^3)$. Since (4.5) holds for any $U \subset \overline{\Omega}^c$ and $\mu_n(\overline{\Omega}^c) = 0$, we have $\operatorname{supp}(\mu) \subseteq \overline{\Omega}$. This implies that $\rho = 0$ a.e. on $\overline{\Omega}^c$. Note that $d|\mu| = |\rho|\,dx = \rho\,dx$. Thus $E[|\mu|] < \infty$.

Step 2. We prove the convergence (4.2), assuming all $Q_n^i \in [-1,1]$ and $d\mu = \rho\,dx$ with $\rho \in L^\infty(\mathbb{R}^3)$ vanishing at a.e. $x \in \overline{\Omega}^c$.

Let $\varphi \in C_c^\infty(\mathbb{R}^3)$ be nonnegative and radially symmetric, satisfying $\operatorname{supp}(\varphi) \subset \overline{B(0,1)}$ and (3.19). Define $\varphi_\lambda(x) = \lambda^{-3}\varphi(x/\lambda)$ for any $\lambda > 0$ and $x \in \mathbb{R}^3$. Recall for any Radon measure ν on $\mathbb{R}^3$ and any $\xi \in C_c(\mathbb{R}^3)$ that the convolusion $\nu * \xi \in C_c^\infty(\mathbb{R}^3)$ is defined by $(\nu * \xi)(x) = \langle \nu, \xi(x - \cdot)\rangle$ $(x \in \mathbb{R}^3)$. Hence,

$$
\begin{aligned}
(\mu_n * \varphi_\lambda)(x) &= \frac{1}{N_n}\sum_{i=1}^{N_n} Q_n^i \varphi_\lambda(x - x_n^i) \qquad \forall x \in \mathbb{R}^3 \ \text{ and } \ \forall n \ge 1, \\
(\mu * \varphi_\lambda)(x) &= \int_{\mathbb{R}^3} \varphi_\lambda(x-y)\,d\mu(y) = \int_{\mathbb{R}^3} \varphi_\lambda(x-y)\rho(y)\,dy \qquad \forall x \in \mathbb{R}^3.
\end{aligned}
$$

We now write

$$
\begin{aligned}
&|E_{\mathrm{d}}[\mu_n] - E[\mu]| \\
&\qquad \le |E_{\mathrm{d}}[\mu_n] - E_{\mathrm{c}}[\mu_n * \varphi_\lambda]| + |E_{\mathrm{c}}[\mu_n * \varphi_\lambda] - E_{\mathrm{c}}[\mu * \varphi_\lambda]| + |E_{\mathrm{c}}[\mu * \varphi_\lambda] - E[\mu]|, \qquad (4.6)
\end{aligned}
$$

where E_{c} is defined in (3.22). We estimate these three terms in three substeps and combine all the estimates to obtain the desired convergence result in the fourth and last substep.

Step 2.1. We claim that there exists a constant $C > 0$ such that

$$
|E_{\mathrm{d}}[\mu_n] - E_{\mathrm{c}}[\mu_n * \varphi_\lambda]| \le C\left(\lambda^2 + r_n^2 + \frac{1}{N_n\lambda}\right) \qquad \forall n \ge 1 \ \text{ and } \ \forall \lambda > 0, \qquad (4.7)
$$

where r_n is given in the geometrical conditions.

Proof of the claim. It follows from the Fubini–Tonelli Theorem that

$$
\begin{aligned}
E_{\mathrm{c}}[\mu_n * \varphi_\lambda] &= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{(\mu_n * \varphi_\lambda)(x)(\mu_n * \varphi_\lambda)(y)}{|x-y|}\,dxdy \\
&= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{1}{|x-y|}\left[\frac{1}{N_n}\sum_{i=1}^{N_n} Q_n^i \varphi_\lambda(x - x_n^i)\right]\left[\frac{1}{N_n}\sum_{j=1}^{N_n} Q_n^j \varphi_\lambda(y - x_n^j)\right] dxdy \\
&= \frac{1}{N_n^2}\sum_{1\le i,j\le N_n} Q_n^i Q_n^j \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi_\lambda(x - x_n^i)\varphi_\lambda(y - x_n^j)}{|x-y|}\,dxdy.
\end{aligned}
$$

Making the change of variables $y \mapsto y + x_j^n$ gives

$$E_{\mathrm{c}}[\mu_n * \varphi_\lambda] = \frac{1}{N_n^2} \sum_{1 \le i,j \le N_n} Q_n^i Q_n^j \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\varphi_\lambda(x - x_n^i)\varphi_\lambda(y)}{|x - y - x_n^j|} \, dx dy,$$

and the further change of variables $x \mapsto y - x + x_n^i$ gives

$$\begin{aligned} E_{\mathrm{c}}[\mu_n * \varphi_\lambda] &= \frac{1}{N_n^2} \sum_{1 \le i,j \le N_n} Q_n^i Q_n^j \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\varphi_\lambda(y - x)\varphi_\lambda(y)}{|x_n^i - x_n^j - x|} \, dx dy \\ &= \frac{1}{N_n^2} \sum_{1 \le i,j \le N_n} Q_n^i Q_n^j \int_{\mathbb{R}^3} \frac{1}{|x_n^i - x_n^j - x|} \left[\int_{\mathbb{R}^3} \varphi_\lambda(y - x)\varphi_\lambda(y) \, dy \right] dx \\ &= \frac{1}{N_n^2} \sum_{1 \le i,j \le N_n} Q_n^i Q_n^j \int_{\mathbb{R}^3} \frac{\vartheta_\lambda(x)}{|x_n^i - x_n^j - x|} \, dx, \end{aligned} \tag{4.8}$$

where $\vartheta_\lambda = \varphi_\lambda * \varphi_\lambda \in C_{\mathrm{c}}^\infty(\mathbb{R}^3)$. Consequently,

$$\begin{aligned} &E_{\mathrm{d}}[\mu_n] - E_{\mathrm{c}}[\mu_n * \varphi_\lambda] \\ &\quad = \frac{1}{N_n^2} \sum_{1 \le i,j \le N_n, i \ne j} Q_n^i Q_n^j \frac{1}{|x_n^i - x_n^j|} - \frac{1}{N_n^2} \sum_{1 \le i,j \le N_n} Q_n^i Q_n^j \int_{\mathbb{R}^3} \frac{\vartheta_\lambda(x)}{|x_n^i - x_n^j - x|} \, dx \\ &\quad = \frac{1}{N_n^2} \sum_{1 \le i,j \le N_n, i \ne j} Q_n^i Q_n^j \int_{\mathbb{R}^3} \left(\frac{1}{|x_n^i - x_n^j|} - \frac{1}{|x_n^i - x_n^j - x|} \right) \vartheta_\lambda(x) \, dx \\ &\qquad - \frac{1}{N_n^2} \sum_{i=1}^{N_n} (Q_n^i)^2 \int_{\mathbb{R}^3} \vartheta_\lambda(x) \frac{1}{|x|} \, dx \\ &\quad =: \alpha_n(\lambda) - \beta_n(\lambda). \end{aligned} \tag{4.9}$$

We first estimate the second term $\beta_n(\lambda)$. Let us denote

$$c_0 = \int_{\mathbb{R}^3} \vartheta(x) \frac{1}{|x|} \, dx = \int_{\mathbb{R}^3} (\varphi * \varphi)(x) \frac{1}{|x|} \, dx,$$

This is a positive number by the local integrability of $1/|x|$ and it depends only on φ. The integral in $\beta_n(\lambda)$ is then found to equal c_0/λ. Since $|Q_n^i| \le 1$ for all n and i, we have

$$|\beta_n(\lambda)| = \frac{1}{N_n^2} \sum_{i=1}^{N_n} (Q_n^i)^2 \int_{\mathbb{R}^3} \vartheta_\lambda(x) \frac{1}{|x|} \, dx = \frac{1}{N_n^2} \sum_{i=1}^{N_n} (Q_n^i)^2 \frac{c_0}{\lambda} \le \frac{c_0}{N_n \lambda}. \tag{4.10}$$

We now estimate the first term $\alpha_n(\lambda)$ in (4.9). Note that $\vartheta_\lambda = \varphi_\lambda * \varphi_\lambda \in C_{\mathrm{c}}^\infty(\mathbb{R}^3)$ is nonnegative, radially symmetric, and supported on $\overline{B(0, 2\lambda)}$. Moreover,

$$\int_{\mathbb{R}^3} \vartheta_\lambda(x) \, dx = \int_{\mathbb{R}^3} \varphi_\lambda(x) \, dx \int_{\mathbb{R}^3} \varphi_\lambda(x) \, dx = 1. \tag{4.11}$$

If $|x_n^i - x_n^j| > 2\lambda$, then Lemma 4.1 implies that

$$\int_{\mathbb{R}^3} \left(\frac{1}{|x_n^i - x_n^j|} - \frac{1}{|x_n^i - x_n^j - x|} \right) \vartheta_\lambda(x)\, dx = 0.$$

For $0 < |x_n^i - x_n^j| \le 2\lambda$, we have that

$$\left| \frac{1}{|x_n^i - x_n^j|} - \frac{1}{|x_n^i - x_n^j - x|} \right| \le \frac{|x|}{|x_n^i - x_n^j||x_n^i - x_n^j - x|},$$

and by Lemma 4.2 that

$$\begin{aligned} \int_{\mathbb{R}^3} \frac{|x|\vartheta_\lambda(x)dx}{|x_n^i - x_n^j - x|} &= \int_{\mathbb{R}^3} \min\left(\frac{1}{|x|}, \frac{1}{|x_n^i - x_n^j|} \right) |x|\vartheta_\lambda(x)\, dx \\ &\le \int_{\mathbb{R}^3} \frac{1}{|x|} |x|\vartheta_\lambda(x)\, dx \\ &= 1. \end{aligned}$$

Therefore, since $|Q_n^i| \le 1$ for all n and i, we obtain from (4.9) that

$$\begin{aligned} |\alpha_n(\lambda)| &= \left| \frac{1}{N_n^2} \sum_{1 \le i,j \le N_n, i \ne j} Q_n^i Q_n^j \int_{\mathbb{R}^3} \left(\frac{1}{|x_n^i - x_n^j|} - \frac{1}{|x_n^i - x_n^j - x|} \right) \vartheta_\lambda(x) dx \right| \\ &\le \frac{1}{N_n^2} \sum_{1 \le i,j \le N, 0 < |x_n^i - x_n^j| \le 2\lambda} \frac{1}{|x_n^i - x_n^j|} \int_{\mathbb{R}^3} \frac{|x|\vartheta_\lambda(x)}{|x_n^i - x_n^j - x|} dx. \\ &= \frac{1}{N_n^2} \sum_{1 \le i,j \le N, 0 < |x_n^i - x_n^j| \le 2\lambda} \frac{1}{|x_n^i - x_n^j|}. \end{aligned} \tag{4.12}$$

Since the balls $B(x_n^i, r_n)$ $(i = 1, \dots, N_n)$ (introduced in the geometrical conditions) are pairwise disjoint, the Mean-Value Theorem for a harmonic function implies that

$$\frac{1}{|x_n^i - x_n^j|} = \frac{1}{(4/3)\pi r_n^3} \int_{B(x_n^j, r_n)} \frac{dy}{|x_n^i - y|} \qquad \text{if } i \ne j.$$

By the geometrical conditions, $N_n r_n^3 \ge 3\tau/(4\pi)$ $(n = 1, 2, \dots)$. Consequently, we obtain from (4.12) that

$$\begin{aligned} |\alpha_n(\lambda)| &\le \frac{1}{N_n^2} \sum_{i=1}^{N_n} \sum_{1 \le j \le N, 0 < |x_n^i - x_n^j| \le 2\lambda} \frac{1}{(4/3)\pi r_n^3} \int_{B(x_n^j, r_n)} \frac{dy}{|x_i^n - y|} \\ &\le \frac{3}{4\pi N_n r_n^3} \int_{B(0, 2\lambda + r_n)} \frac{dy}{|y|} \\ &\le \frac{8\pi}{\tau} \left(2\lambda^2 + r_n^2 \right). \end{aligned}$$

This, together with (4.9) and (4.10), implies (4.7). The claim is proved.

Step 2.2. We prove for any $\lambda > 0$ that

$$\lim_{n\to\infty} E_{\mathrm{c}}[\mu_n * \varphi_\lambda] = E_{\mathrm{c}}[\mu * \varphi_\lambda]. \tag{4.13}$$

We have for any n and x that

$$|\mu_n * \varphi_\lambda(x)| = \left| \frac{1}{N_n} \sum_{i=1}^{N_n} Q_n^i \varphi_\lambda(x - x_n^i) \right| \le \frac{1}{N_n} \sum_{i=1}^{N_n} |Q_n^i| \|\varphi_\lambda\|_\infty \le \|\varphi_\lambda\|_\infty = \lambda^{-3} \|\varphi\|_\infty.$$

Hence,

$$\frac{(\mu_n * \varphi_\lambda)(x)(\mu_n * \varphi_\lambda)(y)}{|x-y|} \le \frac{(\lambda^{-3}\|\varphi\|_\infty)^2}{|x-y|} \qquad \text{a.e. } (x,y) \in \mathbb{R}^3 \times \mathbb{R}^3.$$

The right-hand side of this inequality is locally integrable in $\mathbb{R}^3 \times \mathbb{R}^3$. Since $\mu_n \overset{*}{\rightharpoonup} \mu$ and $\varphi_\lambda(x - \cdot) \in C_{\mathrm{c}}^\infty(\mathbb{R}^3)$, we have

$$\lim_{n\to\infty} (\mu_n * \varphi_\lambda)(x) = (\mu * \varphi_\lambda)(x) \qquad \forall x \in \mathbb{R}^3. \tag{4.14}$$

It then follows from the Dominated Convergence Theorem that

$$\lim_{n\to\infty} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{(\mu_n * \varphi_\lambda)(x)(\mu_n * \varphi_\lambda)(y)}{|x-y|}\, dxdy = \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{(\mu * \varphi_\lambda)(x)(\mu * \varphi_\lambda)(y)}{|x-y|}\, dxdy.$$

This is exactly (4.13).

Step 2.3. We have

$$\lim_{\lambda\to 0^+} E_{\mathrm{c}}[\mu * \varphi_\lambda] = E[\mu]. \tag{4.15}$$

This is a known result; cf. e.g., Lemma A1 in [6]. Here for completeness we provide some details of the proof in our setting.

We have by (4.14) that

$$\begin{aligned} E_{\mathrm{c}}[\mu * \varphi_\lambda] &= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{(\mu * \varphi_\lambda)(x)(\mu * \varphi_\lambda)(y)}{|x-y|}\, dxdy \\ &= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{1}{|x-y|} \left[\int_{\mathbb{R}^3} \varphi_\lambda(x-x')d\mu(x') \right] \left[\int_{\mathbb{R}^3} \varphi_\lambda(y-y')d\mu(y') \right] dxdy \\ &= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \left[\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi_\lambda(x-x')\varphi_\lambda(y-y')}{|x-y|} dxdy \right] d\mu(x')d\mu(y'). \end{aligned}$$

By Lemma 4.2, we have for $y \in \mathbb{R}^3$ and $y \neq 0$ that

$$\int_{\mathbb{R}^3} \frac{\varphi_\lambda(x)\, dx}{|x-y|} \le \frac{1}{|y|} \int_{\mathbb{R}^3} \varphi_\lambda(x)\, dx = \frac{1}{|y|}.$$

Since $\varphi_\lambda \geq 0$, it follows that

$$\begin{aligned}
\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi_\lambda(x-x')\varphi_\lambda(y-y')}{|x-y|}\,dxdy &= \int_{\mathbb{R}^3} \varphi_\lambda(y-y')\left[\int_{\mathbb{R}^3} \frac{\varphi_\lambda(x-x')\,dx}{|x-y|}\right] dy \\
&= \int_{\mathbb{R}^3} \varphi_\lambda(y-y')\left[\int_{\mathbb{R}^3} \frac{\varphi_\lambda(x)\,dx}{|x-(y-x')|}\right] dy \\
&\leq \int_{\mathbb{R}^3} \frac{\varphi_\lambda(y-y')}{|y-x'|}dy \\
&= \int_{\mathbb{R}^3} \frac{\varphi_\lambda(y)}{|y-(x'-y')|}dy \\
&\leq \frac{1}{|x'-y'|} \qquad \text{if } x' \neq y'. \qquad (4.16)
\end{aligned}$$

Since $d\mu = \rho\,dx$ with $\rho \in L^\infty(\mathbb{R}^3)$ and $\rho = 0$ a.e. on $\overline{\Omega}^c$, $1/|x'-y'|$ is integrable on $\mathbb{R}^3\times\mathbb{R}^3$ against $d(\mu\times\mu)(x',y')$. Similar to the calculation leading to (4.8), we can write

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi_\lambda(x-x')\varphi_\lambda(y-y')}{|x-y|}\,dxdy = \int_{\mathbb{R}^3} \frac{\vartheta_\lambda(z)\,dz}{|x'-y'-z|}.$$

Since ϑ is radially symmetric, nonnegative, and of unit mass (cf. (4.11)),

$$\lim_{\lambda\to 0^+} \int_{\mathbb{R}^3} g(z)\vartheta_\lambda(z)\,dz = g(0) \qquad \forall g \in C_0(\mathbb{R}^3).$$

In particular, if $x' \neq y'$ and if $g(\cdot)$ is equal to $1/|x'-y'-\cdot|$ multiplied by a smooth cutoff function equal to 1 in a neighborhood of the origin and supported in a ball of radius less than $|x'-y'|$, we get that

$$\lim_{\lambda\to 0^+} \int_{\mathbb{R}^3} \frac{\vartheta_\lambda(z)dz}{|x'-y'-z|} = \frac{1}{|x'-y'|}.$$

Hence,

$$\lim_{\lambda\to 0^+} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi_\lambda(x-x')\varphi_\lambda(y-y')}{|x-y|}\,dxdy = \frac{1}{|x'-y'|} \qquad \text{a.e. } (x',y') \in \mathbb{R}^3\times\mathbb{R}^3.$$

This and (4.16), together with the Dominated Convergence Theorem, imply (4.15).

Step 2.4. We finally prove the limit (4.2). Given $\varepsilon > 0$. By (4.7) and (4.15), there exists $\lambda > 0$ such that

$$\begin{aligned}
&|E_{\mathrm{d}}[\mu_n] - E_{\mathrm{c}}[\mu_n * \varphi_\lambda]| \leq \frac{\varepsilon}{2} + C\left(r_n^2 + \frac{1}{N_n\lambda}\right) \qquad \forall n \geq 1, \\
&|E_{\mathrm{c}}[\mu * \varphi_\lambda] - E_{\mathrm{c}}[\mu]| < \frac{\varepsilon}{2}.
\end{aligned}$$

These, together with (4.6) and (4.13), the fact that $N_n \to \infty$ and $r_n \to 0$, imply that

$$\limsup_{n\to\infty} |E_{\mathrm{d}}[\mu_n] - E[\mu]| \le \varepsilon.$$

leading to (4.2). The proof is complete. □

We now provide an example to show the convergent subsequence stated in Theorem 4.1 is not unique. Let Ω be a bounded open set as in the theorem. We partition Ω into two parts A and B such that A and B are nonempty open subsets of $\mathbb{R}^3$, $\overline{\Omega} = \overline{A} \cup \overline{B}$, $A \cap B = \emptyset$, and $|\overline{A} \cap \overline{B}| = 0$. Let $Y_n = (2^{-n}\mathbb{Z}^3) \cap \Omega$ and define

$$X_n = \begin{cases} (Y_n \cap B) \cup (Y_{n+1} \cap A) & \text{if } n \text{ is even,} \\ (Y_n \cap A) \cup (Y_{n+1} \cap B) & \text{if } n \text{ is odd.} \end{cases}$$

Denote by N_n the number of distinct points in X_n and set

$$\mu_n = \frac{1}{N_n} \sum_{x_i \in X_n} \delta_{x_i} \qquad (n = 1, 2, \dots).$$

We observe that $X_n \subset X_{n+1}$ for each $n \ge 1$ and that the geometrical conditions are satisfied. Moreover, since X_n is uniformly distributed on each of A and B, but has $2^3 = 8$ times as many points per unit volume in one than the other, hence 8 times the density, we have

$$\mu_{2n} \overset{*}{\rightharpoonup} \mu_{\text{even}} \qquad \text{and} \qquad \mu_{2n-1} \overset{*}{\rightharpoonup} \mu_{\text{odd}},$$

where μ_{even} and μ_{odd} are two Radon measures supported on $\overline{\Omega}$ with distinct densities

$$\rho_{\text{even}} = \frac{8}{8|A| + |B|}\chi_A + \frac{1}{8|A| + |B|}\chi_B$$
$$\rho_{\text{odd}} = \frac{1}{8|B| + |A|}\chi_A + \frac{8}{8|B| + |A|}\chi_B,$$

respectively, where χ_S denotes the characteristic function of a set S. Note that $\|\mu_n\| = 1$ for all n, and $\|\mu_{\text{even}}\| = \|\mu_{\text{odd}}\| = 1$. Note also that these two densities are always different.

If we set specifically

$$\Omega = \{x \in \mathbb{R}^3 : |x| < 2\}, \quad A = \{x \in \mathbb{R}^3 : |x| < 1\}, \quad \text{and} \quad B = \{x \in \mathbb{R}^3 : 1 < |x| < 2\},$$

then the densities are

$$\rho_{\text{even}} = \frac{2}{5\pi^2}\chi_A + \frac{1}{20\pi^2}\chi_B \qquad \text{and} \qquad \rho_{\text{odd}} = \frac{1}{76\pi^2}\chi_A + \frac{2}{19\pi^2}\chi_B,$$

respectively. We now calculate the energies $E[\mu_{\text{even}}]$ and $E[\mu_{\text{odd}}]$. Note that χ_A and χ_B are radially symmetric. By approximations by smooth and radially symmetric functions, we have by Lemma 4.2 that

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\chi_A(x)\chi_A(y)\,dxdy}{|x-y|} = \int_{\mathbb{R}^3} \left[\int_{\mathbb{R}^3} \frac{\chi_A(x)\,dx}{|x-y|}\right] \chi_A(y)\,dy$$

$$
\begin{aligned}
&= \int_{\mathbb{R}^3} \left[\int_{\mathbb{R}^3} \min\left(\frac{1}{|x|}, \frac{1}{|y|}\right) \chi_A(x)\, dx \right] \chi_A(y)\, dy \\
&= \int_A \left[\int_A \min\left(\frac{1}{|x|}, \frac{1}{|y|}\right) dx \right] dy \\
&= (4\pi)^2 \int_0^1 \left[\int_0^1 \min\left(\frac{1}{s}, \frac{1}{t}\right) s^2\, ds \right] t^2\, dt \\
&= (4\pi)^2 \int_0^1 \left[\int_0^t s^2 t\, ds + \int_t^1 s t^2\, ds \right] dt \\
&= \frac{32}{15}\pi^2.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\chi_B(x)\chi_B(y)\, dxdy}{|x-y|} &= \int_B \left[\int_B \min\left(\frac{1}{|x|}, \frac{1}{|y|}\right) dx \right] dy \\
&= (4\pi)^2 \int_1^2 \left[\int_1^2 \min\left(\frac{1}{s}, \frac{1}{t}\right) s^2\, ds \right] t^2\, dt \\
&= \frac{752}{15}\pi^2,
\end{aligned}
$$

and

$$
\begin{aligned}
\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\chi_A(x)\chi_B(y)\, dxdy}{|x-y|} &= \int_B \left[\int_A \min\left(\frac{1}{|x|}, \frac{1}{|y|}\right) dx \right] dy \\
&= (4\pi)^2 \int_1^2 \left[\int_0^1 \min\left(\frac{1}{s}, \frac{1}{t}\right) s^2\, ds \right] t^2\, dt \\
&= (4\pi)^2 \int_1^2 \left(\int_0^1 s^2 t\, ds \right) dt \\
&= 8\pi^2.
\end{aligned}
$$

Therefore, since $d\mu_{\text{even}} = \rho_{\text{even}}\, dx$ and $d\mu_{\text{odd}} = \rho_{\text{odd}}\, dx$, we obtain by a series of calculations that

$$
\begin{aligned}
E[\mu_{\text{even}}] &= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{\text{even}}(x)\, \rho_{\text{even}}(y)\, dxdy}{|x-y|} \\
&= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \left[\frac{2}{5\pi^2}\chi_A(x) + \frac{1}{20\pi^2}\chi_B(x) \right] \left[\frac{2}{5\pi^2}\chi_A(y) + \frac{1}{20\pi^2}\chi_B(y) \right] \frac{dxdy}{|x-y|} \\
&= \frac{59}{75}.
\end{aligned}
$$

Similarly, $E[\mu_{\text{odd}}] = 626/1083$. Note that $E[\mu_{\text{even}}] \neq E[\mu_{\text{odd}}]$.

By Theorem 4.1, there exists a subsequence $\{\mu_n'\}$ of $\{\mu_{2n}\}$ and a subsequence $\{\mu_n''\}$ of $\{\mu_{2n-1}\}$ such that $\mu_n' \overset{*}{\rightharpoonup} \mu_{\text{even}}$ and $\mu_n'' \overset{*}{\rightharpoonup} \mu_{\text{odd}}$. Moveover, $E[\mu_n'] \to E[\mu_{\text{even}}]$ and $E[\mu_n''] \to E[\mu_{\text{odd}}]$, respectively. Note that the sequence $\{\mu_n'\}$ is different from $\{\mu_n''\}$, $\mu_{\text{even}} \neq \mu_{\text{odd}}$, and $E[\mu_{\text{even}}] \neq E[\mu_{\text{odd}}]$. Therefore, the subsequence in Theorem 4.1 is not unique,

5 Minimization of Electrostatic Eenrgy in the Presence of an External Field

Let $\Omega \subseteq \mathbb{R}^3$ be a bounded open set. Given a finite, signed Radon measure ν on $\mathbb{R}^3$ and assume it is compactly supported in $\overline{\Omega}^{\mathrm{c}} = \mathbb{R}^3 \setminus \overline{\Omega}$. We consider minimizing the energy $E[\mu + \nu]$ among all $\mu \in \mathcal{M}(\overline{\Omega})$ (cf. (3.1)). Such minimization has various applications, particularly, in an implicit-solvent model of the charged molecules occupying the region Ω in aqueous (i.e., water or salted water) environment; cf. [7, 8, 28, 33, 39, 41].

Formally,

$$E[\mu + \nu] = E[\mu] + 2E[\mu, \nu] + E[\nu].$$

Since ν is given and fixed, we consider the first two terms here. We define $U^\nu : \overline{\Omega} \to \mathbb{R}$ by

$$U^\nu(x) := \int_{\mathbb{R}^3} \frac{d\nu(y)}{|x-y|} \qquad \forall x \in \overline{\Omega}.$$

Since $\|\nu\| < \infty$ and $\operatorname{supp}(\nu) \subset \overline{\Omega}^{\mathrm{c}}$, $U^\nu(x)$ is well defined and is finite for each $x \in \overline{\Omega}$. If we denote $\delta = \operatorname{dist}(\operatorname{supp}(\nu), \overline{\Omega}) > 0$, then

$$|U^\nu(x)| \le \int_{\mathbb{R}^3} \frac{d|\nu|(y)}{|x-y|} \le \int_{\operatorname{supp}(\nu)} \frac{d|\nu|(y)}{\delta} = \frac{\|\nu\|}{\delta} \qquad \forall x \in \overline{\Omega}. \tag{5.1}$$

Moreover, for any $x, z \in \overline{\Omega}$,

$$\begin{aligned} |U^\nu(x) - U^\nu(z)| &= \left| \int_{\mathbb{R}^3} \frac{d\nu(y)}{|x-y|} - \int_{\mathbb{R}^3} \frac{d\nu(y)}{|z-y|} \right| \\ &\le \int_{\operatorname{supp}(\nu)} \frac{|x-z| d|\nu|(y)}{|x-y||z-y|} \\ &\le \frac{\|\nu\|}{\delta^2} |x-z|. \end{aligned} \tag{5.2}$$

Hence, U^ν is Lipschitz continuous on $\overline{\Omega}$. Therefore, if $\mu \in \mathcal{M}(\overline{\Omega})$, then $E[\mu, \nu]$ is well defined and is finite. In fact, it follows from the Fubini–Tonelli theorem and (5.1) that

$$|E[\mu, \nu]| = \left| \int_{\mathbb{R}^3} U^\nu(x) d\mu(x) \right| \le \int_{\mathbb{R}^3} |U^\nu(x)| \, d|\mu|(x) \le \frac{\|\mu\| \, \|\nu\|}{\delta}. \tag{5.3}$$

We define $J : \mathcal{M}(\overline{\Omega}) \to \mathbb{R} \cup \{+\infty\}$ by

$$J[\mu] = \begin{cases} E[\mu] + 2E[\mu, \nu] & \text{if } E[|\mu|] < \infty \\ \infty & \text{otherwise} \end{cases} \qquad \forall \mu \in \mathcal{M}(\overline{\Omega}).$$

Similarly, we define $J_{\mathrm{d}} : \mathcal{A}(\overline{\Omega}) \to \mathbb{R} \cup \{+\infty\}$ by

$$J_{\mathrm{d}}[\mu] = E_{\mathrm{d}}[\mu] + 2E[\mu, \nu] \qquad \forall \mu \in \mathcal{A}(\overline{\Omega}).$$

where $E_{\mathrm{d}}[\mu]$ for $\mu \in \mathcal{A}(\overline{\Omega})$ is defined in (3.5).

Theorem 5.1. *Let Ω be a nonempty, bounded, open subset of $\mathbb{R}^3$ with a C^2 boundary $\partial\Omega$. Let ν be a compactly supported signed Radon measure on $\mathbb{R}^3$ with* $\operatorname{supp}(\nu) \subset \overline{\Omega}^{\mathrm{c}}$.

(1) *There exists a unique $\underline{\mu} \in \mathcal{M}(\overline{\Omega})$ such that*

$$J[\underline{\mu}] = \inf_{\mu \in \mathcal{M}(\overline{\Omega})} J[\mu].$$

Moreover, $\operatorname{supp}(\underline{\mu}) \subseteq \partial\Omega$.

(2) *For any $\varepsilon > 0$ there exist $\mu_n \in \mathcal{A}(\overline{\Omega})$ $(n = 1, 2, \dots)$ such that*

$$\operatorname{supp}(\mu_n) \subseteq \{x \in \overline{\Omega} : \operatorname{dist}(x, \partial\Omega) < \varepsilon\} \qquad (n = 1, 2, \dots),$$

and

$$\mu_n \overset{*}{\rightharpoonup} \underline{\mu} \qquad \text{and} \qquad J_{\mathrm{d}}[\mu_n] \to J[\underline{\mu}] \qquad \text{as } n \to \infty.$$

Proof. Let $G = \mathbb{R}^3 \setminus \overline{\Omega} = \overline{\Omega}^{\mathrm{c}}$. Since $\partial G = \partial\Omega$ is C^2, it satisfies the exterior cone condition: every point $x \in \partial G$ is accessible from outside of G by a finite cone that does not otherwise intersect $\overline{G}$. Therefore, there exists a unique Radon measure ν' on $\mathbb{R}^3$ with $\operatorname{supp}(\nu') \subseteq \partial\Omega$ and $\|\nu'\| \le \|\nu\|$ such that $U^\nu = U^{\nu'}$ on $\overline{\Omega}$; cf. Chapter 4 of [26]. Note that $\nu' \in \mathcal{M}(\overline{\Omega})$.

Both $E[\nu']$ and $E[\mu, \nu']$ with $\mu \in \mathcal{M}(\overline{\Omega})$ are well defined and finite. In fact, similar to (5.3), we have for $\delta = \operatorname{dist}(\operatorname{supp}(\nu), \partial\Omega) > 0$ that

$$\begin{aligned} E[\nu'] &= \int_{\mathbb{R}^3} U^{\nu'}\, d\nu' = \int_{\partial\Omega} U^\nu(x)\, d\nu'(x) = \int_{\partial\Omega} \int_{\mathbb{R}^3 \setminus \overline{\Omega}} \frac{d\nu'(x)\, d\nu(y)}{|x-y|} \\ &\le \frac{\|\nu'\|\, \|\nu\|}{\delta} \le \frac{\|\nu\|^2}{\delta} < \infty. \end{aligned} \tag{5.4}$$

Moreover, since $\operatorname{supp}(\mu) \subseteq \overline{\Omega}$, we have

$$E[\mu, \nu'] = \int_{\overline{\Omega}} U^{\nu'}\, d\mu = \int_{\overline{\Omega}} U^\nu\, d\mu = E[\mu, \nu],$$

which is finite by (5.3). Thus, for $\mu \in \mathcal{M}(\overline{\Omega})$ with $E[|\mu|] < \infty$,

$$J[\mu] = E[\mu] + 2E[\mu, \nu] = E[\mu] + 2E[\mu, \nu'] + E[\nu'] - E[\nu'] = E[\mu + \nu'] - E[\nu'].$$

Since $\mu + \nu'$ is compactly supported, we have (cf. Theorem 3.10 of [29])

$$J[\mu] = E[\mu + \nu'] = (2\pi)^{-3} \int_{\mathbb{R}^3} \frac{4\pi}{|\xi|^2} \left| \widehat{\mu}(\xi) + \widehat{\nu'}(\xi) \right|^2 d\xi \ge 0,$$

where $\widehat{\alpha}$ is the Fourier transform of a signed Radon measure α. The integral vanishes if and only if $\widehat{\mu} + \widehat{\nu'} = 0$ identically on $\mathbb{R}^3$, which is true if and only if $\mu + \nu' = 0$ (the zero measure) by the uniqueness of the Fourier transform of compactly supported finite measures [29]. Therefore, the functional J is uniquely minimized at $\underline{\mu} = -\nu' \in \mathcal{M}(\overline{\Omega})$, establishing (1). Note the minimum value is then given by $J[-\nu'] = -E[\nu']$.

To prove (2), we note that $E[|\nu'|] < \infty$, which is similar to (5.4). Since $\operatorname{supp}(\underline{\mu}) = \operatorname{supp}(\nu') \subseteq \partial\Omega$, we obtain by Theorem 3.1 a sequence of discrete charge distributions $\mu_n \in \mathcal{A}(\overline{\Omega})$ such that

$$\operatorname{supp}(\mu_n) \subseteq \{x \in \overline{\Omega} : \operatorname{dist}(x, \partial\Omega) < \varepsilon\} \qquad (n = 1, 2, \dots),$$

and

$$\mu_n \overset{*}{\rightharpoonup} \underline{\mu} = -\nu' \qquad \text{and} \qquad E_{\mathrm{d}}[\mu_n] \to E[\underline{\mu}] = E[-\nu'] \qquad \text{as } n \to \infty.$$

Since U^ν is continuous on $\overline{\Omega}$ (cf. (5.2)), all μ_n $(n = 1, 2, \dots)$ and ν' are supported on $\overline{\Omega}$, and $U^\nu = U^{\nu'}$ on $\overline{\Omega}$, we find that

$$\lim_{n\to\infty} E[\mu_n, \nu] = \lim_{n\to\infty} \int_{\overline{\Omega}} U^\nu \, d\mu_n = -\int_{\overline{\Omega}} U^\nu \, d\nu' = -\int_{\overline{\Omega}} U^{\nu'} \, d\nu' = -E[\nu'].$$

Therefore,

$$\begin{aligned}\lim_{n\to\infty} J_{\mathrm{d}}[\mu_n] &= \lim_{n\to\infty} \Big(E_{\mathrm{d}}[\mu_n] + 2E[\mu_n, \nu]\Big) = E[-\nu'] - 2E[\nu'] \\ &= E[\nu'] - 2E[\nu'] = -E[\nu'] = J[-\nu'] = J[\underline{\mu}] = \inf_{\mu \in \mathcal{M}(\overline{\Omega})} J[\mu].\end{aligned}$$

The proof is complete. □

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