AN EXTERNAL DUAL CHARGE APPROACH TO THE
OPTIMAL TRANSPORT WITH COULOMB COST

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Abstract. In this paper, we study the multimarginal optimal
transport with Coulomb cost, also known in the physics literature
as the Strictly-Correlated Electrons (SCE) functional. We prove
that the dual Kantorovich potential is an electrostatic potential in-
duced by an external charge density, which we call the dual charge.
We study its properties and use it to discretize the potential in one
and three space dimensions.

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1. Introduction

In the recent years, Multimarginal Optimal Transport (MOT) has be-
gun to attract considerable attention, due to a wide variety of emerg-
ing applications outside of mathematics, such as economics, finance,
physics and image processing (see [31] for a rather detailed review and
citations therein). As such, it has become of valuable importance to
develop numerical methods to solve this problem, which is plagued with
the infamous curse of dimensionality.

In physics, MOT appears in a variety of applications, e.g. in defining
the Uniform Electron Gas (UEG; see [24]), which in turn serves as a
building block for the very important Local Density Approximation in
Density Functional Theory (DFT; see [25]), a successful computational
modeling method in quantum physics. Another example of MOT in
physics, and closely related to DFT, is the paradigm of classical DFT
(see e.g. [42]), which exactly reformulates as a MOT problem together with entropic regularization.

From a numerical viewpoint, MOT is notoriously hard to solve. Most algorithms require exponential time in the number of marginals and in the discretization size of their supports. While for some specific costs, it is possible to fashion polynomial time methods, in the case of the Coulomb cost the problem is known to be \( \mathcal{NP} \)-hard [3, 2]. Current methods then consist in either adding an entropic regularization [4], which physically translates into adding positive temperature to the system, and which makes the numerics more tractable by heavily exploiting parallel computing; or using ideas from Linear Programming (e.g. leveraging on the sparsity of optimal plans [17]). One can also mention the approach proposed in [1], namely the Moment Constrained Optimal Transport (MCOT), which relies on a neat relaxation of the primal constraints (and somehow closely related to our own approach).

From a physical viewpoint, the Kantorovich dual of the MOT is a very meaningful and interesting object in its own right. In fact, as readily noticed in the literature, the so-called (not necessarily unique) Kantorovich potential can be interpreted as an external potential which forces the particles to live, at equilibrium and zero temperature, on the support of an optimal plan. Moreover, at positive temperature, the dual relates to physics still, and the (unique up to an additive constant) Kantorovich potential is interpreted, from a statistical physics viewpoint, as the external potential which forces the associated canonical ensemble to have the target density of the MOT as its one-particle density.

In this paper, we suggest to parametrize the Kantorovich potential (both at zero and positive temperature) as an electrostatic potential generated by an external charge distribution, which we call the dual charge. While such an approach had already been proposed at zero temperature in [28], here we mainly focus on its the theoretical aspects. Moreover, from a numerical viewpoint, this dual charge seems a rather amenable candidate for discretization, as it allows for a natural “smoothing” from the discretization space to the space of potentials.

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2. Theoretical properties on the dual charge

2.1. Transport at zero temperature. In what follows, we fix an absolutely continuous density \( \rho \in L^1(\mathbb{R}^d, \mathbb{R}^+) \) with \( \int_{\mathbb{R}^d} \rho = N \in \mathbb{N} \) where \( N \geq 2 \) and \( d \geq 3 \), representing the expected charge density of a system of \( N \) indistinguishable electrons interacting through the Coulomb potential. Among all symmetric \( N \)-particle probability measures \( \mathbb{P} \) such that \( \rho \mathbb{P} = \rho \), where

\[
\rho_{\mathbb{P}}(r) = N \int_{\mathbb{R}^{d(N-1)}} \mathbb{P}(r, \text{d}r_2, \ldots, \text{d}r_N),
\]

we want to determine the one(s) yielding the lowest possible electrostatic energy, that is, we seek to solve the following minimization problem

\[
F_{\text{SCE}}(\rho) = \inf_{\rho_{\mathbb{P}} = \rho} \left\{ \int_{\mathbb{R}^{dN}} \sum_{1 \leq i < j \leq N} \frac{1}{|r_i - r_j|^{d-2}} \mathbb{P}(\text{d}r_1, \ldots, \text{d}r_N) \right\}. \tag{SCE}
\]

The (Problem SCE) is known in the physics literature as the Strictly-Correlated Electrons (SCE) \([37, 38]\). The functional \( \rho \mapsto F_{\text{SCE}}(\rho) \) arises in DFT as the semiclassical limit of the celebrated Levy-Lieb functional \([22, 26, 23]\), and is used in the context of strongly-correlated systems. In particular, the SCE approach is to be thought as the exact counterpart to the Kohn-Sham (KS) approach \([19]\), where one seeks to map a many-body system of interacting electrons into another (fictitious) system of non-interacting electrons with the same electronic density, whereas in the SCE approach, the fictitious system is purported to have infinite electronic correlation and zero kinetic energy. We refer the reader to the recent survey \([16]\) for further details regarding (Problem SCE).

As by now well-established \([6, 12]\), the SCE problem reformulates as a MOT problem with all marginals constrained to \( \rho/N \) and cost of transportation given by the Coulomb cost

\[
c(r_1, \ldots, r_N) = \sum_{1 \leq i < j \leq N} \frac{1}{|r_i - r_j|^{d-2}}.
\]

In particular, (Problem SCE) is equivalent to the following maximization problem \([5]\), the so-called Kantorovich dual, which reads

\[
F_{\text{SCE}}(\rho) = \sup_{\int_{\mathbb{R}^d} |v| \rho < +\infty} \left\{ E_N(v) + \int_{\mathbb{R}^d} v(r) \rho(r) \text{d}r \right\}, \tag{SCE_D}
\]
where the infimum runs over all continuous functions \( v \) and where 
\[
E_N(v) = \inf_{r_1, \ldots, r_N} \left\{ c(r_1, \ldots, r_N) - \sum_{i=1}^{N} v(r_i) \right\}.
\]

**Remark 1.** From a numerical viewpoint \( E_N(v) \) is intractable. Instead, one can consider the following problem, which is equivalent to (Problem \( \text{SCE}_D \)):

\[
F_{\text{SCE}}(\rho) = \sup_{\text{s.t. } \int_{\Omega} |v| < +\infty} \left\{ E_{N,\Omega}(v) + \int_{\mathbb{R}^d} v(r) \rho(r) dr \right\}, \quad \text{(SCE}_{D,\Omega})
\]

where \( E_{N,\Omega}(v) \) is defined for any continuous \( v \) similarly to \( E_N(v) \) only with the particles constrained to the support \( \Omega \) of \( \rho \), that is

\[
E_{N,\Omega}(v) = \inf_{r_1, \ldots, r_N \in \Omega} \left\{ c(r_1, \ldots, r_N) - \sum_{i=1}^{N} v(r_i) \right\}.
\]

A maximizer \( v \) of (Problem \( \text{SCE}_{D,\Omega} \)) is called a Kantorovich potential. Notice that (minus) \( v \) can be regarded as a physical potential, and that \( E_N(v) \) is to be understood as the classical counterpart to the ground-state energy in quantum physics. In fact, in the physics literature, \( v \) is coined as the SCE potential, which is to be thought as the effective one-body potential which emulates the SCE system, and which captures the effects of the strongly-correlated regime.

Since (Problem \( \text{SCE}_{D,\Omega} \)) entirely pertains to electrostatics, one might conjecture that \( v \) shall also relate to electrostatics. More precisely, we ask ourselves whether or not there exists a Kantorovich potential \( v \) which is a Coulomb potential, that is, such that there exists a measure \( \rho_{\text{ext}} \in \mathcal{M}(\mathbb{R}^d) \), which we coined as the dual charge, so that \( v(r) = \rho_{\text{ext}} * |r|^{2-d} \), where \( * \) denotes the usual convolution operator. We would expect that \( \rho_{\text{ext}} \) verifies \( \rho_{\text{ext}} \geq 0 \) and \( \text{supp}(\rho_{\text{ext}}) \subset \text{supp}(\rho) \), in order to attract the electrons into an optimal transport plan, which, in the absence of an external potential landscape, would escape to infinity, and that \( \int_{\mathbb{R}^d} \rho_{\text{ext}} = N - 1 \), since each fixed electron “sees” the \( N - 1 \) other electrons, so as to counterbalance the repulsive force created by those electrons.

The following theorem confirms our intuition:

**Theorem 1** (Existence of a dual charge at zero temperature). Given \( \rho \in L^1(\mathbb{R}^d, \mathbb{R}^+) \) with \( \int_{\mathbb{R}^d} \rho = N \geq 2 \), there exists a maximizer \( v \) of (Problem \( \text{SCE}_{D,\Omega} \)) which is an attractive Coulomb potential, that is of...
Figure 1. Example for Theorem 1: the (radial components of a) Kantorovich potential \( \rho_{\text{ext}} \ast |r|^{-1} \) and its associated dual charge \( \rho_{\text{ext}} \) for a two-electron system \( (N = 2) \) with density \( \rho = 2|B_1|^{-1}1_{B_1} \) where \( B_1 \) is the unit ball of \( \mathbb{R}^3 \).

the form \( v(r) = \rho_{\text{ext}} \ast |r|^{2-d} \) for some positive measure \( \rho_{\text{ext}} \) of mass \( \int_{\mathbb{R}^d} \rho_{\text{ext}} \leq N - 1 \). Moreover, if the support \( \Omega \) of \( \rho \) is bounded, one can suppose that \( \text{supp}(\rho_{\text{ext}}) \subset \Omega \) and that \( \int_{\Omega} \rho_{\text{ext}} = N - 1 \).

Remark 2 (Non-uniqueness of dual charges). Let \( \rho_{\text{ext}} \) be a dual charge as in Theorem 1, i.e. \( v(r) = \rho_{\text{ext}} \ast |r|^{2-d} \) is a Kantorovich potential for (Problem SCE). If the support \( \Omega \) of \( \rho \) is bounded, i.e. \( \Omega \subset B_R \) for some \( R > 0 \), then \( \rho_{\text{ext}} = \rho_{\text{ext}} + \sigma_R \) is still an admissible dual charge, where \( \sigma_R \) is the surface measure on \( \partial B_R \). Indeed, \( \sigma_R \) generates a constant potential \( c_R = R^{2-d} \) inside of \( B_R \) and \( \sigma_R \ast |r|^{2-d} \leq c_R \) outside of \( B_R \), so that \( w(r) = \rho_{\text{ext}} \ast |r|^{2-d} \) is still a Kantorovich potential, since

\[
\int_{\mathbb{R}^d} v \rho + E_N(v) = \int_{\mathbb{R}^d} w \rho + \underbrace{E_N(v + c_R)}_{\leq E_N(w)}.
\]

(2)

This shows that dual charges need not be unique. Moreover, by considering \( \rho_{\text{ext}} + c\sigma_R \) with \( c > 0 \), the mass of \( \rho_{\text{ext}} \) can be made arbitrarily large. In fact, even restricting our attention to the dual charges supported on \( \Omega \), the mass \( \int_{\Omega} \rho_{\text{ext}} \) can also be made arbitrarily large, by considering \( \rho_{\text{ext}} + c\chi_{\text{eq}} \) where \( \chi_{\text{eq}} \in M_+(\Omega) \) is the equilibrium measure of \( \Omega \) (see \[20, Chap II.\]). We note that generically (i.e. for « nice » \( \Omega \)), \( \chi_{\text{eq}} \) is supported on \( \partial \Omega \).

\textsuperscript{1}\textsuperscript{1}We will always suppose that measures are \textit{locally finite}. 
Remark 3. In the recent survey [16], it is mentioned as a conjecture [16, Eq. (66)] that, when \( \rho \) is supported over the entire space \( \mathbb{R}^d \), the SCE potential \( v \) shall verify the asymptotic

\[
v(r) \sim \frac{N - 1}{|r|^{d-2}} \quad \text{as } r \to \infty.
\] (3)

We remark that Theorem 1 implies that \( v \) is lower than the asymptotic at (3) — with equality in the case of a compactly supported density \( \rho \), even though in this case the problem is not well-posed since \( v \) can be freely modified outside of the support of \( \rho \).

Though the dual charge need not be unique over the entire space, we obtain uniqueness (among the class of measures which generate Lipschitz Coulomb potentials) over the support of \( \rho \).

Theorem 2 (Uniqueness of the dual charge). Let \( \rho \in L^1(\mathbb{R}^d, \mathbb{R}_+) \) with \( \int_{\mathbb{R}^d} \rho = N \geq 2 \). If \( \rho_{\text{ext}}, \mu_{\text{ext}} \in \mathcal{M}(\mathbb{R}^d) \) are two dual charges for (Problem SCE) such that \( \rho_{\text{ext}} \ast |r|^{2-d} \) and \( \mu_{\text{ext}} \ast |r|^{2-d} \) are Lipschitz, then \( \rho_{\text{ext}} = \mu_{\text{ext}} \) over the (topological) interior of \( \Omega \), where \( \Omega \) is the support of \( \rho \), provided that \( \Omega \) is connected.

The proof of Theorem 2 is consigned in Section 4.3.

2.2. Transport at positive temperature. At positive temperature \( \beta^{-1} > 0 \), i.e. adding an entropic term to (Problem SCE), we are led to the following variational problem

\[
F_{\text{SCE},\beta}(\rho) = \inf_{\rho_{\mathbb{P}} = \rho} \left\{ \int_{\mathbb{R}^{dN}} c(r_1, \ldots, r_N) d\mathbb{P} + \beta^{-1} \text{Ent}(\mathbb{P} \mid \mu^{\otimes N}) \right\}, \quad (\text{SCE}_\beta)
\]

where \( \mu = \rho/N \) and where \( \text{Ent}(\mathbb{P} \mid \mu^{\otimes N}) \geq 0 \) denotes the relative entropy of \( \mathbb{P} \) with respect to the product measure \( \mu^{\otimes N} \), defined for all probability measures \( \mathbb{P} \) which are absolutely continuous with respect to \( \mu^{\otimes N} \) with Radon-Nykodim density \( d\mathbb{P} / d\mu^{\otimes N} \) as

\[
\text{Ent}(\mathbb{P} \mid \mu^{\otimes N}) = \int_{\mathbb{R}^{dN}} \frac{d\mathbb{P}}{d\mu^{\otimes N}}(r_1, \ldots, r_N) \log \left( \frac{d\mathbb{P}}{d\mu^{\otimes N}}(r_1, \ldots, r_N) \right) d\mu^{\otimes N}.
\]

While (Problem SCE_\beta) is an instance of entropy-regularized OT [21, 18], which has received growing interest in the past few years, it originally pertains to the statistical mechanics of non-uniform liquids, which shares substantial connections with the DFT of classical systems [41, 40, 15]. Indeed, the functional \( \rho \mapsto F_{\text{SCE},\beta}(\rho) \) is the Legendre transform of the (canonical) Helmholtz free energy \( F_\beta(v) \) with external (minus)
potential $v$,

$$F_{\text{SCE}, \beta}(\rho) = \sup_v \left\{ \mathcal{F}_\beta(v) + \int_{\mathbb{R}^d} v(\mathbf{r}) \rho(\mathbf{r}) d\mathbf{r} \right\}. \quad (\text{SCE}_{D, \beta})$$

The existence of a maximizer $v_\beta$ for (Problem $\text{SCE}_{D, \beta}$), which is to be thought as the effective one-body potential which forces the system into the constraint density $\rho$, was proved under relatively weak hypotheses through variational techniques in [9, Thm 2.2]. Note that $v_\beta$ is unique up to an additive constant by strict concavity, and that to respect the density constraint it must be that $v_\beta$ is infinite outside of the support of $\rho$.

In what follows, we will make use of the two following assumptions, namely

$$D(\rho) := \iint_{\mathbb{R}^d \times \mathbb{R}^d} \frac{\rho(d\mathbf{r}) \rho(d\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^{d-2}} < \infty, \quad (A1)$$

and

$$\|\rho * |\mathbf{r}|^{2-d}\|_{L^\infty} < \infty. \quad (A2)$$

Remark 4. Appealing to Hardy-Littlewood Sobolev inequality [27, Thm. 4.3], the assumption $[A1]$ is verified as soon as there exists $\varepsilon > 0$ such that $\rho \in L^{\frac{2d}{d+2-\varepsilon}}(\mathbb{R}^d) \cap L^{\frac{2d}{d+2+\varepsilon}}(\mathbb{R}^d)$. Furthermore, it follows from Hölder’s inequality that if there exists $\varepsilon > 0$ such that $\rho \in L^{\frac{2}{d-\varepsilon}}(\mathbb{R}^d) \cap L^{\frac{2}{d+\varepsilon}}(\mathbb{R}^d)$, then the assumption $[A2]$ is verified.

The counterpart of Theorem 1 at positive temperature reads:

**Theorem 3** (Existence of a dual charge at positive temperature). Let $\rho \in L^1(\mathbb{R}^d, \mathbb{R}_+)$ with $\int_{\mathbb{R}^d} \rho = N \geq 2$ which verifies the assumptions $[A1]$ and $[A2]$. Then, the unique (up to an additive constant) maximizer $v_\beta$ of (Problem $\text{SCE}_{D, \beta}$) is an attractive Coulomb potential, i.e. there exists a positive measure $\rho_{\text{ext}, \beta}$ such that $v_\beta(\mathbf{r}) = \rho_{\text{ext}, \beta} * |\mathbf{r}|^{2-d}$ (up to an additive constant) on the support $\Omega$ of $\rho$. Moreover, if $\Omega$ is bounded, one can suppose that $\text{supp}(\rho_{\text{ext}, \beta}) \subset \Omega$.

The proof of Theorem 3 is consigned in Section 4.5.

As one lowers the temperature, it is known [8] that one recovers the zero-temperature problem, i.e. (Problem $\text{SCE}$). In the same spirit, we prove that the dual charge at positive temperature converges to a dual charge at zero temperature in the small temperature limit.

**Theorem 4** (Zero-temperature limit of the dual charge). Let $\rho \in L^1(\mathbb{R}^d, \mathbb{R}_+)$ with $\int_{\mathbb{R}^d} \rho = N \geq 2$ which verifies the assumptions $[A1]$ and $[A2]$, and suppose that the support $\Omega$ of $\rho$ is bounded. Let $\rho_{\text{ext}, \beta}$
with \( \text{supp}(\rho_{\text{ext},\beta}) \subset \Omega \) be as in Theorem 3, i.e. \( v_{\beta}(r) = \rho_{\text{ext},\beta} \ast |r|^{2-d} \) is the unique (up to an additive constant) maximizer of \((\text{Problem SCE}_{\beta})\). Then, the sequence \((\rho_{\text{ext},\beta})_{\beta > 0}\) has at least one accumulation point for the vague topology on \( M(\Omega) \), and any of its accumulation point is an external dual charge for \((\text{Problem SCE}_{\beta})\).

The proof of Theorem 4 is consigned in Section 4.6.

Theorem 4 follows from a more general result, namely the convergence at the level of the Kantorovich potentials, as consigned in Theorem 5 hereafter. While it came to our attention that in [30] it is proved a similar (and decidedly more general) result, our convergence is stronger, though \( a \text{ priori} \) specific to the Coulomb cost.

**Theorem 5** (Zero-temperature limit of the Kantorovich potential). Let \( \rho \in L^{1}(\mathbb{R}^{d}, \mathbb{R}^{+}) \) with \( \int_{\mathbb{R}^{d}} \rho = N \geq 2 \) which verifies the assumptions \((A1)\) and \((A2)\), and suppose that the support \( \Omega \) of \( \rho \) is bounded. Let \( v_{\beta} \) be the unique maximizer of \((\text{Problem SCE}_{\beta})\) which, up to an additive constant, we can suppose to verify \( \mathcal{F}_{\beta}(v_{\beta}) = 0 \). Then, the sequence \((v_{\beta})_{\beta > 0}\) is bounded in \( W^{1,\infty}(\mathbb{R}^{d}) \) uniformly in \( \beta \) in the limit \( \beta \to \infty \), and therefore admits at least one accumulation point \( v \), which is necessarily a Kantorovich potential for \((\text{Problem SCE}_{\beta})\). In particular

\[
v_{\beta} \xrightarrow{\beta \to \infty} v \quad \text{uniformly on every compact set.} \tag{4}
\]

The proof of Theorem 5 is consigned in Section 4.6.

### 3. Numerical investigations

In [28], where it is introduced an analogous of our dual charge, the authors solve \((\text{Problem SCE}_{\beta})\) by discretizing the dual charge as a combination of few Gaussian functions and performing a nested unconstrained optimization. The functional derivative of \( v \mapsto E_{N}(v) \) being intractable, they appealed to derivative-free methods for the outer optimization, while computing \( E_{N}(v) \) through standard quasi-Newton methods. Nevertheless, as noticed by the authors, « the derivative-free methods are not suitable for optimizing with respect to a large number of degrees of freedom. More efficient numerical methods need to be developed in order to obtain the Kantorovich dual solution for more general systems ».

We propose to approximate the solution of \((\text{Problem SCE}_{\beta})\) by considering the problem at positive temperature, which is more amenable for a computational viewpoint. Similarly to [28], we discretize the dual charge as a combination of basis functions. As the temperature is lowered, we shall recover the zero-temperature dual charge. Note that the
idea of approaching numerically the optimal transport by its entropy-
regularized version has gained a lot of popularity in the recent years
[32, 13]. In the context of (Problem \( \text{SCE} \)), this approach has already
been used in [4, 29].

3.1. Discretization of the dual charge. We give ourselves a finite
set of \( M \) basis functions \( B = \{ \rho_i \}_{i=1,...,M} \) where \( \rho_i \in L^1(\mathbb{R}^d, \mathbb{R}^+ ) \) for all
\( i = 1, \ldots, M \), and we seek to approximate the external dual charge of
(Problem \( \text{SCE}_{D,\beta} \)) as a linear combination of the \( \rho_i \)'s, that is by
\( \rho_{\text{ext}}[\nu] \) for some set of weights \( \nu = (\nu_i)_{i=1,...,M} \), where

\[
\rho_{\text{ext}}[\nu] := \sum_{i=1}^{M} \nu_i \rho_i, \quad \nu \in \mathbb{R}^M.
\] (5)

Otherwise stated, we approximate the Kantorovich potential \( v_\beta \) of
(Problem \( \text{SCE}_{D,\beta} \)) by \( v[\nu] \), where \( v[\nu](r) = \rho_{\text{ext}}[\nu] \ast |r|^{2-d} \). We are then
lead to the following optimization problem

\[
G_{\text{SCE,}\beta}(\rho; B) = \sup_{\nu \in \mathbb{R}^M} \left\{ \mathcal{F}_\beta(v[\nu]) + \int_{\mathbb{R}^d} v[\nu](r)\rho(r)dr \right\}. \quad (D_B)
\]

Remark 5. If we define the set of functions \( B' = \{ \rho_i \ast |r|^{2-d} \}_{i=1,...,M} \),
one can show that the following duality for (Problem \( \text{D_B} \)) holds

\[
G_{\text{SCE,}\beta}(\rho; B) = \inf_{\mathbb{P} \in \Pi(\rho; B')} \left\{ \int_{\mathbb{R}^{dN}} c(r_1, \ldots, r_N)d\mathbb{P} + \beta^{-1} \text{Ent}(\mathbb{P}|\mu^{\otimes N}) \right\},
\]

where as previously \( \mu = \rho/N \) and where \( \Pi(\rho; B') \) is defined as the set
of \( N \)-particle probability measures \( \mathbb{P} \) verifying the following moment
constraints for all \( \phi \in B' \)

\[
\int_{\mathbb{R}^{dN}} \sum_{i=1}^{N} \phi(r_i)d\mathbb{P}(r_1, \ldots, r_N) = \int_{\mathbb{R}^d} \phi(r)\rho(r)dr.
\] (6)

Therefore (Problem \( \text{D_B} \)) can be regarded as the dual approach to the
Moment Constrained Optimal Transport (MCOT) as introduced in [1].

Remark 6. According to Theorem [3] the dual charge is a positive
measure. Moreover, in the small temperature limit the dual charge can be
assumed to have total mass no greater than \( N - 1 \) according to Theorem [1]. Therefore, it seems natural to consider the following constrained
version of (Problem \( \text{D_B} \))

\[
\sup_{\nu \in \Delta_B} \left\{ \mathcal{F}_\beta(v[\nu]) + \int_{\mathbb{R}^d} v[\nu](r)\rho(r)dr \right\}
\]
where $\Delta_B$ is the convex set defined as

$$
\Delta_B = \left\{ \nu \in \mathbb{R}_+^M : \sum_{i=1}^{M} \nu_i \int_{\mathbb{R}^d} \rho_i \leq N - 1 \right\}.
$$

Nevertheless, the optimum $\nu^*$ of (Problem $D_B$) need not be in $\Delta_B$. In fact, one should dismiss this additional constraint when dealing with rather crude discretizations, as it might yield far-from-optimal results.

Denoting by $G[\nu]$ the objective of (Problem $D_B$), we note that $\nu \mapsto G[\nu]$ is strictly concave. We can solve (Problem $D_B$) using a classical steepest ascent maximization algorithms. A straightforward computation shows that, for all $i = 1, \ldots, M$, we have

$$
\partial_{\nu_i} G[\nu] = D(\rho_i, \rho - \rho[\nu])
$$

where $\rho[\nu]$ denotes the one-particle density of the configurational canonical ensemble with external potential (minus) $v[\nu]$, and where for any two measures $\mu, \nu \in \mathcal{M}(\mathbb{R}^d)$ we define

$$
D(\mu, \nu) = \int_{\mathbb{R}^d} \frac{\mu(dr)\nu(dr')}{|r - r'|^{d-2}}.
$$

From a numerical perspective, the quantity $D(\rho_i, \rho)$ can easily be computed for all $i = 1, \ldots, M$. In fact, all the computational burden is hidden in the computation of $\rho[\nu]$. Nevertheless, we notice that

$$
D(\rho_i, \rho[\nu]) = \left\langle \sum_{j=1}^{N} \rho_i \ast |r_j|^{2-d} \right\rangle_{\beta, \nu}
$$

where $\langle \cdot \rangle_{\beta, \nu}$ denotes the expectation value with respect to the canonical ensemble. Therefore, we can appeal to Monte-Carlo (MC) methods. At high temperature (and in the compactly-supported case), one can resort to vanilla MC with uniform proposals over the support of $\rho$. At low temperature, as the ensemble crystallizes onto a minimizer of (Problem $SCE$), one needs to resort to fancier sampling methods since minimizers are believed to be generically singular. For the canonical ensemble is the unique invariant ergodic measure of the (overdamped) Langevin diffusion, we can for example produce approximate samples of the ensemble through a myriad of algorithms [35, 7].

3.2. Numerical investigations.
3.2.1. One-dimensional system. We start, as a sanity check, with a one-dimensional system, i.e., $d = 1$. This problem is amenable for numerical investigations, as it is entirely solvable for all $N \geq 2$, as stated in Theorem 6 below. Recall that, in one-dimension, the Coulomb potential is given by $-|r-r'|$. We have not considered this specific case (nor the two-dimensional case where the Coulomb potential is given by $-\ln|r-r'|$) in our main theorems to avoid potential problems due to the divergence of both potentials at infinity. Nevertheless, we expect similar results to hold (see Remark 9 below).

**Theorem 6** ([10], Thm. 1.1). Let $\rho \in L^1(\mathbb{R}, \mathbb{R}_+)$ with $\int_\mathbb{R} \rho = N \geq 2$, and suppose that $\int_{\mathbb{R}} |r| \rho < \infty$. Then, there exists an explicit measurable map $t : \mathbb{R} \to \mathbb{R}$ such that, denoting $t^{(j)}$ the $j$-th fold composition of $t$ with itself, the probability measure

$$
\mathbb{P}_t(r_1, \ldots, r_N) = \frac{\rho(r_1)}{N} \otimes \delta(r_2 - t(r_1)) \otimes \cdots \otimes \delta(r_N - t^{(N-1)}(r_1)) \tag{9}
$$

is a minimizer for the (Problem SCE) in dimension $d = 1$, that is

$$
\inf_{\rho' = \rho} \left\{ -\int_{\mathbb{R}^N} \sum_{1 \leq i < j \leq N} |r_i - r_j| d\mathbb{P}(r_1, \ldots, r_N) \right\}.
$$

Moreover, given $\ell_1 < \cdots < \ell_{N-1}$ such that $\int_{\ell_i}^{\ell_{i+1}} \rho = 1$ for all $i = 0, \ldots, N$, with $\ell_0 = -\infty$ and $\ell_N = +\infty$, the function $v$ defined as

$$
v(r) = -\left( \sum_{i=1}^{N-1} \delta_{\ell_i} \right) * |r|
$$

is a Kantorovich potential for the (Problem SCE) in $d = 1$. In particular, the comb $\sum_{i=1}^{N-1} \delta_{\ell_i}$ is, according to our terminology, a dual charge, which only depends on $\rho$ through the $\ell_i$’s.

**Remark 7.** The result in [10] Thm. 1.1 does not per se apply to the one-dimensional Coulomb potential as claimed above, for it is not strictly convex. Nevertheless, it is straightforward to prove that $t$ remains an optimal transport plan which in this case need not be unique. In fact, there might exist optimal plans which are not of the form (9) and which carry entropy. For instance, for any $N \geq 2$ and $\rho = 1_{[-N/2,N/2]}$, the following probability measure

$$
\mathbb{P}_N = \frac{1}{N!} \sum_{i_1, \ldots, i_N = 0, \ldots, N-1} 1_{[\ell_{i_1}, \ell_{i_1+1}]}(r_1) \otimes \cdots \otimes 1_{[\ell_{i_N}, \ell_{i_N+1}]}(r_N) \tag{10}
$$

is a minimizer.
is optimal. We conjecture that among all minimizers of (Problem SCE) for this given density $\rho$, $P_N$ is the one which maximizes the entropy. Therefore, if one considers the one-dimensional problem at positive temperature $\beta^{-1}$, then in the small temperature limit $\beta \to \infty$, one shall recover $P_N$.

**Remark 8.** We see from Theorem 6 that in one-dimension (Problem SCE)$_D$ is degenerate with respect to $\rho$. Indeed, the maximizer $v$ only depends on the positions $\ell_i$’s, and not on the “shape” of the density $\rho$ inside each segment $[\ell_i, \ell_{i+1}]$. This pertains to the special case of the one-dimensional Coulomb force, which does not depend on the distance between the particles — *i.e.* when the electrons are consigned to their respective segment, the potential felt by them is effectively constant, so that their exact positions inside the segments are irrelevant.

We run our algorithm with $N = 4$ at inverse temperature $\beta = 10$ with density $\rho = 1_{[-2,2]}$. We select a crude discretization where the elements of $B$ are indicator functions of evenly-spaced segments of width $2/M$, that is

$$\rho_i = 1_{i M/2, (i+1) M/2]} \quad \text{for all } i = 0, \ldots, M - 1$$

with $M = 10$, the segment $[-2, 0]$ being dealt with symmetrically. The results obtained, which are displayed at Figure 3, are consistent with Theorem 6.

**Remark 9 (Extension of the main theorems to the one-dimensional case).** In one-dimension, we see that Theorem 1, which is stated only for $d \geq 3$, remains valid according to Theorem 6. Similar uniqueness
Figure 3. One-dimensional four-electron droplet, i.e. \( \rho = 1_{[-2,2]} \) and \( \beta = 10 \). Left: the approximate Kantorovich potential \( v[\nu] \) for \( \nu \) obtained with our algorithm compared to the exact Kantorovich potential given by Theorem 6. Right: the associated dual charge compared to the exact dual charge.

results as in Theorem 2 holds in one-dimension. At positive temperature \( \beta^{-1} \), the existence of a dual charge (i.e. Theorem 3) also remains valid. In fact, we even have a stronger result in the one-dimensional case, namely that the dual charge \( \rho_{\text{ext},\beta} = -\frac{1}{2} v''_\beta \) at positive temperature has mass \( N-1 \), as in the zero-temperature case. Indeed, suppose that the support \( \Omega \) of \( \rho \) is connected, that is of the form \( [a,b] \). Then, we have

\[
-\frac{1}{2} \int_{[a,b]} v''_\beta(r)dr = \frac{1}{2} (v'_\beta(a) - v'_\beta(b)).
\]

Now, appealing to the equation verified by \( v_\beta \) (see Equation (52) below in the case \( d \geq 3 \)), we have

\[
v'_\beta(r) = -\int_{\mathbb{R}^{N-1}} \sum_{i=2}^{N} \text{sgn}(r - r_i)d\overline{G}_\beta(r_2, \ldots, r_N),
\]

where \( \overline{G}_\beta \) is the (normalized) Gibbs measure defined as in (53) below. Therefore, we have \( v'_\beta(a) = N - 1 \) and \( v'_\beta(b) = -(N - 1) \), leading to the claimed fact. Finally, regarding the convergence of the Kantorovich potential (Theorem 5) and the dual charge (Theorem 4) at positive temperature in the small temperature limit \( \beta \to \infty \), these results also remain veracious in one-dimension (using similar arguments).

3.2.2. Three-dimensional droplets. We now consider uniform droplets in three-dimension, that is, \( \rho = N|B_1|^{-1}1_{B_1} \) where \( B_1 \) is the unit ball.
of $\mathbb{R}^3$. Uniform droplets were numerically investigated in [33] up to $N = 30$ using the now called Seidl’s maps, which are believed to furnish a minimizer of (Problem SCE) and which, irrespective of its conjectured optimality, is known to be near-optimal. In the special two-electron case, the problem is analytically solvable. The unique minimizer of (Problem SCE) is known to be

$$\frac{\rho(r_1)}{2} \otimes \delta(r_2 - t(r_1)) \quad \text{where} \quad t(r) = -\frac{r}{|r|}(1 - |r|^3)^{1/3}. \quad (13)$$

Given a Lipschitz Kantorovich potential $v$ (which always exists; see Section 4.1), we have for almost-every $r \in B_1$

$$\nabla v(r) = -\frac{r - t(r)}{|r - t(r)|^3}. \quad (14)$$

Then $v$ can be retrieved by integrating (14). Conversely, the dual charge associated to $v$ is found to be $-\Delta v(r)/4\pi$ where $\Delta$ denotes the usual Laplacian operator, that is, for almost-every $r \in B_1$

$$\rho_{\text{ext}}(r) = \frac{(4\pi)^{-1}}{|r|(1 - |r|^3)^{\frac{2}{3}}(|r| + (1 - |r|^3)^{\frac{1}{3}})^3}. \quad (15)$$

We run our algorithm with $N = 2$ and $\rho = 2|B_1|^{-1}1_{B_1}$ at decreasing temperatures. The dual charge is discretized into $M = 15$ evenly-spaced concentric shells in which the charge is constant. The results obtained at Figure 4 are consistent. We then select a fixed temperature $\beta = 50$ and we run our algorithm for an increasing number of particles up to $N = 30$. We use the same discretization as for the two-particle case, except when $N = 30$, in which case $M$ is raised up to 25. Given the discretized version of (Problem DB) at zero-temperature, that is

$$F_{\text{SCE}}[\nu] = E_N(v[\nu]) + \int_{\mathbb{R}^d} v[\nu](r)\rho(r)dr,$$

we can assess the performance of our procedure by comparing $F_{\text{SCE}}[\nu]$ with the values obtained in [33], which are known to be (near-)optimal. The results obtained are displayed at Figure 5. We notice that, even appealing to rather crude discretization, our algorithm yields near-optimal values. The case $N = 30$ was obtained in $\sim 6$ min on a personal computer using the programming language Julia.

3.3. Implementation and bottlenecks. Given the gradient $\nabla G[\nu_t]$ of the objective at the iteration point $\nu_t$, the outer optimization in (Problem DB) can be conducted using first-order or quasi-Newton methods. In our experiments, we used a Gradient Ascent algorithm with
Figure 4. Two-electron droplet, i.e. $\rho = 2|B_1|^{-1}1_{B_1}$ where $B_1$ is the unit ball of $\mathbb{R}^3$. Left: the Kantorovich potentials $v[\nu]$ for $\nu$ obtained with our algorithm at decreasing temperatures compared to the exact Kantorovich potential (defined up to an additive constant). Right: the associated dual charges for the corresponding temperatures compared to the exact dual charge.

Figure 5. Droplets, i.e. $\rho = N|B_1|^{-1}1_{B_1}$ where $B_1$ is the unit ball of $\mathbb{R}^3$. The inverse temperature is fixed to $\beta = 50$, and the number of electrons increases until $N = 30$. We compare the total energy of the system at zero temperature with the values in [33]. We also display the approximate Kantorovich potentials obtained, macroscopically rescaled i.e. $v[\nu]/N$. 

| $N$ | $F_{\text{SCE}}[\nu]$ | In [33] |
|-----|----------------------|---------|
| 3   | 2.300               | 2.327   |
| 4   | 4.922               | 4.935   |
| 5   | 8.519               | 8.626   |
| 10  | 43.022              | 43.140  |
| 14  | 90.454              | 90.808  |
| 20  | 195.607             | 196.198 |
| 30  | 462.423             | 463.807 |
fixed step-size and added momentum, more precisely the Nesterov's Accelerated Gradient (NAG) procedure. The objective \( G \) being extremely expansive to compute because of the free energy term \( F_\beta \), classical line search procedures are impracticable. Note that it would be interesting to implement a procedure which bypasses the usual line searches algorithms to only enforce approximate orthogonality of the gradient with the search direction.

The inner optimization for (Problem \([DB]\)) consists in determining the gradient \( \nabla G[\nu_t] \). As mentioned above, this can be done using many different algorithms, the simplest of them being the Unadjusted Langevin Algorithm (ULA; see [34]). Though the original ULA is not a priori tailored for compactly supported densities, we found it to perform rather well — at least in the case of the droplets. Evidently, an important bottleneck is that, as the temperature is decreased, it becomes harder to sample from the canonical ensemble.

4. Proofs

4.1. On duality theory at zero temperature. We briefly recall some important facts regarding the duality theory for (Problem \([SCE]\)). In [5 11], it is proved that the electrons cannot overlap at optimality, in the sense that there exists \( \alpha > 0 \) such that any minimizer \( \mathbb{P} \) of (Problem \([SCE]\)) is supported away from \( D_\alpha \), i.e. \( \mathbb{P}(D_\alpha) = 0 \), where

\[
D_\alpha = \{(r_1, \ldots, r_N) : \exists i \neq j \text{ such that } |r_i - r_j| \leq \alpha \}.
\]

In particular, one can substitute to \( c \) the truncated Coulomb cost \( c_\alpha \), where

\[
c_\alpha(r_1, \ldots, r_N) = \sum_{1 \leq i < j \leq N} \min \left\{ \frac{1}{\alpha^{d-2}}, \frac{1}{|r_i - r_j|^{d-2}} \right\}.
\]

Using this fact, one can prove [5 Thm. 2.6] that (Problem \([SCE]\)) admits the following dual formulation, which is equivalent to (Problem \([SCE]\)):

\[
F_{SCE}(\rho) = \max_{\int_R [v | \rho] < +\infty} \left\{ E_{N,\alpha}(v) + \int_{R^d} v(r) \rho(r) dr \right\}, \quad (D_\alpha)
\]

where \( E_{N,\alpha}(v) \) is defined similarly to \( E_N(v) \), only with the truncated cost \( c_\alpha \) substituted to \( c \), that is

\[
E_{N,\alpha}(v) = \inf_{r_1, \ldots, r_N} \left\{ c_\alpha(r_1, \ldots, r_N) - \sum_{i=1}^N v(r_i) \right\}.
\]
For brevity, we drop the subscript $\alpha$ in (18) from now on. Moreover, according to [5, Lem. 3.3 and Thm. 3.6], there exists a maximizer $v$ of (Problem D$_\alpha$) which verifies
\[
v(r) = \inf_{r_2, \ldots, r_N} \left\{ c_\alpha(r, r_2, \ldots, r_N) - \sum_{i=2}^N v(r_i) \right\} .
\] (19)

Note that, for a Kantorovich potential $v$ which verifies (19), it holds that $E_{N-1}(v) = 0$. Moreover, we have the following lemma.

**Lemma 7.** Let $v$ be a Kantorovich potential for (Problem SCE$_D$) verifying Equation (19). Then, $v$ is Lipschitz and uniformly bounded. Moreover, it satisfies the following limit
\[
\lim_{|r| \to \infty} v(r) = E_{N-1}(v) < 0
\] (20)
where, according to (18), we have
\[
E_{N-1}(v) = \inf_{r_2, \ldots, r_N} \left\{ c_\alpha(r_2, \ldots, r_N) - \sum_{i=2}^N v(r_i) \right\} .
\]

**Proof of Lemma 7.** From [5, Thm. 3.4 and Thm. 3.6], we know that $v$ is uniformly bounded and Lipschitz. Now, using Equation (19), for all $r$ we have
\[
v(r) \geq \inf_{r_2, \ldots, r_N} \left\{ c_\alpha(r_2, \ldots, r_N) - \sum_{i=2}^N v(r_i) \right\} = E_{N-1}(v).
\] (21)

Moreover, for all $r$ and $(r_2, \ldots, r_N)$, we have
\[
v(r) \leq c_\alpha(r, r_2, \ldots, r_N) - \sum_{i=2}^N v(r_i),
\] (22)
which entails that
\[
\limsup_{|r| \to \infty} v(r) \leq c_\alpha(r_2, \ldots, r_N) - \sum_{i=2}^N v(r_i).
\] (23)

Taking the infimum with respect to $r_2, \ldots, r_N$ then leads to the conclusion that $\lim_{|r| \to \infty} v(r) = E_{N-1}(v)$. Then, letting $|r_i| \to \infty$ for all $i = 2, \ldots, N$ in (22), we obtain
\[
E_{N-1}(v) \leq -(N-1)E_{N-1}(v),
\] (24)
which implies that $E_{N-1}(v) \leq 0$. If $E_{N-1}(v) = 0$, then, once again appealing to (21) and (22) and letting $|r_i| \to \infty$ for $i = 2, \ldots, N$, we would obtain $v \equiv 0$, which is impossible. Therefore $E_{N-1}(v) < 0$. □
4.2. Proof of Theorem 1. Let us turn to the proof of Theorem 1 regarding the existence of a dual charge at zero temperature. As mentioned above, there exists a Kantorovich potential \( v \) for \((\text{Problem SCE}_{\mathcal{D}})\) which verifies
\[
v(r) = \inf_{r_2, \ldots, r_N} \left\{ c_{\alpha}(r, r_2, \ldots, r_N) - \sum_{i=2}^{N} v(r_i) \right\}.
\] (25)
We will show that this particular potential arises from a charge. Indeed, for any \( r_2, \ldots, r_N \), the function
\[
r \mapsto c_{\alpha}(r, r_2, \ldots, r_N) - \sum_{i=2}^{N} v(r_i)
\]
is superharmonic (see [20, Chap I.2]) and uniformly Lipschitz in the \( r_i \)'s. Therefore, any \( v \) which verifies (25) remains superharmonic as the pointwise infimum of a set of uniformly Lipschitz superharmonic functions. Now, we recall the following theorem:

**Theorem 8** (Riesz’s decomposition theorem [20, Thm 1.24]). Let \( f : \mathbb{R}^d \to \mathbb{R} \) be a superharmonic function which admits a harmonic minorant, i.e. there exists a harmonic function \( m : \mathbb{R}^d \to \mathbb{R} \) with \( m(r) \leq f(r) \) for all \( r \in \mathbb{R}^d \). Then, there exists a positive measure \( \mu \in \mathcal{M}_+(\mathbb{R}^d) \) and a harmonic function \( h : \mathbb{R}^d \to \mathbb{R} \) such that
\[
f(r) = \mu \ast |r|^{2-d} + h(r) \quad \text{for all } r \in \mathbb{R}^d.
\] (26)

We are now ready to provide the proof of Theorem 1.

**Proof of Theorem 1.** Let us consider \( v \) a Kantorovich potential for \((\text{Problem SCE}_{\mathcal{D}})\) which verifies (25). As noted above, \( v \) is superharmonic. Moreover, according to Lemma 7, \( v \) is uniformly bounded. Therefore, according to Theorem 8 above, there exists a positive measure \( \rho_{\text{ext}} \in \mathcal{M}_+(\mathbb{R}^d) \) and an harmonic function \( h \) such that \( v(r) = \rho_{\text{ext}} \ast |r|^{2-d} + h(r) \). But \( h \) must be bounded from above, so that Liouville’s theorem entails that \( h \) is constant. This provides the existence of a dual charge as stated by Theorem 1. In fact, let us prove that the constant is provided by \( E_{N-1}(v) \) the limit of \( v \) at infinity (see Lemma 7). This is not entirely trivial, as the limit of a Coulomb potential need not to be zero. Nevertheless, we have the following result, whose proof is given below.

**Lemma 9.** Let \( \mu \in \mathcal{M}_+(\mathbb{R}^d) \) be any locally finite measure such that \( \mu \ast |r|^{2-d} \) is bounded at the origin, i.e. \( \int_{\mathbb{R}^d} |r|^{2-d} \mu(dr) < \infty \). Then
\[
\liminf_{|r| \to \infty} \mu \ast |r|^{2-d} = 0.
\] (27)
In fact, because \( v \) admits a limit at infinity, Lemma 9 implies the stronger result that \( \rho_{\text{ext}}^*|r|^{2-d} \) converges to zero everywhere at infinity:

\[
\lim_{|r| \to \infty} \rho_{\text{ext}}^*|r|^{2-d} = 0. \tag{28}
\]

Let us prove that the total mass of the dual charge \( \rho_{\text{ext}} \) cannot exceed \( N - 1 \). In what follows, we denote \( v_{\text{ext}}(r) = \rho_{\text{ext}}^*|r|^{2-d} \). Note that, according to (28) and Lemma 7, we have for all \( r \in \mathbb{R}^d \):

\[
v(r) = v_{\text{ext}}(r) + E_{N-1}(v). \tag{29}
\]

Moreover, for \( E_N(v) = 0 \), we have the following inequality for all \( r \) and \( (r_2, \ldots, r_N) \)

\[
v_{\text{ext}}(r) \leq c_\alpha(r, r_2, \ldots, r_N) - \sum_{i=2}^{N} v_{\text{ext}}(r_i) - E_N(v_{\text{ext}}). \tag{30}
\]

We first claim that \( E_N(v_{\text{ext}}) = E_{N-1}(v_{\text{ext}}) \). Indeed, according to (29) and still appealing to the fact that \( E_N(v) = 0 \), we have

\[
E_N(v_{\text{ext}}) = NE_{N-1}(v). \tag{31}
\]

Furthermore, we have

\[
E_{N-1}(v) = E_{N-1}(v_{\text{ext}}) - (N-1)E_{N-1}(v). \tag{32}
\]

This entails that \( NE_{N-1}(v) = E_{N-1}(v_{\text{ext}}) \), and ultimately implies the claim that \( E_N(v_{\text{ext}}) = E_{N-1}(v_{\text{ext}}) \). Now, because \( v_{\text{ext}} \) vanishes at infinity, we have the following sequence of inequalities

\[
E_{N-K}(v_{\text{ext}}) \leq E_{N-K+1}(v_{\text{ext}}) \quad \text{for all } K = 1, \ldots, N-1,
\]

where the limiting case \( K = N - 1 \) corresponds to the case where all electrons but one are sent to infinity, that is

\[
E_1(v_{\text{ext}}) = \inf_r \{-v_{\text{ext}}(r)\}.
\]

As the supremum of \( v \) cannot be attained at infinity, we deduce the existence of a lowest \( K \in \{1, \ldots, N-1\} \) such that

\[
E_{N-1}(v_{\text{ext}}) = E_{N-2}(v_{\text{ext}}) = \cdots = E_{N-K}(v_{\text{ext}}) < E_{N-K-1}(v_{\text{ext}}). \tag{34}
\]

The last inequality implies that the infimum \( E_{N-K}(v_{\text{ext}}) \) is attained inside a compact set for some \( \hat{r}_1, \ldots, \hat{r}_{N-K} \). Now, plugging \( \hat{r}_1, \ldots, \hat{r}_{N-K} \) into (30), we obtain

\[
v_{\text{ext}}(r) \leq \sum_{k=1}^{N-K} \frac{1}{|r - \hat{r}_k|^{d-2}}, \quad \text{for all } r \in \mathbb{R}^d, \tag{35}
\]
which entails, as claimed in Theorem 1, that
\[ \int_{\mathbb{R}^d} \rho_{\text{ext}} \leq N - K \leq N - 1. \]  
(36)

Finally, for the last item of Theorem 1, namely that we can suppose \( \text{supp}(\rho_{\text{ext}}) \subset \Omega \) in the case where \( \Omega \) is bounded, it suffices to consider the balayage of \( \rho_{\text{ext}} \) onto \( \Omega \), as stated in the following technical theorem.

**Theorem 10** (Balayage [20, Thm 4.2, Thm 4.4]). Let \( G \subset \mathbb{R}^d \) be a region with compact boundary. Given any \( \mu \in \mathcal{M}_+^{+}(\mathbb{R}^d) \) such that \( \text{supp}(\mu) \subset G \), there exists a measure \( \nu \in \mathcal{M}_+^{+}(\mathbb{R}^d) \), the so-called balayage measure of \( \mu \) onto \( \partial G \), which verifies that \( \text{supp}(\nu) \subset \partial G \), and that \( \nu \ast |r|^{d-2} = \mu \ast |r|^{d-2} \) for all \( r \in \mathbb{R}^d \setminus G \) and \( \nu \ast |r|^{d-2} \leq \mu \ast |r|^{d-2} \) for all \( r \in \partial G \). Moreover, we have \( \int_{\mathbb{R}^d} \nu \leq \int_{\mathbb{R}^d} \mu \).

This concludes the proof of Theorem 1. \( \square \)

We now turn to the proof of Lemma 9.

**Proof of Lemma 9.** It suffices to consider the case where \( \mu \) is radial, that is \( \mu(RA) = \mu(A) \) for all Borel sets \( A \subset \mathbb{R}^d \) and all rotations \( R \in SO(d) \). Indeed, we always have
\[ 0 \leq \liminf_{|r| \to \infty} \mu \ast |r|^{2-d} \leq \liminf_{|r| \to \infty} \tilde{\mu} \ast |r|^{2-d} \]  
(37)
where \( \tilde{\mu} \in \mathcal{M}_+^{+}(\mathbb{R}^d) \) is the radial measure defined as
\[ \tilde{\mu}(A) = \int_{SO(d)} \mu(RA) \nu(dR). \]  
(38)
where \( \nu \) is the Haar measure of \( SO(d) \). Therefore, let us suppose that \( \mu \) is radial. According to Newton’s theorem (see, e.g. [27, Thm 9.7]), we have
\[ \mu \ast |r|^{2-d} = \frac{1}{|r|^{d-2}} \int_{B_{|r|}} \mu(dr') + \int_{\mathbb{R}^d \setminus B_{|r|}} \mu(dr') |r'|^{d-2}. \]  
(39)
Let \( (r_n)_{n \geq 0} \) be any sequence such that \( |r_n| \to \infty \) as \( n \to \infty \), and suppose that \( r_0 = 0 \). We write \( r_n = |r_n| \) and \( \mu(r_n) = \mu(B_{r_n}) \). Up to a subsequence, since \( \mu \) is locally finite, we can suppose that
\[ \mu(r_{n-1}) \leq \sqrt{r_n}, \quad \text{for all } n \geq 1. \]  
(40)
But, we can write
\[ \int_{\mathbb{R}^d} \frac{\mu(dr')}{|r'|^{d-2}} = \sum_{n \geq 1} \int_{B_{r_n} \setminus B_{r_{n-1}}} \frac{\mu(dr')}{|r'|^{d-2}} \geq \sum_{n \geq 1} \frac{1}{r_n} (\mu(r_n) - \mu(r_{n-1})). \]  
(41)
By assumption, \( \int_{\mathbb{R}^d} |r'|^{2-d} \mu(dr') < \infty \), so it must be that
\[
\frac{1}{r_n} (\mu(r_n) - \mu(r_{n-1})) \xrightarrow{n \to \infty} 0. \tag{42}
\]
But, according to (40), we have
\[
\frac{1}{r_n} \mu(r_{n-1}) \leq \frac{1}{\sqrt{r_n}} \xrightarrow{n \to \infty} 0, \tag{43}
\]
so that
\[
\frac{1}{r_n} \mu(r_n) \xrightarrow{n \to \infty} 0. \tag{44}
\]
Now, still appealing to Newton’s theorem, we have
\[
\mu \ast |r|^{2-d}(r_n) = \frac{1}{r_n} \mu(r_n) + \int_{\mathbb{R}^d \setminus B_{r_n}} \frac{\mu(dr')}{|r'|^{d-2}} \xrightarrow{n \to \infty} 0, \tag{45}
\]
which yields the thesis of Lemma 9. □

4.3. Proof of Theorem 2. The uniqueness of the dual charge is intrinsically linked to that of the uniqueness of the Kantorovich potential — and, as such, follows from the following proposition:

**Proposition 11.** Let \( \rho \in L^1(\mathbb{R}^d, \mathbb{R}_+) \) with \( \int_{\mathbb{R}^d} \rho = N \geq 2 \), and suppose that \( \rho \) has connected support \( \Omega \). Let \( v \) and \( w \) be two Lipschitz Kantorovich potentials for (Problem SCE\( \mathcal{D} \)). Then \( v \) and \( w \) are equal up to an additive constant on the support \( \Omega \) of \( \rho \).

**Proof of Proposition 11.** It follows from [36, Thm 1.15] that, for any two almost-everywhere differentiable Kantorovich potentials \( v \) and \( w \), we have
\[
\nabla v(r) = \nabla w(r) \quad \text{for almost-all } r \in \Omega, \tag{46}
\]
where the gradients \( \nabla v \) and \( \nabla w \) are to be understood in the Fréchet sense. Since Lipschitz functions are differentiable almost-everywhere according to Rademacher’s theorem, the above equality makes sense. Furthermore, it is known [14] that the gradient of a Lipschitz function identifies with its distributional gradient. Therefore, it must be that
\[
v(r) = w(r) + c, \quad \text{for all } r \in \Omega, \quad c \in \mathbb{R}. \tag{47}
\]

**Proof of Theorem 2.** This follows immediately from Proposition 11 by considering the distributional Laplacian in (47). □
4.4. On duality theory at positive temperature. We recall important facts regarding the duality theory for \((\text{Problem SCE}_\beta)\). As mentioned above, the SCE problem at positive temperature can be viewed as the Legendre transform

\[
F_{\text{SCE},\beta}(\rho) = \sup_v \left\{ F_\beta(v) + \int_{\mathbb{R}^d} v(r) \rho(r) dr \right\},
\]

(48)

where \(F_\beta(v)\) is the Helmholtz free energy of the canonical ensemble with external potential (minus) \(v\), that is

\[
F_\beta(v) = -\beta^{-1} \ln z_\beta(v)
\]

where \(z_\beta(v)\) is defined as the volume \(\int_{\mathbb{R}^d} dG_\beta(v)\) of the configurational canonical ensemble \(G_\beta(v)\) defined as the Gibbs-Boltzmann measure whose density with respect to \(\mu \otimes N\) is given by

\[
dG_\beta(v)(r_1, \ldots, r_N) = \exp \left[-\beta \left( c(r_1, \ldots, r_N) - \sum_{i=1}^N v(r_i) \right) \right] d\mu \otimes N.
\]

(49)

Appealing to the strict concavity of \((\text{Problem SCE}_{D,\beta})\), one can formally take the functional derivative of the objective and solve for the first-order optimality condition. One finds

\[
\frac{\delta}{\delta v(r)} \left( F_\beta(v) + \int_{\mathbb{R}^d} v(r) \rho(r) dr \right) = \rho_{G_\beta(v)}(r) - \rho(r)
\]

(50)

where \(\rho_{G_\beta(v)}\) is the one-particle density of the ensemble \(G_\beta(v)\), that is

\[
\rho_{G_\beta(v)}(r) = N \int_{\mathbb{R}^{d(N-1)}} G_\beta(v)(r, dr_2, \ldots, dr_N).
\]

(51)

Therefore \((\text{Problem SCE}_{D,\beta})\) amounts to finding the unique (up to an additive constant) potential \(v_\beta\) such that the one-particle density of the associated canonical ensemble is \(\rho\). We will always write \(G_\beta\) for \(G_\beta(v_\beta)\).

**Convention 1.** Up to an additive constant, we will always assume that \(v_\beta\) verifies \(z_\beta(v_\beta) = N\).

Note that the first-order optimality condition \(\rho_{G_\beta} = \rho\) rewrites under the above convention as the fixed-point equation

\[
v_\beta(r) = -\beta^{-1} \ln \int_{\mathbb{R}^{d(N-1)}} G^r_\beta(r_2, \ldots, r_N) d\mu \otimes (N-1)(r_2, \ldots, r_N)
\]

(52)

for almost all \(r \in \Omega\), where \(\Omega\) is the support of \(\rho\) and where \(G^r_\beta\) is defined as

\[
G^r_\beta(r_2, \ldots, r_N) = \exp \left[-\beta \left( c(r, r_2, \ldots, r_N) - \sum_{i=2}^N v_\beta(r_i) \right) \right].
\]

(53)
Convention 2. Since in (49) the Gibbs measure $G_\beta$ is defined only with respect to $\rho$, in the first-order optimality condition (50) one can free modified $v_\beta$ outside of the support $\Omega$ of $\rho$. Furthermore, although Equation (52) is only valid inside of $\Omega$, the right-hand side is well-defined for all $r$ and can be used to extend $v_\beta$ over the entire space. In what follows we will always suppose that $v_\beta$ is defined everywhere according to Equation (52).

Finally, let us indicate that the equality at (48) between (Problem $\text{SCE}_\beta$) and (Problem $\text{SCE}_{D,\beta}$) follows from classical Convex Optimization theorem, see e.g. [39, Thm 5.17], and that the above argument leading to the equation (52) was made rigorous in [9] under the assumption that (i.e. see (A1))

$$\int\int_{\mathbb{R}^d \times \mathbb{R}^d} \rho(dr)\rho(dr') \frac{|r-r'|}{d-2} < \infty.$$

(54)

4.5. Proof of Theorem 3. Let us start with the following lemma:

Lemma 12. Let $\rho \in L^1(\mathbb{R}^d, \mathbb{R}_+)$ with $\int_{\mathbb{R}^d} \rho = N \geq 2$ be such that the assumptions (A1) and (A2) are verified. Then, the unique maximizer $v_\beta$ of (Problem $\text{SCE}_{D,\beta}$) under Conventions 1–2 is a twice continuously differentiable superharmonic function, i.e. $v_\beta \in C^2(\mathbb{R}^d)$ and $-\Delta v_\beta \geq 0$.

Proof of Lemma 12. It follows from dominated convergence that $v_\beta$ is twice continuously differentiable. To prove that $v_\beta$ is superharmonic, it then suffices to check that $-\Delta v_\beta \geq 0$ [20, p.56-57]. We denote by $G_\beta^r$ the Gibbs-Boltzmann measure $G_\beta$ normalized to unity. We have

$$\nabla v_\beta(r) = -\int_{\mathbb{R}^{d(N-1)}} \nabla_r c(r, r_2, \ldots, r_N) dG_\beta^r(r_2, \ldots, r_N)$$

(55)

and, taking the divergence with respect to $r$ above, we obtain

$$-\beta^{-1} \Delta v_\beta(r) = \int_{\mathbb{R}^{d(N-1)}} |\nabla_r c(r, r_2, \ldots, r_N)|^2 dG_\beta^r$$

$$-\left| \int_{\mathbb{R}^{d(N-1)}} \nabla_r c(r, r_2, \ldots, r_N) dG_\beta^r \right|^2 .$$

(56)

The thesis is then obtained by appealing to Jensen’s inequality. Note that for any $r$, the function $(r_2, \ldots, r_N) \mapsto \nabla_r c(r_2, \ldots, r_N)$ is integrable against the Gibbs measure $G_\beta^r$ for the latter vanishes exponentially fast as $r_j \to \infty$ for all $j = 2, \ldots, N$. Therefore, the above equation makes sense for all $r$. □

Lemma 13. Let $\rho \in L^1(\mathbb{R}^d, \mathbb{R}_+)$ with $\int_{\mathbb{R}^d} \rho = N \geq 2$ be such that the assumptions (A1) and (A2) are verified. Then, the unique maximizer
$v_\beta$ of (Problem $\text{SCE}_{D,\beta}$) under Conventions 1–2 is bounded in $L^\infty(\mathbb{R}^d)$ independently in $\beta$ in the limit $\beta \to \infty$. More precisely, we have

$$\sup_{r \in \mathbb{R}^d} v_\beta(r) \leq \|\rho * |r|^{2-d}\|_{L^\infty} + \frac{1}{2} D(\rho).$$

(57)

and

$$\inf_{r \in \mathbb{R}^d} v_\beta(r) \geq -(N-1)(\|\rho * |r|^{2-d}\|_{L^\infty} + \frac{1}{2} D(\rho)).$$

(58)

Proof of Lemma 13. The upper bound (57) follows by appealing to Jensen’s inequality in Equation (52). Indeed, we have

$$v_\beta(r) \leq \int_{\mathbb{R}^d} (c(r, r_2, \ldots, r_N) - \sum_{i=2}^N v_\beta(r_i)) d\mu^{\otimes N-1},$$

(59)

which implies

$$v_\beta(r) \leq (N-1)\mu * |r|^{2-d} + \left(\frac{N-1}{2}\right) D(\mu)$$

$$- (N-1) \int_{\mathbb{R}^d} v_\beta(r) \mu(dr).$$

(60)

Now, recalling that $\mu = \rho/N$, we have by definition

$$F_{\text{SCE},\beta}(\rho) = -\beta^{-1} \ln z_\beta(v_\beta) + N \int_{\mathbb{R}^d} v_\beta(r) \mu(dr).$$

(61)

Therefore, using the above equality and the fact that $z_\beta(v_\beta) = N$ (see Convention 1), we obtain

$$v_\beta(r) \leq (N-1)\mu * |r|^{2-d} + \left(\frac{N-1}{2}\right) D(\mu)$$

$$- \frac{(N-1)}{N} (F_{\text{SCE},\beta}(\rho) + \beta^{-1} \ln N).$$

(62)

Finally, from the fact that $F_{\text{SCE},\beta}(\rho)$ is positive and converges to $F_{\text{SCE}}(\rho)$ as $\beta \to \infty$, we obtain the upper bound (57) as claimed. Now using the positivity of the Coulomb cost, we have

$$v_\beta(r) \geq -\beta^{-1}(N-1) \ln \left(\int_{\mathbb{R}^d} e^{\beta v_\beta(r')} \mu(dr')\right)$$

(63)

and plugging the upper bound (57) into (63) we obtain the lower bound (58).

□

We can now provide the proof of Theorem 3.
Proof of Theorem 3. From Lemma 12 and Lemma 13, we known that $v_\beta$ (under Conventions 1–2) is superharmonic and bounded from below. Therefore, the proof of Theorem 3 regarding the existence of a dual charge at positive temperature, is identical to that of the proof of Theorem 1 regarding the existence of a dual charge at zero temperature. □

4.6. Proofs of Theorem 4 and Theorem 5. We start with the proof of Theorem 5 regarding the convergence of the Kantorovich potential $v_\beta$ to a Kantorovich potential for (Problem SCE$_{D,\beta}$) in the limit $\beta \to \infty$.

Lemma 14. Let $\rho \in L^1(\mathbb{R}^d, \mathbb{R}_+)$ with $\int_{\mathbb{R}^d}\rho = N \geq 2$ be such that the assumptions (A1) and (A2) are verified, and such that the support $\Omega$ of $\rho$ is bounded. Then, the unique maximizer $v_\beta$ of (Problem SCE$_{D,\beta}$) under Conventions 1–2 is bounded in $W^{1,\infty}(\mathbb{R}^d)$ independently in $\beta$ in the limit $\beta \to \infty$.

Proof of Lemma 14. According to Lemma 13, we know that $v_\beta$ is bounded in $L^\infty(\mathbb{R}^d)$ uniformly in $\beta$ in the small temperature limit, so that it only remains to prove that $\nabla V_\beta$ is also bounded in $L^\infty(\mathbb{R}^d)$ uniformly in $\beta$ as $\beta \to \infty$. Recall that

$$\nabla v_\beta(r) = -\int_{\mathbb{R}^d(N-1)} \nabla c(r, r_2, \ldots, r_N) dG(r_2, \ldots, r_N)$$

where $G$ is the Gibbs-Boltzmann measure $G_{\beta}$ normalized to unity. Using the fact that $G_{\beta}$ is symmetric, we have

$$|\nabla v_\beta(r)| \leq (N-1) \int_{\mathbb{R}^{d(N-1)}} \frac{dG(r_2, \ldots, r_N)}{|r - r_2|^{d-1}}. \quad (64)$$

For all $\beta > 0$ and all $r \in \mathbb{R}^d$, we have supp$(G_{\beta}) \subset \Omega$, where $\Omega$ is the support of $\rho$. Therefore, since $\Omega$ is by hypothesis bounded, we have

$$\int_{\mathbb{R}^{d(N-1)}} \frac{dG(r_2, \ldots, r_N)}{|r - r_2|^{d-1}} = \frac{1}{|r|^{d-1}} + o_{|r| \to \infty}(1),$$

where the $o_{|r| \to \infty}(1)$ is independent of $\beta$. Therefore, for a large enough compact set $K$, the gradient $\nabla V_\beta$ is bounded in $L^\infty(\mathbb{R}^d \setminus K)$ uniformly in $\beta$ in the limit $\beta \to \infty$. It remains to control $|\nabla V_\beta|$ inside of $K$.

Let us define the (unnormalized) Gibbs-Boltzmann measure $H^r_{\beta}$ as

$$dH^r_{\beta}(r_2, \ldots, r_N) = \frac{G^r_{\beta}(r_2, \ldots, r_N)}{|r - r_2|^{d-1}} d\mu^{\otimes(N-1)}(r_2, \ldots, r_N),$$

and let $H^r_{\beta}$ be the associated probability measure, i.e. $H^r_{\beta}$ normalized to unity. We denote by $g_\beta(r)$ the volume of $G^r_{\beta}$, i.e. $g_\beta(r) = \int_{\mathbb{R}^{d(N-1)}} dG^r_{\beta},$
and by $h_\beta(r)$ the volume of $H^r_\beta$. We can then rewrite

$$A(r) := \int_{\mathbb{R}^{d(N-1)}} \frac{dG_\beta(r_2, \ldots, r_N)}{|r - r_2|^{d-1}} = \frac{h_\beta(r)}{g_\beta(r)}$$  \hspace{1cm} (66)

According to the *Gibbs Variational Principle*, the free energies associated with $G^r_\beta$ and $H^r_\beta$ can be rewritten as

$$-\beta^{-1} \ln g_\beta(r) = F(G^r_\beta) = \min_{\mathbb{P}} F(\mathbb{P})$$ \hspace{1cm} (67)

and

$$-\beta^{-1} \ln h_\beta(r) = F'(H^r_\beta) = \min_{\mathbb{P}} F'(\mathbb{P}),$$ \hspace{1cm} (68)

where the minimum runs over all probability measures $\mathbb{P}$ on $\mathbb{R}^{d(N-1)}$ and where the functionals $F$ and $F'$ are defined as the total energies

$$F(\mathbb{P}) = \int_{\mathbb{R}^{d(N-1)}} \mathcal{H}^r(r_2, \ldots, r_N) d\mathbb{P} + \beta^{-1} \text{Ent}(\mathbb{P} | \mu^\otimes(N-1))$$ \hspace{1cm} (69)

and

$$F'(\mathbb{P}) = F(\mathbb{P}) + \beta^{-1} \int_{\mathbb{R}^{d(N-1)}} \ln |r - r_2|^{d-1} d\mathbb{P},$$ \hspace{1cm} (70)

where $\mathcal{H}^r$ is the Hamiltonian defined as

$$\mathcal{H}^r(r_2, \ldots, r_N) = c(r, r_2, \ldots, r_N) - \sum_{i=2}^N v_\beta(r_i).$$

Therefore, we obtain

$$-\beta^{-1} \ln A(r) = F'(H^r_\beta) - F(G^r_\beta) \geq F'(H^r_\beta) - F(H^r_\beta),$$ \hspace{1cm} (71)

and the preceding inequality rewrites as

$$A(r) \leq \exp \left( - \int_{\mathbb{R}^{d(N-1)}} \ln |r - r_2|^{d-1} dH^r_\beta \right).$$ \hspace{1cm} (72)

Using the inequality $-\log t^{d-1} \leq t^{2-d}$ for $t > 0$, we then obtain

$$A(r) \leq \exp \left( \int_{\mathbb{R}^{d(N-1)}} \frac{dH^r_\beta}{|r - r_2|^{d-2}} \right).$$ \hspace{1cm} (73)

Now, let us appeal to the Gibbs Variational Principle once again to further the inequality (73). Indeed, for any probability measure $\mathbb{P}$, we have (by definition) that $F'(H^r_\beta) \leq F'(\mathbb{P})$. Using the fact that the entropy and the Coulomb cost are positive, we are led to

$$\int_{\mathbb{R}^{d(N-1)}} \frac{dH^r_\beta}{|r - r_2|^{d-2}} \leq F'(\mathbb{P})$$

$$+ \int_{\mathbb{R}^{d(N-1)}} \left( \sum_{i=2}^N v_\beta(r_i) - \beta^{-1} \log |r - r_N|^{d-1} \right) dH^r_\beta.$$  \hspace{1cm} (74)
Using that $v_\beta$ is uniformly bounded in $\beta$ in the limit $\beta \to \infty$, say $\|v_\beta\|_{L^\infty(\mathbb{R}^d)} \leq M$ for all $\beta$ as $\beta \to \infty$, we further obtain

\[
(1 - \beta^{-1}) \int_{\mathbb{R}^d} \frac{dH_\beta}{|r - r_2|^{d-2}} \leq F'(P) + (N - 1)M. \tag{75}
\]

Now, it suffices to put, e.g. $P = |\Omega|^{-(N-1)}I_{\Omega}^{\otimes(N-1)}$, in (75). One can check that the bound then obtained is bounded in $L^\infty(K)$ uniformly in the temperature $\beta$, yielding the thesis of Lemma 14. \hfill \square

**Lemma 15.** Let $\rho \in L^1(\mathbb{R}^d, \mathbb{R}^+)$ with $\int_{\mathbb{R}^d} \rho = N \geq 2$ be such that the assumptions (A1) and (A2) are verified, and let $v_\beta$ be the unique maximizer of (Problem $SCE_{D,\beta}$) under Conventions 1–2. Then there exists $v_\infty \in W^{1,\infty}(\mathbb{R}^d)$ such that, up to a subsequence $\beta' \to \infty$, we have

\[
v_\beta \xrightarrow{\beta \to \infty} v_\infty \text{ uniformly on every compact set.} \tag{76}
\]

Moreover, $v_\infty$ is a Kantorovich potential for (Problem $SCE_{D,\Omega}$).

**Proof of Lemma 15.** The Kantorovich potential $v_\beta$ being bounded in $W^{1,\infty}(\mathbb{R}^d)$ uniformly in $\beta$ in the limit $\beta \to \infty$, it follows that there exists $v_\infty \in W^{1,\infty}(\mathbb{R}^d)$ such that (up to a subsequence $\beta' \to \infty$)

\[
v_\beta \to v_\infty \text{ weakly in } W^{1,\infty}(\mathbb{R}^d) \text{ and locally uniformly in } L^\infty(\mathbb{R}^d). \tag{77}
\]

We claim that $v_\infty$ is a Kantorovich potential for (Problem $SCE_{D,\Omega}$). Since $F_{SCE,\beta}(\rho) \to F_{SCE}(\rho)$ as $\beta \to \infty$, we have

\[
F_{SCE,\beta}(\rho) = -\beta^{-1} \ln N + \int_{\Omega} v_\beta \rho \xrightarrow{\beta \to \infty} \int_{\Omega} v_\infty \rho = F_{SCE}(\rho). \tag{78}
\]

Now, by duality we have

\[
E_{N,\Omega}(v_\infty) + \int_{\Omega} v_\infty \rho \leq F_{SCE}(\rho) = \int_{\Omega} v_\infty \rho, \tag{79}
\]

where the last equality follows from (78). Therefore, we will have proved that $v_\infty$ is a Kantorovich potential for (Problem $SCE_{D,\Omega}$) if we can prove that $E_{N,\Omega}(v_\infty) \geq 0$ — which will eventually imply that $E_{N,\Omega}(v_\infty) = 0$. Let us then define

\[
A_\varepsilon = \left\{ (r_1, \ldots, r_N) \in \Omega^N : \sum_{i=1}^N v_\infty(r_i) > c_\alpha(r_1, \ldots, r_N) + \varepsilon \right\}.
\]

By convention, we have $z_\beta(v_\beta) = N$ for all $\beta > 0$. Appealing to Fatou’s lemma, we have

\[
N \geq \int_{A_\varepsilon} \liminf_{\beta \to \infty} G_\beta(r_1, \ldots, r_N) d\mu^\otimes N(r_1, \ldots, r_N) \tag{80}
\]
But, by definition of $A_\varepsilon$, for all $(r_1, \ldots, r_N) \in A_\varepsilon$ we have
\[
\liminf_{\beta \to \infty} G_\beta(r_1, \ldots, r_N) = +\infty.
\tag{81}
\]
Therefore, in regards of (80) and (81), it must be that
\[
\mu^N(A_\varepsilon) = 0.
\]
Since $A_\varepsilon$ is open in $\Omega^N$, we necessarily have that $A_\varepsilon$ is empty for all $\varepsilon > 0$. Therefore, we obtain $E_{N,\Omega}(v_\infty) \geq 0$ as wanted, yielding the thesis that $v_\infty$ is a Kantorovich potential for Problem $SCE_{D,\Omega}$. □

Proof of Theorem 5. The proof of Theorem 5 now follows entirely from Lemma 14 and Lemma 15. □

We now turn to the proof of Theorem 4. Given two measures $\mu, \nu \in M(\mathbb{R}^d)$, their Coulomb energy is defined as
\[
D(\mu, \nu) = \int \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{\mu(dr)\nu(dr')}{|r - r'|^{d-2}},
\]
and we use the shorthand notation $D(\mu) := D(\mu, \mu)$ to denote the self-energy of $\mu$. If we define the space $\mathcal{E}(\mathbb{R}^d) \subset M(\mathbb{R}^d)$ as
\[
\mathcal{E}(\mathbb{R}^d) = \{ \mu \in M(\mathbb{R}^d) : D(\mu) < \infty \},
\]
then $(\mu, \nu) \mapsto D(\mu, \nu)$ defines an inner product which endows $\mathcal{E}(\mathbb{R}^d)$ with a Hilbert space structure [20, Thm 1.18]. In particular, the weak topology on $\mathcal{E}(\mathbb{R}^d)$ is defined as follows: given $(\mu_n)_n \subset \mathcal{E}(\mathbb{R}^d)$, we say that the sequence $(\mu_n)_n$ weakly converge (in energy) to $\mu$ if, for all $\nu \in \mathcal{E}(\mathbb{R}^d)$, we have
\[
D(\mu_n, \nu) \xrightarrow{n \to \infty} D(\mu, \nu).
\]
This weak topology is stronger than that of the vague topology on $M(\mathbb{R}^d)$ [20, Lem 1.3]. In particular, $\{ \mu \in \mathcal{E}(\mathbb{R}^d) : D(\mu) < c \}$ is compact for the vague topology for any $c > 0$.

Proof of Theorem 4. Let $\rho_{ext, \beta}$ be the dual charge associated with $v_\beta$ which is not yet “swept” onto $\Omega$ using Theorem 10. We claim that $D(\rho_{ext, \beta})$ is bounded uniformly in $\beta$ in the limit $\beta \to \infty$. Integrating by parts, we have
\[
D(\rho_{ext, \beta}) = \frac{1}{c_d} \int_{\mathbb{R}^d} |\nabla v_\beta(r)|^2 dr \quad \text{where} \quad c_d = \frac{d(d-2)\pi^{d/2}}{\Gamma\left(\frac{d}{2} + 1\right)}.
\]
Now, as in the proof of Theorem 5, we have
\[
|\nabla v_\beta(r)|^2 \leq (N-1)^2 \int_{\mathbb{R}^{d(N-1)}} \frac{dG_\beta(r_2, \ldots, r_N)}{|r - r_2|^{2(d-1)}}.
\]
Outside a large enough compact set $K$, the above integral is bounded in $L^2(\mathbb{R}^d \setminus K)$ uniformly in $\beta$ in the limit $\beta \to \infty$. It then remains to control the $L^2$-norm of $\nabla v_{\beta}$ inside $K$. The strategy to do so is completely analogous to that of the proof of Theorem 5.

Now, if $\rho_{\text{ext}, \beta}$ is swept onto $\Omega$, its self-energy does not increase [20, Thm. 4.4.]. Therefore, according to what precedes, the self-energy of the balayage measure remains uniformly bounded in $\beta$ in the limit $\beta \to \infty$. As such, there exists $\rho_\infty \in \mathcal{E}(\mathbb{R}^d)$ such that

$$\rho_{\text{ext}, \beta} \rightharpoonup \rho_\infty \quad \text{in } \mathcal{M}(\mathbb{R}^d), \quad \text{(82)}$$

and we have that $\rho_\infty$ is a dual charge for (Problem $\text{SCE}_{D, \Omega}$). Indeed, we know that (up to a subsequence; see Theorem 5)

$$\rho_{\text{ext}, \beta} * \lvert \mathbf{r} \rvert^{2-d} \underset{\beta \to \infty}{\longrightarrow} v_\infty \quad \text{uniformly on } \Omega, \quad \text{(83)}$$

where $v_\infty$ is a Kantorovich potential for (Problem $\text{SCE}_{D, \Omega}$). Therefore, using (82), we obtain $\rho_\infty * \lvert \mathbf{r} \rvert^{2-d} = v_\infty$, yielding that $\rho_\infty$ is a dual charge for (Problem $\text{SCE}_{D, \Omega}$). $\square$

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