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Thomas–Fermi theory of out-of-plane charge screening in graphene

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This paper provides a variational treatment of the effect of external charges on the free charges in an infinite free-standing graphene sheet within the Thomas–Fermi theory. We establish existence, uniqueness and regularity of the energy minimizers corresponding to the free charge densities that screen the effect of an external electrostatic potential at the neutrality point. For the potential due to one or several off-layer point charges, we also prove positivity and a precise universal asymptotic decay rate for the screening charge density, as well as an exact charge cancellation by the graphene sheet. We also treat a simpler case of the non-zero background charge density and establish similar results in that case.

1. Introduction

Graphene is a classical example of a two-dimensional material whose electronic properties give rise to a number of unusual characteristics that make it a prime target for both fundamental research and multiple applications [1–5]. A key feature of the electrons in single-layer graphene sheets is the presence of the Dirac cone in their dispersion relation that makes the elementary excitations (electrons and holes) of the ground state behave as massless relativistic fermions [6,7]. This presents challenges in the theoretical treatment of those excitations, as their kinetic energy, which is of the order of $E_K \sim \hbar v_F/r$, where $v_F \simeq 1 \times 10^8\ \mathrm{cm\,s^{-1}}$ is the Fermi velocity and r is the radius of the wave packet containing a single charge, remains comparable to the Coulombic interaction energy $E_C \sim e^2/(\epsilon_d r)$ of two charges at distance r independently of the scale r (here e is the elementary charge, in the CGS units, $\epsilon_d \sim 1$ is the effective dielectric constant, and it is noted that $e^2/(\hbar v_F) \simeq 2.2$). As a result, many-body effects need to be taken into consideration in the studies of electronic properties of graphene. In particular, these effects are significant in determining the way the massless ultrarelativistic fermions screen the electric field of supercritical charged impurities [6].

The problem of characterizing the charged impurity screening by the graphene sheet has been studied, using a number of theoretical approaches [8–14] (this list is not intended to be exhaustive). Note that a similar question arises in the studies of graphene-based devices in the proximity of a conducting electrode, or when a scanning tunnelling microscope tip approaches a graphene sheet [15]. In particular, in this situation, the electric charge the layer is exposed to may exceed the elementary charge e by many orders of magnitude. Under such conditions, a fully nonlinear treatment of the screening problem is, therefore, necessary.

In conventional quantum systems, a good starting point for the analysis of electric field screening is the Thomas–Fermi (TF) theory, as it yields an asymptotically exact response of a system of interacting electrons to a large external charge [16]. Such a theory for massless relativistic fermions was developed by DiVincenzo and Mele in the context of charged impurity screening in graphite intercalated compounds [8]. They conducted numerical studies of the resulting equations for the screening charge density and noted a highly non-local character of the response. More recently, Katsnelson carried out a formal analysis of the asymptotic behaviour of the screening charge density away from a single impurity ion in a graphene monolayer [11]. His results were further clarified an extended by Fogler *et al.*, who also confirmed the predictions about the decay of the screening charge density by numerical simulations [17]. The non-local character of the response and its dependence on the level of doping have been confirmed by the direct experimental observations of the screening charge density [18–20]. Note that these observations are at variance with the prediction of a purely local dielectric response at the Dirac point from the linear response theory for massless relativistic fermions within the random phase approximation [12].

This paper is a mathematical counterpart of the studies in [8,11,17] that provides a suitable variational framework for the study of the charge screening problem described by the TF theory of graphene (for a closely related TF–von Weizsäcker model and some further discussion, see [14]). The setting turns out to be rather delicate, as the presence of a bare Coulombic potential from an impurity leads to heavy tails in the potential term that are precisely balanced with the Coulombic interaction term. Within our setting, we prove existence, uniqueness, radial symmetry and monotonicity of the minimizer of the graphene TF energy for an off-layer external point charge in a free-standing graphene sheet. More generally, we provide existence, uniqueness, the Euler–Lagrange equation that is understood in a suitable sense, and regularity of the minimizer for a general class of external potentials arising as Coulombic potentials of appropriate collections of external charges. Back to a single off-layer charge in a free-standing graphene sheet, we establish the precise asymptotic decay of the screening charge density at infinity, which agrees with the one obtained by Katsnelson using formal arguments.

The decay of the screening charge density turns out to be a borderline power law decay modulated by a logarithmic factor that makes it barely integrable. The latter presents a significant technical difficulty in the handling of the appropriate barrier functions that control the decay of the solution at infinity. In particular, we prove that the decay indeed turns out to be universal, independently of the strength of the external charge and remains the same for a finite collection of charges of the same sign.

As a by-product of our analysis, we also demonstrate the existence of sign-changing minimizers in the case of positive fast decaying potentials for the closely related TF–von Weizsäcker model studied in [14] in the regime when the latter is well approximated by the TF model. This gives a partial answer to the question raised in [14]. Finally, we present the corresponding results for the biased layer. The treatment of the latter is significantly simpler due to the expected fast power law decay of the screening charge density.

Our paper is organized as follows. In §2, we introduce the TF energy functional for a free-standing graphene sheet and then discuss several issues associated with its definition in the context of the associated variational problem for charge screening that requires a modified formulation compared with the classical TF theory. Within these modifications, we then state the main results of our paper in theorems 2.1 and 2.2, and corollary 2.6. In §3, we give the precise variational setting for the modified TF energy of the free-standing graphene sheet and establish general existence and regularity results for the minimizers.

Then, in §4, we focus on the case of the potential from a single off-layer external point charge. In particular, in §4a, we reformulate the Euler–Lagrange equation for the minimizers in terms of a convenient auxiliary variable and establish several properties of the solutions associated with a comparison principle that we establish for this equation, and in §4b we establish further implications of the comparison principle on the positivity of solutions. This leads us, in §4c, to establish existence of sign-changing solutions to the closely related TF–von Weizsäcker model considered by us in [14].

The key computation of the paper is carried out in §4d, where a logarithmic barrier is established, which is then used in §4e to prove the asymptotic decay rate of the solution at infinity for the external potential of a point charge. Furthermore, in §4f, we show the complete charge screening and in §4g, we establish the universality of the decay. We conclude this section by showing how the statements of our main results in §2 follow from the various technical results obtained in §§3 and 4.

Finally, in §5, we outline the analogous treatment of the case of a doped graphene sheet characterized by the presence of a uniform background charge, where the main results are contained in theorems 5.2 and 5.4.

(a) Notation

Throughout the paper, for $f(t), g(t) \geq 0$, we use the asymptotic notation as $t \to +\infty$

- $f(t) \lesssim g(t)$ if there exists $C > 0$ independent of t such that $f(t) \leq Cg(t)$ for all t sufficiently large;
- $f(t) \sim g(t)$ if $f(t) \lesssim g(t)$ and $g(t) \lesssim f(t)$;
- $f(t) \simeq g(t)$ if $f(t) \sim g(t)$ and $\lim_{t\to+\infty}(f(t)/g(t)) = 1$.

As usual, $B_R(x) := \{y \in \mathbb{R}^N : |y - x| < R\}$, $B_R := B_R(0)$, and C, c, c_1 etc., denote generic positive constants. By $C^\alpha(\mathbb{R}^2)$, we denote the space of all locally Hölder continuous functions of order $\alpha \in (0, 1]$ on $\mathbb{R}^2$, and $C^{k,\alpha}(\mathbb{R}^2)$ denotes higher order Hölder spaces for $k = 1, 2, \ldots$. For an open set $\Omega \subseteq \mathbb{R}^2$, by $C_c^\infty(\Omega)$, we denote the space of all compactly supported infinitely differentiable function with the support in Ω, while $\mathcal{D}'(\Omega)$ is the space of distributions on Ω, i.e. the dual space of $C_c^\infty(\Omega)$. For a function $f \in L^1_{\mathrm{loc}}(\Omega)$, unless specified otherwise, the inequality $f \geq 0$ in Ω is always understood in the distributional sense, i.e. that $\int_{\mathbb{R}^2} f(x)\varphi(x)dx \geq 0$ for all $0 \leq \varphi \in C_c^\infty(\Omega)$. We similarly define $f \leq 0$. When we want to emphasize a *pointwise* (in)equality, we always write explicitly $f(x)$.

2. Model and main results

TF energy for massless relativistic fermions in a free-standing graphene layer in the presence of the external electrostatic potential V takes the following form, after a suitable non-dimensionalization [11]:

$$\mathcal{E}_0^{TF}(\rho) = \frac{2}{3}\int_{\mathbb{R}^2} |\rho|^{3/2}\,\mathrm{d}^2x - \int_{\mathbb{R}^2} \rho(x)V(x)\,\mathrm{d}^2x + \frac{1}{4\pi}\iint_{\mathbb{R}^2\times\mathbb{R}^2} \frac{\rho(x)\rho(y)}{|x-y|}\,\mathrm{d}^2x\,\mathrm{d}^2y. \qquad (2.1)$$

Here, $\rho : \mathbb{R}^2 \to \mathbb{R}$ is the *charge density* of charge carrying fermionic quasi-particles (electrons and holes). The density ρ is a sign-changing function with $\rho > 0$ corresponding to electrons and $\rho < 0$ to holes. The first, *TF term*, is an approximation of the kinetic energy of the uniform gas of non-interacting particles. The exponent 3/2 can be deduced from scaling considerations. The last, non-local *Coulomb term*

$$\mathcal{D}(\rho, \rho) := \frac{1}{4\pi} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} \frac{\rho(x)\rho(y)}{|x-y|} \, d^2x \, d^2y, \tag{2.2}$$

is the like-charged inter-particle repulsion energy which is inherited from $\mathbb{R}^3$. The middle term is the *potential energy* due to the interaction with the *external potential* $V : \mathbb{R}^2 \to \mathbb{R}$. In the case of a *single* external point charge of magnitude $Z \in \mathbb{R}$ located in $\mathbb{R}^3$ at distance $d \geq 0$ away from the graphene layer the external potential is

$$V_{Z,d}(x) := \frac{Z}{2\pi \sqrt{d^2 + |x|^2}}, \tag{2.3}$$

but more general potentials $V(x)$ could be considered, e.g. those involving multiple point charge configurations,

$$V_N(x) := \sum_{i=1}^{N} V_{Z_i, d_i}(x - x_i), \tag{2.4}$$

for some $Z_i \in \mathbb{R}$, $d_i \geq 0$ and $x_i \in \mathbb{R}^2$. Importantly, for an unscreened system of uncompensated external charges (i.e. when $\sum_i Z_i \neq 0$ in (2.4)), one has $V_N(x) \sim 1/|x|$ as $|x| \to \infty$, since the quasi-particle–charge interaction is according to Coulomb's Law in $\mathbb{R}^3$. For a more detailed discussion of various terms in the energy and the non-dimensionalization, see [14, section 2]. Note that the energy in (2.1) is invariant with respect to the transformation

$$\rho \to -\rho \quad \text{and} \quad V \to -V, \tag{2.5}$$

hence when dealing with the potential $V_{Z,d}$ it is sufficient to restrict attention to the case $Z > 0$.

Our principal goal is to prove the existence of global minimizers of $\mathcal{E}_0^{TF}$ and establish their fundamental properties, such as regularity and decay estimates. At first glance, the TF energy $\mathcal{E}_0^{TF}$ looks similar to its classical three-dimensional atomic counterpart [16,21,22]. However, there are fundamental differences within the variational framework for graphene modelling

— Unlike in the classical TF theory for atoms and molecules where $\rho \geq 0$, the density ρ in graphene is a sign-changing function. As a consequence, $\mathcal{D}(|\rho|, |\rho|) \geq \mathcal{D}(\rho, \rho)$, which means that oscillating profiles could be energetically more favourable.

— All three terms in $\mathcal{E}_0^{TF}$ with $V = V_{Z,0}$ scale at the same rate under the charge-preserving rescaling $\rho_\lambda(x) = \lambda^2 \rho(\lambda x)$. Hence, $\mathcal{E}_0^{TF}(\rho_\lambda) = c\lambda$ when $d = 0$ for some $c \in \mathbb{R}$. Physically, this is a manifestation of the non-perturbative role of the Coulomb interaction in graphene. Mathematically, this reveals the critical tuning of the three different terms in the energy.

— The non-local term $\mathcal{D}(\rho, \rho)$ is formally identical to the usual Coulomb term in $\mathbb{R}^3$. However, the integral kernel $|x-y|^{-1}$ in $\mathbb{R}^2$ is associated with the Green function of the fractional Laplacian operator $(-\Delta)^{1/2}$. As a consequence, the Euler–Lagrange equation for $\mathcal{E}_0^{TF}$ transforms into a fractional semilinear partial differential equation (PDE) involving $(-\Delta)^{1/2}$, instead of the usual Laplace operator $-\Delta$ of the classical three-dimensional TF theory.

Note that the total number of electrons and holes in the graphene sheet is neither fixed nor bounded *a priori*. As a consequence, unlike in the atomic and molecular three-dimensional models, it is unclear if the minimizers of $\mathcal{E}_0^{TF}$ should have a finite total charge, i.e. if they are L^1-functions. This implies that regular distributions should be included as admissible densities. Indeed, even if the density ρ is a sign-changing continuous function, it is not *a priori* clear if ρ can be interpreted as a charge density in the sense of potential theory (i.e. whether $d\mu = \rho\, dx$ can be associated with a signed measure μ on $\mathbb{R}^2$, making the Coulomb energy $\mathcal{D}(\rho, \rho)$ meaningful in the sense of the Lebesgue integration, see [14, example 4.1] and further references therein. This makes the analysis of the minimizers of $\mathcal{E}_0^{TF}$ mathematically challenging.

We avoid these issues by identifying the Coulomb term $\mathcal{D}(\rho,\rho)$ with one-half of the square of the $\mathring{H}^{-1/2}(\mathbb{R}^2)$ norm of ρ. The energy we consider is then

$$\mathcal{E}_0(\rho) := \frac{2}{3}\int_{\mathbb{R}^2} |\rho|^{3/2}\,\mathrm{d}^2x - \langle \rho, V\rangle + \frac{1}{2}||\rho||^2_{\mathring{H}^{-1/2}(\mathbb{R}^2)}, \tag{2.6}$$

where $\langle\cdot,\cdot\rangle$ is a duality pairing between the function $V \in L^1_{\mathrm{loc}}(\mathbb{R}^2)$ and the linear functional generated by ρ, to be specified shortly. Sometimes, we also write $\mathcal{E}_0^V$ to emphasize the dependence on V. It is easy to see that the definition of $\mathcal{E}_0$ in (2.6) agrees with that of $\mathcal{E}_0^{TF}$ when $\rho \in C_c^\infty(\mathbb{R}^2)$ and $\langle \rho, V\rangle = \int_{\mathbb{R}^2} V\rho\,\mathrm{d}^2x$.

The natural domain of definition of $\mathcal{E}_0$ is the class

$$\mathcal{H}_0 := \mathring{H}^{-1/2}(\mathbb{R}^2) \cap L^{3/2}(\mathbb{R}^2). \tag{2.7}$$

Clearly, $\mathcal{H}_0$ is a Banach space with the norm $||\cdot||_{\mathcal{H}_0} = ||\cdot||_{L^{3/2}(\mathbb{R}^2)} + ||\cdot||_{\mathring{H}^{-1/2}(\mathbb{R}^2)}$. Its dual space $\mathcal{H}_0'$ can be identified with the Banach space $\mathring{H}^{1/2}(\mathbb{R}^2) + L^3(\mathbb{R}^2)$.[1] Therefore, one may define $\langle\cdot,\cdot\rangle$ as the duality pairing between $\mathcal{H}_0'$ and $\mathcal{H}_0$. More precisely, for every $\rho \in \mathcal{H}_0$ and every $V = V_1 + V_2$, where $V_1 \in \mathring{H}^{1/2}(\mathbb{R}^2)$ and $V_2 \in L^3(\mathbb{R}^2)$, we may define

$$\langle \rho, V\rangle := {}_{\mathring{H}^{-1/2}(\mathbb{R}^2)}\langle \rho, V_1\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} + \int_{\mathbb{R}^2} \rho(x)V_2(x)\,\mathrm{d}^2x. \tag{2.8}$$

See §3 for further details and precise definitions.

Our first result establishes the existence of a unique minimizer for $\mathcal{E}_0$.

Theorem 2.1. *For every $V \in \mathring{H}^{1/2}(\mathbb{R}^2) + L^3(\mathbb{R}^2)$, there exists a unique minimizer $\rho_V \in \mathcal{H}_0$ such that $\mathcal{E}_0(\rho_V) = \inf_{\rho\in\mathcal{H}_0}\mathcal{E}_0(\rho)$. The minimizer ρ_V satisfies the Euler–Lagrange equation*

$$\int_{\mathbb{R}^2} \mathrm{sgn}(\rho_V)|\rho_V|^{1/2}\varphi\,\mathrm{d}^2x - \langle \varphi, V\rangle + \langle \rho_V, \varphi\rangle_{\mathring{H}^{-1/2}(\mathbb{R}^2)} = 0, \quad \forall \varphi \in \mathcal{H}_0. \tag{2.9}$$

Furthermore,

(i) if $(-\Delta)^{1/2}V \geq 0$ then $\rho_V \geq 0$,
(ii) if $V \in \mathring{H}^{1/2}(\mathbb{R}^2) \cap C^\alpha(\mathbb{R}^2)$ for some $\alpha \in (0,1]$ then $\rho_V \in \mathcal{H}_0 \cap C^\alpha(\mathbb{R}^2)$ and $\rho_V(x) \to 0$ as $|x| \to \infty$.

Note that the statements of this theorem, including the ones about the positivity and Hölder continuity of the minimizer apply to $V = V_{Z,d}$ for all $Z > 0$ and $d > 0$. The positivity of the minimizer follows from the well-known formula

$$(-\Delta)^{1/2}V_{Z,d}(x) = -\frac{\mathrm{d}}{\mathrm{d}t}V_{Z,t+d}(x)\bigg|_{t=0} = \frac{Zd}{2\pi(d^2+|x|^2)^{3/2}} \quad x \in \mathbb{R}^2, \tag{2.10}$$

that is obtained from the interpretation of the half-Laplacian in $\mathbb{R}^2$ via harmonic extension to $\mathbb{R}^2 \times (0,\infty)$ (see also the direct calculations in [23, p. 258 and (6.5)]). From this formula, it also follows that $V = V_{Z,d} \in \mathring{H}^{1/2}(\mathbb{R}^2)$ for all $Z > 0$ and $d > 0$, due to the fact that $(-\Delta)^{1/2}V_{Z,d} \in L^{4/3}(\mathbb{R}^2) \subset \mathring{H}^{-1/2}(\mathbb{R}^2)$ in this case.

[1] Recall that

$$\mathring{H}^{1/2}(\mathbb{R}^2) + L^3(\mathbb{R}^2) = \{f \in L^1_{\mathrm{loc}}(\mathbb{R}^2) : f = f_1 + f_2,\ f_1 \in \mathring{H}^{1/2}(\mathbb{R}^2), f_2 \in L^3(\mathbb{R}^2)\}$$

is a Banach space with the norm $||f||_{\mathring{H}^{1/2}(\mathbb{R}^2)+L^3(\mathbb{R}^2)} := \inf(||f_1||_{\mathring{H}^{1/2}(\mathbb{R}^2)} + ||f_2||_{L^3(\mathbb{R}^2)})$, where the infimum is taken over all admissible pairs (f_1, f_2).

If e.g. $\rho_V \in L^{4/3}(\mathbb{R}^2)$, then (2.9) implies that

$$\mathrm{sgn}(\rho_V(x))|\rho_V(x)|^{1/2} - V(x) + \frac{1}{2\pi}\int_{\mathbb{R}^2} \frac{\rho_V(y)}{|x-y|}\,\mathrm{d}^2y = 0 \quad \text{for a.e. } x \in \mathbb{R}^2. \tag{2.11}$$

However, (2.11) is not valid for a general $V \in \mathcal{H}_0$, since the non-local term may not be well defined as the Lebesgue integral. Nevertheless, we show that for any $V \in \mathring{H}^{1/2}(\mathbb{R}^2)$ the Euler–Lagrange equation (2.9) is equivalent to the fractional semilinear PDE

$$(-\Delta)^{1/2}u + |u|u = (-\Delta)^{1/2}V \quad \text{in } \mathring{H}^{1/2}(\mathbb{R}^2), \tag{2.12}$$

and

$$u_V := \mathrm{sgn}(\rho_V)|\rho_V|^{1/2} \in \mathring{H}^{1/2}(\mathbb{R}^2) \tag{2.13}$$

is the unique solution of (2.12). We further show that (2.12) satisfies suitable weak maximum and comparison principles. This allows us to employ barrier techniques to study the decay of the solution u_V. With the aid of explicit log-barrier functions constructed in §4d, we establish the main result of this work.

Theorem 2.2. *Let $Z > 0$, $d > 0$ and let $V_{Z,d}$ be defined in (2.3). Then the minimizer $\rho_{V_{Z,d}} \in \mathcal{H}_0$ of $\mathcal{E}_0$ with $V = V_{Z,d}$ is Hölder continuous, radially symmetric non-increasing and satisfies*

$$0 < \rho_{V_{Z,d}}(x) \le V_{Z,d}(x) \quad \textit{for all } x \in \mathbb{R}^2 \tag{2.14}$$

and

$$\rho_{V_{Z,d}}(x) \simeq \frac{1}{|x|^2\log^2|x|} \quad \textit{as } |x| \to \infty. \tag{2.15}$$

In particular, $\rho_{V_{Z,d}} \in L^1(\mathbb{R}^2)$ and $||\rho_{V_{Z,d}}||_{L^1(\mathbb{R}^2)} = Z$.

Note that the asymptotic decay rate in (2.15) is *universal*, i.e. it does not depend on either the value of the charge Z or d for large $|x|$. Such 'universality of decay' is well known in the standard atomic TF theory, going back to Sommerfeld [24], cf. [25, section 5] for a discussion. In TF theory for graphene, a similar universality was observed by Katsnelson [11] (see also [17]).

Remark 2.3. The order of the estimate in (2.15) remains valid for a more general class of external potentials V with sufficiently fast decay at infinity, see proposition 4.10. The significance of the log-decay becomes clear if we note that $p = 2$ plays a role of the Serrin's critical exponent [26, (1.7)] for the equation

$$(-\Delta)^{1/2}u + |u|^{p-1}u = f \quad \text{in } \mathring{H}^{1/2}(\mathbb{R}^2), \tag{2.16}$$

with $p > 1$ and (for simplicity) non-negative $f \in C_c^\infty(\mathbb{R}^2)$. If $p > 2$, the linear part in (2.16) dominates, and solutions must decay as the Green function of $(-\Delta)^{1/2}$, i.e. $|x|^{-1}$. For $3/2 < p < 2$, the nonlinear part in (2.16) dominates, and the solutions should have 'nonlinear' decay rate $|x|^{-1/(p-1)}$. In the Serrin's critical regime $p = 2$, the linear and nonlinear parts balance each other, which leads to the log-correction in the decay asymptotics, correctly captured by Katsnelson [11]. Such log-correction is well known for the local Laplacian $-\Delta$ [27, theorem 3.1]. We are not aware of similar results in the fractional Laplacian case.

Remark 2.4. If $d = 0$ then $V_{Z,0}(x) = Z/(2\pi|x|) \notin (\mathring{H}^{1/2}(\mathbb{R}^2) + L^3(\mathbb{R}^2))$ and $\mathcal{E}_0$ with $V = V_{Z,0}$ is unbounded below, for any $Z \neq 0$. In fact, by scaling, $V_{Z,d}(x) = d^{-1}V_{Z,1}(x/d)$ and $\rho_{V_{Z,d}}(x) = d^{-2}\rho_{V_{Z,1}}(x/d)$. Then

$$\mathcal{E}_0^{V_{Z,d}}(\rho_{V_{Z,d}}) = d^{-1}\mathcal{E}_0^{V_{Z,1}}(\rho_{V_{Z,1}}) \to -\infty, \tag{2.17}$$

as $d \to 0$. Note also that by scaling, $||\rho_{V_{Z,d}}||_{L^1(\mathbb{R}^2)} = ||\rho_{V_{Z,1}}||_{L^1(\mathbb{R}^2)}$.

Remark 2.5. Observe that by (2.10), we have $(-\Delta)^{1/2}V_{Z,d} \to Z\delta_0$ in $\mathcal{D}'(\mathbb{R}^2)$ as $d \to 0$, so in the case $V = V_{Z,0}$ equation (2.12) formally becomes

$$(-\Delta)^{1/2}u + u^2 = Z\delta_0 \quad \text{in } \mathcal{D}'(\mathbb{R}^2). \tag{2.18}$$

Such an equation has no positive distributional solutions, see [26, theorem 4.2].

Lastly, as a corollary to theorem 2.2, we have the following result that is relevant to the experiments on ion cluster screening in single graphene sheets [19]. This result is a direct consequence of the universal decay estimate in (2.15) and the comparison principle for (2.12).

Corollary 2.6. *Let $N \geq 2$ be an integer, let $x_i \in \mathbb{R}^2$ and let $Z_i > 0$ and $d_i > 0$ for all $i = 1, \dots, N$. Then the minimizer $\rho_{V_N} \in \mathcal{H}_0$ of $\mathcal{E}_0$ with $V = V_N$, where V_N is given by (2.4), satisfies the conclusions of theorem 2.2.*

In physical terms, this result implies that a cluster of out-of-plane charges of the same sign exhibits the same universal decay at infinity of the induced charge density in a graphene layer as a single point charge and is independent of the charge magnitude. Therefore, surprisingly, measuring the behaviour of the induced charge density far from the cluster does not provide any information about the cluster itself.

3. Variational setting at the neutrality point

(a) Space $\mathring{H}^{1/2}(\mathbb{R}^2)$

Recall that the homogeneous Sobolev space $\mathring{H}^{1/2}(\mathbb{R}^2)$ can be defined as the completion of $C_c^\infty(\mathbb{R}^2)$ with respect to the Gagliardo norm

$$||u||^2_{\mathring{H}^{1/2}(\mathbb{R}^2)} := \frac{1}{4\pi}\iint_{\mathbb{R}^2\times\mathbb{R}^2} \frac{|u(x)-u(y)|^2}{|x-y|^3}\, d^2x\, d^2y. \tag{3.1}$$

By the fractional Sobolev inequality [28, theorem 8.4], [29, theorem 6.5],

$$||u||^2_{\mathring{H}^{1/2}(\mathbb{R}^2)} \geq \sqrt{\pi}\, ||u||^2_{L^4(\mathbb{R}^2)}, \qquad \forall\, u \in C_c^\infty(\mathbb{R}^2). \tag{3.2}$$

In particular, the space $\mathring{H}^{1/2}(\mathbb{R}^2)$ is a well-defined space of functions and

$$\mathring{H}^{1/2}(\mathbb{R}^2) \subset L^4(\mathbb{R}^2). \tag{3.3}$$

The space $\mathring{H}^{1/2}(\mathbb{R}^2)$ is also a Hilbert space, with the scalar product associated with (3.1) given by

$$\langle u, v\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} := \frac{1}{4\pi}\iint_{\mathbb{R}^2\times\mathbb{R}^2} \frac{(u(x)-u(y))(v(x)-v(y))}{|x-y|^3}\, d^2x\, d^2y. \tag{3.4}$$

Recall (cf. [30]) that if $u \in \mathring{H}^{1/2}(\mathbb{R}^2)$ then $u^+, u^- \in \mathring{H}^{1/2}(\mathbb{R}^2)$ and $||u^\pm||_{\mathring{H}^{1/2}(\mathbb{R}^2)} \leq ||u||_{\mathring{H}^{1/2}(\mathbb{R}^2)}$. Moreover, $\langle u^+, u^-\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} \leq 0$.

The dual space to $\mathring{H}^{1/2}(\mathbb{R}^2)$ is denoted $\mathring{H}^{-1/2}(\mathbb{R}^2)$. According to the Riesz representation theorem, for every $F \in \mathring{H}^{-1/2}(\mathbb{R}^2)$, there exists a uniquely defined *potential* $U_F \in \mathring{H}^{1/2}(\mathbb{R}^2)$ such that

$$\langle U_F, \varphi\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} = \langle F, \varphi\rangle \quad \forall\, \varphi \in \mathring{H}^{1/2}(\mathbb{R}^2), \tag{3.5}$$

where $\langle F, \cdot\rangle : \mathring{H}^{1/2}(\mathbb{R}^2) \to \mathbb{R}$ denotes the bounded linear functional generated by F, $\langle \cdot, \cdot\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)}$ is the inner product in $\mathring{H}^{1/2}(\mathbb{R}^2)$, and $\langle \cdot, \cdot\rangle_{\mathring{H}^{-1/2}(\mathbb{R}^2)}$ will be similarly defined as the inner product in

$\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)$. Moreover,

$$||U_F||_{\overset{\circ}{H}{}^{1/2}(\mathbb{R}^2)} = ||F||_{\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)}, \tag{3.6}$$

so the duality (3.5) is an isometry.

The potential $U_F \in \overset{\circ}{H}{}^{1/2}(\mathbb{R}^2)$ satisfying (3.5) is interpreted as the *weak solution* of the linear equation

$$(-\Delta)^{1/2} U_F = F \quad \text{in } \mathbb{R}^2, \tag{3.7}$$

and we recall that for functions $u \in C_c^\infty(\mathbb{R}^2)$, the fractional Laplacian $(-\Delta)^{1/2}$ can be defined as

$$(-\Delta)^{1/2} u(x) = \frac{1}{4\pi} \int_{\mathbb{R}^2} \frac{2u(x) - u(x+y) - u(x-y)}{|y|^3} \, \mathrm{d}^2 y \quad (x \in \mathbb{R}^2), \tag{3.8}$$

cf. [29, proposition 3.3].

(b) Regular distributions in $\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)$ and potentials

Recall that $\rho \in \overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2) \cap L^1_{\mathrm{loc}}(\mathbb{R}^2)$ means that ρ is a *regular distribution* in $\mathcal{D}'(\mathbb{R}^2)$, i.e.

$$\langle \rho, \varphi \rangle := \int_{\mathbb{R}^2} \rho(x) \varphi(x) \, \mathrm{d}^2 x \quad \forall \varphi \in C_c^\infty(\mathbb{R}^2), \tag{3.9}$$

and $\langle \rho, \varphi \rangle$ is bounded by a multiple of $||\varphi||_{\overset{\circ}{H}{}^{1/2}(\mathbb{R}^2)}$. Then $\langle \rho, \cdot \rangle$ is understood as the unique continuous extension of (3.9) to $\overset{\circ}{H}{}^{1/2}(\mathbb{R}^2)$. Caution, however, is needed as not every regular distribution $\rho \in \overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2) \cap L^1_{\mathrm{loc}}(\mathbb{R}^2)$ admits an integral representation (3.9) on all of $\overset{\circ}{H}{}^{1/2}(\mathbb{R}^2)$. In other words, $\rho \in \overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2) \cap L^1_{\mathrm{loc}}(\mathbb{R}^2)$ does not necessarily imply that $\rho w \in L^1(\mathbb{R}^2)$ for every $w \in \overset{\circ}{H}{}^{1/2}(\mathbb{R}^2)$. Examples of this type go back to H. Cartan (cf. [31,32], or [14, remark 5.1] for an example from $\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2) \cap C^\infty(\mathbb{R}^2)$ and further references). As a consequence, the Coulomb energy term in $\mathcal{E}^{TF}$ may not be defined in the sense of Lebesgue's integration for all $\rho \in \mathcal{H}_0$ and should be interpreted *in the distributional sense*, i.e. in the definition of $\mathcal{E}_0^{TF}$ one should replace $\mathcal{D}(\rho, \rho)$ with $||\rho||^2_{\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)}$. Recall, however, that every non-negative distribution is a measure [28, theorem 6.22].

An alternative reinterpretation of $\mathcal{D}(\rho, \rho)$ can be given in terms of potentials. Given $\rho \in \overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2) \cap L^1_{\mathrm{loc}}(\mathbb{R}^2)$, let $U_\rho \in \overset{\circ}{H}{}^{1/2}(\mathbb{R}^2)$ be the uniquely defined potential of ρ, defined as in (3.9) by Riesz's representation theorem. If $\rho \in L^1(\mathbb{R}^2, (1+|x|)^{-1} \, \mathrm{d}^2 x)$ then the potential U_ρ could be identified with the Riesz potential of the function ρ, so that

$$U_\rho(x) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \frac{\rho(y)}{|x-y|} \, \mathrm{d}^2 y \quad \text{a.e. in } \mathbb{R}^2 \tag{3.10}$$

(see [31, (1.3.10)]). Furthermore, according to the Hardy–Littlewood–Sobolev (HLS) inequality (cf. [33, section 5.1, theorem 1]), if $\rho \in L^s(\mathbb{R}^2)$ with $s \in (1,2)$ then $U_\rho \in L^t(\mathbb{R}^2)$ with $1/t = (1/s) - (1/2)$, and

$$||U_\rho||_{L^t(\mathbb{R}^2)} \leq C ||\rho||_{L^s(\mathbb{R}^2)}. \tag{3.11}$$

Even if (3.10) is valid, $\rho U_\rho \notin L^1(\mathbb{R}^2)$ in general. However, if $\varphi \in \overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2) \cap L^{4/3}(\mathbb{R}^2)$, then $\varphi U_\rho \in L^1(\mathbb{R}^2)$ by the HLS inequality and

$$\frac{1}{2\pi} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} \frac{\rho(x)\varphi(y)}{|x-y|} \, \mathrm{d}^2 x \, \mathrm{d}^2 y = \int_{\mathbb{R}^2} U_\rho(x) \varphi(x) \, \mathrm{d}^2 x = \langle U_\rho, U_\varphi \rangle_{\overset{\circ}{H}{}^{1/2}(\mathbb{R}^2)} = \langle \rho, \varphi \rangle_{\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)}. \tag{3.12}$$

In particular,

$$\mathcal{D}(\rho, \rho) = \int_{\mathbb{R}^2} U_\rho(x) \rho(x) \, \mathrm{d}^2 x = ||U_\rho||^2_{\overset{\circ}{H}{}^{1/2}(\mathbb{R}^2)} = ||\rho||^2_{\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)}, \tag{3.13}$$

which means that $L^{4/3}(\mathbb{R}^2) \subset \overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)$ and the Coulomb energy is well defined on $L^{4/3}(\mathbb{R}^2)$ in the sense of Lebesgue's integration.

(c) Existence, uniqueness and regularity of the minimizers

Consider the unconstrained minimization problem

$$E_0 := \inf_{\rho \in \mathcal{H}_0} \mathcal{E}_0(\rho). \tag{3.14}$$

It is easy to prove the following.

Proposition 3.1 (Existence). *For every $V \in \overset{\circ}{H}{}^{1/2}(\mathbb{R}^2) + L^3(\mathbb{R}^2)$, the TF-energy $\mathcal{E}_0$ admits a unique minimizer $\rho_V \in \mathcal{H}_0$ such that $\mathcal{E}_0(\rho_V) = E_0$. The minimizer ρ_V satisfies the Euler–Lagrange equation*

$$\int_{\mathbb{R}^2} \operatorname{sgn}(\rho_V)|\rho_V|^{1/2}\varphi \, \mathrm{d}^2x - \langle \varphi, V\rangle + \langle \rho_V, \varphi\rangle_{\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)} = 0 \quad \forall \varphi \in \mathcal{H}_0. \tag{3.15}$$

Proof. It is standard to conclude from $V \in \overset{\circ}{H}{}^{1/2}(\mathbb{R}^2) + L^3(\mathbb{R}^2)$ that $\mathcal{E}_0$ is bounded below on $\mathcal{H}_0$, i.e. that $E_0 > -\infty$.

Consider a minimizing sequence $(\rho_n) \subset \mathcal{H}_0$. Clearly,

$$\sup_n ||\rho_n||_{L^{3/2}(\mathbb{R}^2)} \le C \quad \text{and} \quad \sup_n ||\rho_n||_{\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)} \le C. \tag{3.16}$$

Using weak-$*$ compactness of the closed unit ball in $\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)$, we may extract a subsequence, still denoted by (ρ_n), such that

$$\rho_n \rightharpoonup \rho_V \quad \text{in } L^{3/2}(\mathbb{R}^2) \tag{3.17}$$

and

$$\rho_n \overset{*}{\rightharpoonup} F \quad \text{in } \overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2), \tag{3.18}$$

for some $\rho_V \in L^{3/2}(\mathbb{R}^2)$ and $F \in \overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)$. By the definition, (3.17) and (3.18) mean that

$$\int_{\mathbb{R}^2} \rho_n(x)\varphi(x) \, \mathrm{d}^2x \to \int_{\mathbb{R}^2} \rho_V(x)\varphi(x) \, \mathrm{d}^2x \quad \forall \varphi \in L^3(\mathbb{R}^2) \tag{3.19}$$

and

$$\langle \rho_n, \varphi\rangle = \int_{\mathbb{R}^2} \rho_n(x)\varphi(x) \, \mathrm{d}^2x \to \langle F, \varphi\rangle \quad \forall \varphi \in \overset{\circ}{H}{}^{1/2}(\mathbb{R}^2). \tag{3.20}$$

Therefore, passing to the limit, we obtain

$$\int_{\mathbb{R}^2} \rho_V(x)\varphi(x) \, \mathrm{d}^2x = \langle F, \varphi\rangle \quad \forall \varphi \in L^3(\mathbb{R}^2) \cap \overset{\circ}{H}{}^{1/2}(\mathbb{R}^2). \tag{3.21}$$

In particular, $\rho_V \in \overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)$ defines a regular distribution in $\mathcal{D}'(\mathbb{R}^2)$ and we may identify $F = \rho_V$. This implies that

$$\mathcal{E}_0(\rho_V) \le \liminf_{n\to\infty} \mathcal{E}_0(\rho_n) = E_0, \tag{3.22}$$

which follows from the weak lower semicontinuity of the $|| \cdot ||_{L^{3/2}(\mathbb{R}^2)}$ and $|| \cdot ||_{\overset{\circ}{H}{}^{-1/2}(\mathbb{R}^2)}$ norms, and the weak continuity of the linear functionals $\langle \cdot, V\rangle$ on $\mathcal{H}_0$.

The uniqueness of the minimizer $\rho_V \in \mathcal{H}_0$ is a consequence of the strict convexity of the energy $\mathcal{E}_0$, which is the sum of the strictly convex kinetic energy, linear external potential energy and positive definite quadratic Coulomb energy.

The derivation of the Euler–Lagrange equation (3.15) is standard, we omit the details. ∎

Remark 3.2. As was already mentioned, if $\rho_V \in \mathcal{H}_0 \cap L^{4/3}(\mathbb{R}^2)$ then (3.15) can be interpreted pointwise as the integral equation (2.11). However, in general, the Euler–Lagrange equation (3.15) for $\mathcal{E}_0$ should be interpreted as

$$\operatorname{sgn}(\rho_V)|\rho_V(x)|^{1/2} + U_{\rho_V} = V \quad \text{in } \mathcal{D}'(\mathbb{R}^2), \tag{3.23}$$

where $U_{\rho_V} \in \mathring{H}^{1/2}(\mathbb{R}^2)$ is the potential of ρ_V defined via (3.5). In particular, if $\rho_V \geq 0$ then $U_{\rho_V} \geq 0$ (see [34, theorem 3.14]) which implies $V \geq 0$ and

$$0 \leq \rho_V \leq V^2 \quad \text{in } \mathcal{D}'(\mathbb{R}^2). \tag{3.24}$$

Remark 3.3. The mapping $V \mapsto \rho_V$ is a bijection between $\mathcal{H}_0' = \mathring{H}^{1/2}(\mathbb{R}^2) + L^3(\mathbb{R}^2)$ and $\mathcal{H}_0$. Indeed, the uniqueness of the minimizer implies that ρ_V is injective. Further, it is clear that for any $\rho \in \mathcal{H}_0$,

$$V := U_\rho + \operatorname{sgn}(\rho)|\rho(x)|^{1/2} \in \mathring{H}^{1/2}(\mathbb{R}^2) + L^3(\mathbb{R}^2), \tag{3.25}$$

which means that the mapping ρ_V is also surjective. In particular, this shows that non-regular *at infinity* distributions in $\mathring{H}^{-1/2}(\mathbb{R}^2)$ could occur among the minimizers. Simply choose a regular distribution $\rho \in \mathcal{H}_0$ such that $\rho\varphi \notin L^1(\mathbb{R}^2)$ for some $\varphi \in \mathring{H}^{1/2}(\mathbb{R}^2)$ (e.g. [14, example 4.1.] for an explicit example) and generate the corresponding potential V via (3.25).

While for a generic $V \in \mathring{H}^{1/2}(\mathbb{R}^2) + L^3(\mathbb{R}^2)$, the information $\rho_V \in \mathcal{H}_0$ is optimal, under additional restrictions on the potential V, the regularity of the minimizer can be improved up to the regularity of V.

Lemma 3.4 (Hölder regularity). *Assume that $V \in \mathring{H}^{1/2}(\mathbb{R}^2) \cap C^\alpha(\mathbb{R}^2)$ for some $\alpha \in (0,1]$. Then the minimizer $\rho_V \in \mathcal{H}_0$ additionally satisfies $\rho_V \in \mathcal{H}_0 \cap C^\alpha(\mathbb{R}^2)$, and $\rho_V(x) \to 0$ as $|x| \to \infty$. Furthermore, the potential U_ρ could be identified with the Riesz potential of ρ as in (3.10) and $U_{\rho_V} \in C^{1/3}(\mathbb{R}^2)$.*

Proof. According to (3.23), the minimizer $\rho_V \in \mathcal{H}_0$ satisfies

$$\operatorname{sgn}(\rho_V)|\rho_V|^{1/2} = V - U_{\rho_V} \quad \text{in } \mathcal{D}'(\mathbb{R}^2). \tag{3.26}$$

Since $\rho_V \in \mathcal{H}_0 \subset L^{3/2}(\mathbb{R}^2)$, by the HLS-inequality (3.11) with $s = 3/2$, we have

$$U_{\rho_V} \in L^6(\mathbb{R}^2), \tag{3.27}$$

and in particular, the potential U_ρ could be identified with the Riesz potential of ρ as in (3.10).

Also, by the Sobolev inequality (3.2),

$$V \in \mathring{H}^{1/2}(\mathbb{R}^2) \cap C^\alpha(\mathbb{R}^2) \subset L^4(\mathbb{R}^2) \cap C^\alpha(\mathbb{R}^2). \tag{3.28}$$

This implies

$$V^2 \in L^2(\mathbb{R}^2) \cap C^\alpha(\mathbb{R}^2). \tag{3.29}$$

In particular, both V and V^2 are bounded and decay to zero as $|x| \to \infty$. Note also that $U_{\rho_V}^2 \in L^3(\mathbb{R}^2)$. Hence,

$$|\rho_V| = (V - U_{\rho_V})^2 = V^2 - 2VU_{\rho_V} + U_{\rho_V}^2 \in L^{3/2}(\mathbb{R}^2) \cap L^3(\mathbb{R}^2). \tag{3.30}$$

Furthermore, by Hölder estimates on Riesz potentials, we conclude that $U_{\rho_V} \in C^{1/3}(\mathbb{R}^2)$, see [14, lemma 4.1] or [34, theorem 2]. Then,

$$|\rho_V| = (V - U_{\rho_V})^2 \in C^\beta(\mathbb{R}^2), \tag{3.31}$$

where $\beta = \min\{\alpha, 1/3\}$ and $\rho_V(x) \to 0$ as $|x| \to \infty$. If $\alpha \leq 1/3$, we are done. If $\alpha > 1/3$ then (3.31) implies $U_{\rho_V} \in C^{1,1/3}(\mathbb{R}^2)$, see [35, proposition 2.8]. Therefore, ρ_V has at least the same Hölder regularity as V. ∎

Remark 3.5. Similarly, one can establish higher Hölder regularity of ρ_V assuming higher regularity of V. For instance, using [35, proposition 2.8], we can conclude that if $V \in C^{1,\alpha}(\mathbb{R}^2)$ then $\rho_V \in C^{1,\beta}(\mathbb{R}^2)$, where $\beta = \min\{\alpha, 1/3\}$. However, in general, the Hölder regularity of ρ_V can not be improved beyond the Hölder regularity of V.

4. Positivity and decay

(a) Half-Laplacian representation, positivity and comparison

Let $\rho_V \in \mathcal{H}_0$ be the minimizer of $\mathcal{E}_0$. Introduce the substitution

$$u_V := \operatorname{sgn}(\rho_V)|\rho_V|^{1/2}. \tag{4.1}$$

Then $\rho_V = |u_V|u_V$ and (3.15) transforms into

$$\int_{\mathbb{R}^2} u_V(x)\varphi(x)\,\mathrm{d}^2x - \langle\varphi, V\rangle + \langle U_{|u_V|u_V}, \varphi\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} = 0 \quad \forall\,\varphi \in \mathcal{H}_0. \tag{4.2}$$

Proposition 4.1 (Equivalent fractional PDE). *Let $V \in \mathring{H}^{1/2}(\mathbb{R}^2)$ and u_V be defined by (4.1). Then $u_V \in \mathring{H}^{1/2}(\mathbb{R}^2)$ and is the unique solution of the problem*

$$(-\Delta)^{1/2}u + |u|u = (-\Delta)^{1/2}V \quad \textit{in } \mathring{H}^{1/2}(\mathbb{R}^2). \tag{4.3}$$

Proof. Let $\psi \in C_c^\infty(\mathbb{R}^2)$. Then $(-\Delta)^{1/2}\psi \in C^\infty(\mathbb{R}^2) \cap L^1(\mathbb{R}^2) \subset L^{4/3} \cap L^1(\mathbb{R}^2) \subset \mathcal{H}_0$ [35, section 2.1]. Test (4.2) with $\varphi = (-\Delta)^{1/2}\psi$ and take into account that in view of (3.12),

$$\langle|u_V|u_V, \varphi\rangle_{\mathring{H}^{-1/2}(\mathbb{R}^2)} = \langle U_{|u_V|u_V}, (-\Delta)^{1/2}\psi\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} \tag{4.4}$$

$$= \int_{\mathbb{R}^2} |u_V|u_V(x)\psi(x)\,\mathrm{d}^2x \quad \forall\,\psi \in C_c^\infty(\mathbb{R}^2). \tag{4.5}$$

Then (4.2) yields

$$\int_{\mathbb{R}^2} u_V(-\Delta)^{1/2}\psi\,\mathrm{d}^2x - \langle(-\Delta)^{1/2}\psi, V\rangle + \int_{\mathbb{R}^2} |u_V|u_V(x)\psi(x)\,\mathrm{d}^2x = 0 \quad \forall\,\psi \in C_c^\infty(\mathbb{R}^2), \tag{4.6}$$

or equivalently,

$$(-\Delta)^{1/2}u_V - (-\Delta)^{1/2}V + |u_V|u_V = 0 \quad \text{in } \mathcal{D}'(\mathbb{R}^2), \tag{4.7}$$

where $(-\Delta)^{1/2}V \in \mathring{H}^{-1/2}(\mathbb{R}^2)$, $|u_V|u_V = \rho_V \in \mathring{H}^{-1/2}(\mathbb{R}^2)$. Hence $u_V \in \mathring{H}^{1/2}(\mathbb{R}^2)$, and (4.7) also holds weakly in $\mathring{H}^{1/2}(\mathbb{R}^2)$ by density.

The uniqueness for (4.3) follows from the comparison principle of lemma 4.3 below. ∎

Proposition 4.2 (Positivity). *Let $V \in \mathring{H}^{1/2}(\mathbb{R}^2)$. Assume that $(-\Delta)^{1/2}V \geq 0$ in $\mathbb{R}^2$. Then $u_V \geq 0$ in $\mathbb{R}^2$. If, in addition, $V \neq 0$ then $u_V \neq 0$.*

Proof. Decompose $u_V = u_V^+ - u_V^-$ and recall that $u_V^+, u_V^- \in \mathring{H}^{1/2}(\mathbb{R}^2)$ and $\langle u_V^+, u_V^-\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} \leq 0$. Testing (4.3) by $u_V^- \geq 0$ and taking into account that $u_V|u_V|u_V^- \leq 0$, we obtain

$$0 \leq \langle V, u_V^-\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} = \langle u_V, u_V^-\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} + \int_{\mathbb{R}^2} u_V|u_V|\,u_V^-\,\mathrm{d}^2x \leq -\langle u_V^-, u_V^-\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} \leq 0. \tag{4.8}$$

We conclude that $u_V^- = 0$.

Further, if $V \neq 0$ then $u = 0$ is not a solution of (4.3) and hence $u_V \neq 0$. ∎

Lemma 4.3 (Comparison principle). *Let $V \in \mathring{H}^{1/2}(\mathbb{R}^2)$. Assume that $u, v \in \mathring{H}^{1/2}(\mathbb{R}^2) \cap L^3(\mathbb{R}^2)$ are a super and a subsolution to (4.3) in a smooth domain $\Omega \subseteq \mathbb{R}^2$, respectively, i.e.*

$$(-\Delta)^{1/2}u + u|u| \geq (-\Delta)^{1/2}V \quad \textit{in } \mathcal{D}'(\Omega) \tag{4.9}$$

and

$$(-\Delta)^{1/2}v + v|v| \leq (-\Delta)^{1/2}V \quad \textit{in } \mathcal{D}'(\Omega). \tag{4.10}$$

If $\mathbb{R}^2 \setminus \Omega \neq \varnothing$, we also assume $u \geq v$ in $\mathbb{R}^2 \setminus \bar{\Omega}$. Then $u \geq v$ in $\mathbb{R}^2$.

Proof. Subtracting one inequality from another, we obtain

$$(-\Delta)^{1/2}(v-u)+v|v|-u|u|\leq 0 \quad \text{in } \mathcal{D}'(\Omega). \tag{4.11}$$

Let $H_0^{1/2}(\Omega)$ denotes the completion of $C_c^\infty(\Omega)$ with respect to the Gagliardo's norm $||\cdot||^2_{\mathring{H}^{1/2}(\mathbb{R}^2)}$, defined in (3.1). With this definition, $H_0^{1/2}(\Omega)$ is automatically a closed subspace of $H_0^{1/2}(\mathbb{R}^2)$. By density, (4.11) is also valid in $H_0^{1/2}(\Omega)$, in the sense that

$$\langle v-u,\varphi\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)}+\int_{\mathbb{R}^2}(v|v|-u|u|)\varphi\,\mathrm{d}^2x\leq 0 \quad \forall\, 0\leq\varphi\in H_0^{1/2}(\Omega). \tag{4.12}$$

Note that $(v-u)^+\in\mathring{H}^{1/2}(\mathbb{R}^2)$. If $\mathbb{R}^2\setminus\Omega\neq\varnothing$ then $u\geq v$ in $\mathbb{R}^2\setminus\bar{\Omega}$ and hence $(v-u)^+=0$ in $\mathbb{R}^2\setminus\bar{\Omega}$. This implies $(v-u)^+\in H_0^{1/2}(\Omega)$ (e.g. [36, theorem 10.1.1]). Testing (4.12) by $(v-u)^+$, taking into account $\langle (v-u)^-,(v-u)^+\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)}\leq 0$ and monotone increase of the nonlinearity, we obtain

$$\begin{aligned}0&\geq\langle v-u,(v-u)^+\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)}+\int_{\mathbb{R}^2}(v|v|-u|u|)(v-u)^+\,\mathrm{d}^2x\\&\geq\langle (v-u)^+,(v-u)^+\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)}=||(v-u)^+||^2_{\mathring{H}^{1/2}(\mathbb{R}^2)}.\end{aligned} \tag{4.13}$$

We conclude that $(v-u)^+=0$. ■

The comparison principle immediately implies that (4.3) can have at most one solution in $\mathring{H}^{1/2}(\mathbb{R}^2)$. Hence, the solution u_V constructed from the minimizer ρ_V via (4.1) is the unique solution of (4.3). A consequence of the uniqueness is the following.

Corollary 4.4. *Assume that $V\in\mathring{H}^{1/2}(\mathbb{R}^2)$ and $(-\Delta)^{1/2}V\geq 0$ in $\mathbb{R}^2$. If $(-\Delta)^{1/2}V\in L^{4/3}(\mathbb{R}^2)$ is a radially symmetric non-increasing function, then u_V is also radially symmetric and non-increasing.*

Proof. Note that u_V is the unique global minimizer of the convex energy

$$J_V(u)=\frac{1}{2}||u||^2_{\mathring{H}^{1/2}(\mathbb{R}^2)}+\frac{1}{3}||u||^3_{L^3(\mathbb{R}^2)}-\langle u,V\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)}$$

on $\mathring{H}^{1/2}(\mathbb{R}^2)\cap L^3(\mathbb{R}^2)$. Since $(-\Delta)^{1/2}V\in L^{4/3}(\mathbb{R}^2)$,

$$\langle u_V,V\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)}=\int_{\mathbb{R}^2}u_V(-\Delta)^{1/2}V\,\mathrm{d}^2x,$$

where the latter integral is finite by the HLS inequality. Then the symmetric-decreasing rearrangement u_V^* is also a minimizer of J_V, by [28, theorem 3.4 and lemma 7.17]. Hence, the assertion follows from the uniqueness of the minimizer. ■

Another straightforward, but important consequence of the comparison principle is the following upper bound on u_V.

Corollary 4.5. *Assume that $V\in\mathring{H}^{1/2}(\mathbb{R}^2)$ and $V\geq 0$. Then*

$$u_V\leq V \quad \mathit{in}\,\mathbb{R}^2. \tag{4.14}$$

Proof. We simply note that V is a supersolution to (4.3) in $\mathbb{R}^2$, i.e.

$$(-\Delta)^{1/2}V+V^2\geq(-\Delta)^{1/2}V \quad \text{in } \mathcal{D}'(\mathbb{R}^2). \tag{4.15}$$

Hence, (4.14) follows from the comparison principle in $\mathbb{R}^2$. ■

The comparison principle can be used as an alternative tool to prove the existence of the solution u_V of (4.3), via construction of appropriate sub- and super-solutions. In the next section, we construct an explicit barrier which later will be used to obtain lower and upper solution with matching sharp asymptotics at infinity. This will lead to the sharp decay estimates on u_V and ρ_V.

(b) Super-harmonicity of the potential is essential

We are going to show that the assumptions $(-\Delta)^{1/2}V \geq 0$ is in a certain sense necessary for the positivity of the minimizer ρ_V.

Proposition 4.6. *Let* $V \in \mathring{H}^{1/2}(\mathbb{R}^2) \cap C^\alpha(\mathbb{R}^2)$ *for some* $\alpha \in (0, 1]$. *Assume that* $V \neq 0$ *and*

$$\lim_{|x|\to\infty} |x|V(x) = 0. \tag{4.16}$$

Then ρ_V *changes sign in* $\mathbb{R}^2$.

Remark 4.7. The assumption (4.16) implicitly necessitates that $(-\Delta)^{1/2}V$ cannot be non-negative. Indeed, if $(-\Delta)^{1/2}V \geq 0$ then $\lim_{|x|\to\infty} |x|V(x) > 0$ (cf. (4.18) below), which is incompatible with (4.16).

Proof. According to (3.23) and lemma 3.4, we know that $\rho_V \in \mathcal{H}_0 \cap C^\alpha(\mathbb{R}^2)$, U_ρ could be identified with the Riesz potential of the function ρ as in (3.10), $U_{\rho_V} \in C^{1/3}(\mathbb{R}^2)$, and

$$\mathrm{sign}(\rho_V)|\rho_V|^{1/2}(x) = V(x) - U_{\rho_V}(x) \quad \text{for all } x \in \mathbb{R}^2. \tag{4.17}$$

Assume that $\rho_V \geq 0$ in $\mathbb{R}^2$. Then, for each $x \in \mathbb{R}^2$,

$$U_\rho(x) \geq \frac{1}{2\pi} \int_{B_{2|x|}(x)} \frac{\rho(y)}{|x-y|}\, \mathrm{d}^2y \geq \frac{1}{4\pi|x|} \int_{B_{2|x|}(x)} \rho(y)\, \mathrm{d}^2y. \tag{4.18}$$

In particular,

$$\liminf_{|x|\to\infty} |x|U_{\rho_V}(x) > 0, \tag{4.19}$$

and hence, in view of (4.16),

$$\limsup_{|x|\to\infty} |x|\mathrm{sign}(\rho_V)|\rho_V|^{1/2}(x) = \limsup_{|x|\to\infty} |x|(V(x) - U_{\rho_V}(x)) < 0, \tag{4.20}$$

a contradiction. A symmetric argument shows that $\rho_V \leq 0$ is also impossible. ■

Remark 4.8. For example, we can consider the dipole potential

$$W_Z(x) = \frac{Z}{2\pi(1+|x|^2)^{3/2}}.$$

Note that $W_Z(x) = -(\mathrm{d}/\mathrm{d}t V_{Z,t}(x)|_{t=1}$. While $W_Z > 0$, it is not difficult to see, using the harmonic extension of W_Z, that

$$(-\Delta)^{1/2}W_Z(|x|) = \frac{Z(2-|x|^2)}{2\pi(1+|x|^2)^{5/2}},$$

which is a sign-changing function. Clearly, W_Z satisfies the assumptions of proposition 4.6, so the minimizer ρ_{W_Z} changes sign for any $Z > 0$.

(c) Sign-changing minimizer in Thomas–Fermi–Dirac–von Weizsäcker model

A density functional theory of Thomas–Fermi–Dirac–von Weizsäcker (TFW) type to describe the response of a single layer of graphene to a charge V was developed in [14]. For $\varepsilon > 0$, and in the notation of the present paper, the TFW energy studied in [14] has the form

$$\mathcal{E}_{0,\varepsilon}(\rho) := \varepsilon \| |\rho|^{-1/2}\rho \|^2_{\mathring{H}^{1/2}(\mathbb{R}^2)} + \mathcal{E}_0(\rho) : \mathcal{H}_0 \to \mathbb{R} \cup \{+\infty\}. \tag{4.21}$$

The existence of a minimizer for $\mathcal{E}_{0,\varepsilon}$ with $V \in \mathring{H}^{1/2}(\mathbb{R}^2)$ was established in [14, theorem 3.1]. We are going to show that if $V \geq 0$ satisfies the assumptions of proposition 4.6 then for sufficiently small $\varepsilon > 0$ the TFW energy $\mathcal{E}_{0,\varepsilon}$ *admits a sign-changing minimizer*. This gives a partial answer to one of the questions left open in [14] (see discussions in [14, section 3]).

To show the existence of a sign-changing minimizer for $\mathcal{E}_{0,\varepsilon}$, assume that $V \geq 0$ and the assumptions of proposition 4.6 holds. Then the minimizer ρ_V of $\mathcal{E}_0$ changes sign. Let

$$E_0 := \inf_{\mathcal{H}_0} \mathcal{E}_0 = \mathcal{E}_0(\rho_V).$$

Similarly to proposition 3.1, we can also minimize convex energy $\mathcal{E}_0$ on the weakly closed set $\mathcal{H}_0^+$ of non-negative functions in $\mathcal{H}_0$. Let $\rho_V^+ \in \mathcal{H}_0^+$ be the minimizer of $\mathcal{E}_0$ on $\mathcal{H}_0^+$ and set

$$E_0^+ := \inf_{\mathcal{H}_0^+} \mathcal{E}_0 = \mathcal{E}_0(\rho_V^+).$$

It is clear that $E_0^+ < 0$ and hence $\rho_V^+ \neq 0$ (just take trial functions $0 \leq \varphi \in \mathcal{D}'(\mathbb{R}^2)$ such that $\langle V, \varphi \rangle > 0$). By an adaptation of arguments in [28, theorem 11.13], the minimizer ρ_V^+ satisfies the TF equation

$$(\rho_V^+)^{3/2} = \left(V - U_{\rho_V^+}\right)^+ \quad \text{in } \mathcal{D}'(\mathbb{R}^2). \tag{4.22}$$

Observe that $\operatorname{supp}(\rho_V^+) \neq \mathbb{R}^2$. Indeed, assume that $\rho_V^+ > 0$ in $\mathbb{R}^2$. Then $\rho_V^+ > 0$ satisfies the Euler–Lagrange equation

$$(\rho_V^+)^{3/2} = V - U_{\rho_V^+} \quad \text{in } \mathcal{D}'(\mathbb{R}^2), \tag{4.23}$$

which contradicts to the uniqueness, since (4.23) has a sign-changing solution ρ_V by proposition 4.6. Crucially, by the strict convexity of $\mathcal{E}_0$, we can also conclude that

$$E_0 < E_0^+. \tag{4.24}$$

Next, for $\varepsilon > 0$ consider the TFW energy $\mathcal{E}_{0,\varepsilon}$. Set

$$E_{0,\varepsilon} := \inf_{\mathcal{H}_0} \mathcal{E}_{0,\varepsilon}.$$

The existence of a minimizer for $E_{0,\varepsilon}$ was established in [14, theorem 3.1]. Without loss of a generality, we may assume that ρ_V is regular enough and $|\rho_V|^{-1/2}\rho \in \mathring{H}^{1/2}(\mathbb{R}^2)$ (otherwise we may approximate ρ_V by smooths functions). Then

$$E_{0,\varepsilon} \leq \varepsilon \| |\rho_V|^{-1/2} \rho_V \|^2_{\mathring{H}^{1/2}(\mathbb{R}^2)} + E_0 \to E_0 \quad \text{as } \varepsilon \to 0.$$

Similarly,

$$E_0^+ \leq E_{0,\varepsilon}^+ := \inf_{\mathcal{H}_0^+} \mathcal{E}_{0,\varepsilon}.$$

Taking into account the strict inequality (4.24), for sufficiently small $\varepsilon > 0$, we have

$$E_0 < E_{0,\varepsilon} < E_0^+ \leq E_{0,\varepsilon}^+.$$

In particular, $E_{0,\varepsilon} < E_{0,\varepsilon}^+$ and we conclude that a minimizer for $E_{0,\varepsilon}$ must change sign. For example, a dipole, or any compactly supported non-negative potential should give rise to a sign-changing global minimizer in the TFW model.

(d) Logarithmic barrier

Recall (cf. [23, theorem 1.1]) that for a radial function $u \in C^2(\overline{\mathbb{R}_+})$ such that

$$\int_0^\infty \frac{|u(r)|}{(1+r)^3}\, r\, \mathrm{d}r < \infty, \tag{4.25}$$

the following representation of the fractional Laplacian $(-\Delta)^{1/2}$ in $\mathbb{R}^2$ is valid:

$$(-\Delta)^{1/2} u(r) = \frac{1}{2\pi r} \int_1^\infty \left(u(r) - u(r\tau) + \frac{u(r) - u(r/\tau)}{\tau} \right) \mathcal{K}(\tau)\, \mathrm{d}\tau, \tag{4.26}$$

where

$$\mathcal{K}(\tau) := 2\pi \tau^{-2}\, {}_2F_1\left(\frac{3}{2}, \frac{3}{2}, 1, \tau^{-2}\right), \tag{4.27}$$

see [23, p. 246]. Note that $\mathcal{K}(\tau) > 0$,

$$\mathcal{K}(\tau) \sim (\tau - 1)^{-2} \quad \text{as } \tau \to 1^+ \tag{4.28}$$

and

$$\mathcal{K}(\tau) \sim \tau^{-2} \quad \text{as } \tau \to +\infty, \tag{4.29}$$

so the kernel $\mathcal{K}(\tau)$ is integrable as $\tau \to +\infty$, but it is *singular* as $\tau \to 1^+$.

Denote

$$\Phi_u(r,\tau) := u(r) - u(r\tau) + \frac{u(r) - u(r/\tau)}{\tau}. \tag{4.30}$$

Clearly, $\Phi_u(r,1) = 0$. A direct computation shows that

$$\partial_\tau \Phi_u(r,1) = 0, \quad \partial_\tau^2 \Phi_u(r,1) = -2r^2 \mathscr{L}u(r), \tag{4.31}$$

where the differential expression

$$\mathscr{L}u(r) := u''(r) + \frac{2}{r}u'(r), \tag{4.32}$$

acts on $u(r)$ as the radial Laplacian in three dimensions. In particular, the integral in (4.26) converges as $\tau \to 1^+$.

We now define a barrier function $U \in C^2(\overline{\mathbb{R}_+})$ such that $U(r)$ is monotone decreasing and

$$U(r) = \frac{1}{r\log(er)} \quad \forall r > 1. \tag{4.33}$$

Clearly, if $u(x) := U(|x|)$ then $u \in H^1(\mathbb{R}^2)$. By interpolation between $L^2(\mathbb{R}^2)$ and $H^1(\mathbb{R}^2)$ (cf. [37, proposition 1.52]), we also conclude that $u \in H^{1/2}(\mathbb{R}^2)$.

Lemma 4.9. *There exists $R > 2$ such that*

$$(-\Delta)^{1/2}U(r) \sim -\frac{1}{r^2(\log(r))^2} \quad \textit{for all } r > R. \tag{4.34}$$

Proof. Our strategy is to split the representation in (4.26) into three parts $\int_1^2 + \int_2^r + \int_r^\infty$ and then either estimate each part from above and below or compute the integrals explicitly, see (4.46) and (4.47).

For $r > 2$, we compute

$$\mathscr{L}U(r) = \frac{\log(e^3 r)}{(r\log(er))^3} > 0. \tag{4.35}$$

Next, we claim that for all $r > 2$ the following inequalities hold:

$$\Phi_U(r,\tau) < U(r) \quad \forall \tau \in [r, +\infty), \tag{4.36}$$

$$\Phi_U(r,\tau) \le 0 \quad \forall \tau \in [1, r] \tag{4.37}$$

and

$$\Phi_U(r,\tau) \ge -4r^2 \mathscr{L}U(r)(\tau - 1)^2 \quad \forall \tau \in [1,2]. \tag{4.38}$$

We begin by noting that by monotonicity and positivity of U, we have

$$\Phi_U(r,\tau) < U(r), \tag{4.39}$$

which yields (4.36). To deduce (4.37), observe that for $r > 2$ and $1 \le \tau \le r$, we have

$$\Phi_U(r,\tau) = \frac{1}{r}\left\{\frac{1}{\log(er)} - \frac{1}{\log(er/\tau)} + \frac{1}{\tau}\left(\frac{1}{\log(er)} - \frac{1}{\log(er\tau)}\right)\right\}. \tag{4.40}$$

It is elementary to see that (4.37) is equivalent to

$$\frac{\log(er\tau)}{\log(er/\tau)} \ge \frac{1}{\tau}, \tag{4.41}$$

the latter is true for any $r > 1$ and $\tau \in [1, r]$ (since in this range the left-hand side is bigger than one).

To derive (4.38), let $A := \log(er)$ and observe that for $r > 2$ and $\tau \in [1, 2]$, we have $A > 1$ and

$$\begin{aligned} &r\{\Phi_U(r,\tau) + 4\mathscr{L}U(r)r^2(\tau-1)^2\} \\ &= \frac{1}{\log(er)} - \frac{1}{\log(er)-\log(\tau)} + \frac{1}{\tau}\left(\frac{1}{\log(er)} - \frac{1}{\log(er)+\log(\tau)}\right) + \frac{4\log(e^3 r)}{(\log(er))^3}(\tau-1)^2 \\ &= \frac{1}{A}\left(1+\frac{1}{\tau}\right) - \left(\frac{1}{A-\log(\tau)} + \frac{1}{\tau(A+\log(\tau))}\right) + \frac{4(2+A)}{A^3}(\tau-1)^2 \\ &\geq \frac{1}{A}\left(1+\frac{1}{\tau}\right) - \left(\frac{1}{A-\log(\tau)} + \frac{1}{\tau(A+\log(\tau))}\right) + \frac{4}{A^2}(\log(\tau))^2, \end{aligned} \tag{4.42}$$

where we used the fact that $\log(\tau) < \tau - 1$ for $\tau \geq 1$. It is convenient to substitute $\tau = e^x$, where $x \in [0, \log(2)]$. Then, taking into account that $A \geq \log(2e) > 2x$, we rewrite the right-hand side of (4.42) as

$$\begin{aligned} &\frac{1}{A} - \frac{1}{A-x} + e^{-x}\left(\frac{1}{A} - \frac{1}{A+x}\right) + \frac{4x^2}{A^2} = \frac{x}{A}\left\{-\frac{1}{A-x} + \frac{e^{-x}}{A+x} + \frac{4x}{A}\right\} \\ &\geq \frac{x}{A^2}\left\{-1 - \frac{2x}{A} + (1-x)\left(1-\frac{x}{A}\right) + 4x\right\} \\ &\geq \frac{3x^2}{A^2}\left\{1 - \frac{1}{A}\right\} \geq 0 \quad \text{for all } x \in [0, \log(2)]. \end{aligned} \tag{4.43}$$

Now, for $r > 2$, we compute explicitly, using again the substitution $\tau = e^x$ and a standard asymptotic expansion of the integral,

$$\begin{aligned} \int_2^r r\Phi_U(r,\tau)\tau^{-2}\,d\tau &= \int_{\log(2)}^{z^{-1}} \left(\frac{xz^2e^{-x}}{(z+1)(xz+z+1)} + \frac{z}{(x-1)z-1} + \frac{z}{z+1}\right)e^{-x}\,dx \\ &= -\frac{7+6\log(2)}{16}z^2 + O(z^3) \quad \text{as } z \to 0^+, \end{aligned} \tag{4.44}$$

where we defined $z := 1/\log(r)$. Similarly, we have

$$\left|\int_r^\infty r\Phi_U(r,\tau)\tau^{-2}\,d\tau\right| \leq \int_{z^{-1}}^\infty \frac{ze^{-x}}{z+1}\,dx + U(0)e^{z^{-1}}\int_{z^{-1}}^\infty e^{-2x}\,dx \leq (1+\tfrac{1}{2}U(0))e^{-z^{-1}}. \tag{4.45}$$

Therefore, taking into account (4.29) and using (4.36), (4.37) and (4.44), for $r > 2$, we estimate

$$\begin{aligned} (-\Delta)^{1/2}U(r) &\lesssim r^{-1}\int_2^r \Phi_U(r,\tau)\tau^{-2}\,d\tau + r^{-1}U(r)\int_r^\infty \tau^{-2}\,d\tau, \\ &\sim -\frac{1}{r^2(\log(r))^2} + \frac{1}{r^3\log(r)} \sim -\frac{1}{r^2(\log(r))^2} \quad \text{as } r \to \infty. \end{aligned} \tag{4.46}$$

To deduce a lower estimate, we use (4.38), (4.45) and (4.44) to obtain

$$\begin{aligned} (-\Delta)^{1/2}U(r) &\gtrsim -r\mathscr{L}U(r) + r^{-1}\left(\int_2^r + \int_r^\infty\right)\Phi_U(r,\tau)\tau^{-2}\,d\tau, \\ &\gtrsim -\frac{1}{r^2(\log(r))^2} - \frac{1}{r^2(\log(r))^2} - \frac{1}{r^3} \sim -\frac{1}{r^2(\log(r))^2} \quad \text{as } r \to \infty, \end{aligned} \tag{4.47}$$

which completes the proof. ■

(e) Decay estimate

Proposition 4.10. *Let $V \in \mathring{H}^{1/2}(\mathbb{R}^2) \cap C^\alpha(\mathbb{R}^2)$ for some $\alpha \in (0, 1]$. Assume that $(-\Delta)^{1/2}V \geq 0$, $V \not\equiv 0$, and for some $R > 0$ and $C > 0$,*

$$(-\Delta)^{1/2}V \leq \frac{C}{|x|^2(\log|x|)^2} \quad \text{for } |x| \geq R. \tag{4.48}$$

Then the unique solution $u_V \in H^{1/2}(\mathbb{R}^2) \cap C^\alpha(\mathbb{R}^2)$ of (4.3) satisfies

$$0 < u_V(x) \le V(x) \quad \text{for all } x \in \mathbb{R}^2 \tag{4.49}$$

and

$$u_V(x) \sim \frac{1}{|x| \log |x|} \quad \text{as } |x| \to \infty. \tag{4.50}$$

In particular, $u_V \in L^2(\mathbb{R}^2)$.

Remark 4.11. We do not assume radial symmetry of V or u_V. The assumptions $(-\Delta)^{1/2}V \ge 0$ and $V \ne 0$ ensure the positivity of u_V, while the upper bound (4.48) controls the logarithmic decay rate (4.50). The bound (4.48) together with $(-\Delta)^{1/2}V \ge 0$ implicitly necessitates that V is positive in $\mathbb{R}^2$, $(-\Delta)^{1/2}V \in L^1(\mathbb{R}^2)$ and

$$\lim_{|x|\to\infty} 2\pi |x| V(x) = ||(-\Delta)^{1/2}V||_{L^1(\mathbb{R}^2)}, \tag{4.51}$$

see lemma 4.12 below.

Proof. Note that $(-\Delta)^{1/2}V \ge 0$ implies that $V \ge 0$ (this could be seen similarly to the argument in the proof of proposition 4.2 but without the nonlinear term). Then the upper bound in (4.49) follows by corollary 4.5. Next, recall that $u_V \in C^\alpha(\mathbb{R}^2)$ by lemma 3.4 and $u_V \ne 0$ by proposition 4.2. Therefore, with $c := ||u_V||_{L^\infty(\mathbb{R}^2)}$, we get

$$((-\Delta)^{1/2} + c)u_V = (c - u_V)u_V + (-\Delta)^{1/2}V \ge 0 \quad \text{in } \mathbb{R}^2.$$

This implies that $u_V(x) > 0$ for all $x \in \mathbb{R}^2$, cf. [14, lemma 7.1].

To derive (4.50), set $U_\lambda := \lambda U$, where U is the logarithmic barrier function defined in (4.33). Recall that $U \in H^{1/2}(\mathbb{R}^2) \subset \mathring{H}^{1/2}(\mathbb{R}^2)$. Using (4.34) to estimate $(-\Delta)^{1/2}U_\lambda$, we conclude that there exist positive constants c_1, c_2, C such that for some $R' > R$ and all sufficiently large $\lambda > 0$,

$$\begin{aligned}(-\Delta)^{1/2}U_\lambda &+ bU_\lambda^2 - (-\Delta)^{1/2}V \\ &\ge -\frac{c_1\lambda}{|x|^2(\log(|x|))^2} + \frac{\lambda^2}{|x|^2(\log(e|x|))^2} - \frac{C}{|x|^2(\log|x|)^2} \ge 0 \quad \text{for } |x| \ge R'.\end{aligned} \tag{4.52}$$

Similarly, for some $R' > R$ and all sufficiently small $\lambda > 0$,

$$(-\Delta)^{1/2}U_\lambda + bU_\lambda^2 - (-\Delta)^{1/2}V \le -\frac{c_2\lambda}{|x|^2(\log(|x|))^2} + \frac{\lambda^2}{|x|^2(\log(e|x|))^2} \le 0 \quad \text{for } |x| \ge R'. \tag{4.53}$$

Therefore, for suitable values of λ, we can use U_λ as a sub- or super-solution in the comparison principle of lemma 4.3 with $\Omega = B_R^c$.

To construct a lower barrier for the solution u_V, set $\lambda_0 := \min_{\bar{B}_R} u_V > 0$. Then

$$u_V \ge U_{\lambda_0} \quad \text{in } \bar{B}_R. \tag{4.54}$$

Taking into account (4.53), we conclude by lemma 4.3 that

$$u_V \ge U_\lambda \quad \text{in } \mathbb{R}^2, \tag{4.55}$$

for a sufficiently small $\lambda \le \lambda_0$.

To construct an upper barrier for u_V, choose $\mu > 0$ such that

$$u_V \le U_\mu \quad \text{in } \bar{B}_R. \tag{4.56}$$

Using (4.52), we conclude by lemma 4.3 that

$$u_V \le U_\lambda \quad \text{in } \mathbb{R}^2, \tag{4.57}$$

for a sufficiently large $\lambda \ge \mu$. ∎

(f) Charge estimate

In the case of the standard Newtonian kernel $|x|^{-1}$ on $\mathbb{R}^3$ it is well known that for a non-negative $f \in L^1_{rad}(\mathbb{R}^3)$, $|x|^{-1} * f = ||f||_{L^1(\mathbb{R}^3)}|x|^{-1} + o(|x|^{-1})$ as $|x| \to \infty$ (cf. [38] for a discussion). The result becomes non-trivial when we consider the convolution kernel $|x|^{-1}$ on $\mathbb{R}^2$, or more generally the Riesz kernel $|x|^{-(N-\alpha)}$ on $\mathbb{R}^N$ with $\alpha \in (0, N)$. It is known that if $\alpha \in (1, N)$ and $f \in L^1(\mathbb{R}^N)$ is positive radially symmetric then $|x|^{-(N-\alpha)} * f = O(|x|^{-(N-\alpha)})$ (see [38, theorem 5(i)]). The same remains valid if $\alpha \in (0, 1]$ and f is in addition monotone decreasing (see [39, lemma 2.2 (4)]). However, without assuming monotonicity of f, $|x|^{-(N-\alpha)} * f$ with $\alpha \in (0, 1]$ could have arbitrary fast growth at infinity [38, theorem 5].

We are going to show that if f is monotone non-increasing and decays faster than $|x|^{-2}$, then the sharp asymptotics of $|x|^{-1} * f$ on $\mathbb{R}^2$ is recovered. The proof is easily extended to Riesz kernels with $N \geq 2$ and $\alpha \in (0, N)$.

Lemma 4.12 (Asymptotic Newton's type theorem). *Let $0 \leq f \in L^1(\mathbb{R}^2)$ be a function dominated by a radially symmetric non-increasing function $\varphi : \mathbb{R}_+ \to \mathbb{R}_+$ that satisfies*

$$\lim_{|x|\to\infty} \varphi(x)|x|^2 = 0. \tag{4.58}$$

Then

$$\int_{\mathbb{R}^2} \frac{f(y)}{|x-y|}\, d^2y = \frac{||f||_{L^1(\mathbb{R}^2)}}{|x|} + o(|x|^{-1}) \quad as\, |x| \to \infty. \tag{4.59}$$

Proof. Fix $0 \neq x \in \mathbb{R}^2$ and decompose $\mathbb{R}^2$ as the union of $B = \{y : |y - x| < |x|/2\}$, $A = \{y \notin B : |y| \leq |x|\}$, $C = \{y \notin B : |y| > |x|\}$.

We want to estimate the quantity

$$\left|\int_{A\cup C} f(y)\left(\frac{1}{|x-y|} - \frac{1}{|x|}\right) d^2y\right| \leq \int_{A\cup C} f(y)\left|\frac{1}{|x-y|} - \frac{1}{|x|}\right| d^2y. \tag{4.60}$$

Since $|x|/2 \leq |x-y| \leq 2|x|$ for all $y \in A$, by the mean value theorem, we have

$$\left|\frac{1}{|x-y|} - \frac{1}{|x|}\right| \leq \frac{4|y|}{|x|^2} \quad (y \in A). \tag{4.61}$$

Thus

$$\left|\int_{A} f(y)\left(\frac{1}{|x-y|} - \frac{1}{|x|}\right) d^2y\right| \leq \frac{4}{|x|^2}\int_{A} f(y)|y|\, d^2y. \tag{4.62}$$

On the other hand, since $|x-y| > |x|/2$, for all $y \in C$ then

$$\left|\frac{1}{|x|} - \frac{1}{|x-y|}\right| \leq \frac{1}{|x|} \quad (y \in C), \tag{4.63}$$

from which we compute that

$$\left|\int_{C} f(y)\left(\frac{1}{|x-y|} - \frac{1}{|x|}\right) d^2y\right| \leq \frac{1}{|x|}\int_{C} f(y)\, d^2y. \tag{4.64}$$

Then

$$\begin{aligned}&\left|\int_{\mathbb{R}^2} \frac{f(y)}{|x-y|}\, d^2y - \frac{||f||_{L^1(\mathbb{R}^2)}}{|x|}\right| \\ &\quad\leq \frac{4}{|x|^2}\int_{A} f(y)|y|\, d^2y + \int_{B} \frac{f(y)}{|x-y|}\, d^2y + \frac{1}{|x|}\int_{B\cup C} f(y)\, d^2y =: I_1 + I_2 + I_3.\end{aligned} \tag{4.65}$$

Using (4.58), for $|x| \gg 2$, we estimate

$$I_1 = \frac{4}{|x|^2}\int_{|y|\leq|x|} f(y)|y|\, d^2y \leq \frac{8\pi}{|x|^2}\underbrace{\int_0^{|x|} \varphi(t)t^2\, dt}_{o(|x|)} = o(|x|^{-1}) \quad (|x| \to \infty). \tag{4.66}$$

Also, using the monotonicity of f and (4.58), for $|x| \gg 2$, we obtain

$$I_2 = \int_{|y-x|\leq|x|/2} \frac{f(y)}{|x-y|}\, dy \leq \varphi(|x|/2) \int_{|z|\leq|x|/2} \frac{dz}{|z|} = \pi\varphi(|x|/2)|x| = o(|x|^{-1}). \tag{4.67}$$

Finally, $I_3 = o(|x|^{-1})$ as $|x| \to \infty$ since $f \in L^1(\mathbb{R}^2)$, so the assertion follows. ∎

Proposition 4.13. *Assume that the assumptions of proposition 4.10 hold and*

$$\lim_{|x|\to\infty} 2\pi|x|V(x) = Z > 0. \tag{4.68}$$

Then $||\rho_V||_{L^1(\mathbb{R}^2)} = Z$.

Proof. According to (3.23), the minimizer $\rho_V \in \mathcal{H}_0 \cap C^\alpha(\mathbb{R}^2)$ satisfies

$$\rho_V^{1/2}(x) = V(x) - U_{\rho_V}(x) \quad \text{for all } x \in \mathbb{R}^2. \tag{4.69}$$

Taking into account (2.15), by lemma 4.12 above, we conclude that

$$\lim_{|x|\to\infty} 2\pi|x|U_{\rho_V}(x) = ||\rho_V||_{L^1(\mathbb{R}^2)}. \tag{4.70}$$

Then the assertion follows since $\lim_{|x|\to\infty} |x|\rho_V^{1/2}(x) = 0$. ∎

(g) Universality of decay

We next prove that in the case $V = V_{Z,d}$ the behaviour of $\rho_{V_{Z,d}}$ for large $|x|$ does not depend on the values of Z and d.

Proposition 4.14. *Let $Z > 0$, $d > 0$ and let $V = V_{Z,d}$ as defined in* (2.3). *Then*

$$u_V(x) \simeq \frac{1}{|x|\log|x|} \quad \textit{as } |x| \to \infty. \tag{4.71}$$

Proof. We start by noting that proposition 4.10 applies to $V_{Z,d}$ (see (2.10)). To prove the sharp asymptotic decay of the minimizer when $V = V_{Z,d}$, we use the idea in the computation of Katsnelson [11], also giving the latter a precise mathematical meaning. To this end, we first note that since $\rho_V \in L^1(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2)$, we have that (2.11) holds. In terms of $u_V > 0$ defined in (2.13), this equation reads

$$u_V(x) = V(x) - \frac{1}{2\pi}\int_{\mathbb{R}^2} \frac{u_V^2(y)}{|x-y|}\, \mathrm{d}^2y \quad \text{for all } x \in \mathbb{R}^2, \tag{4.72}$$

where we used the regularity of u_V and V. In turn, since $u_V(x) = u(|x|)$, applying Fubini's theorem, we obtain after an explicit integration

$$u(r) = \frac{Z}{2\pi\sqrt{d^2+r^2}} - \frac{1}{2\pi}\int_0^\infty\int_0^{2\pi} \frac{u^2(r')\, r'\, \mathrm{d}r'\, \mathrm{d}\theta}{\sqrt{r^2+r'^2-2rr'\cos\theta}} \tag{4.73}$$

$$= \frac{Z}{2\pi\sqrt{d^2+r^2}} - \frac{2}{\pi}\int_0^\infty \frac{r'u^2(r')}{r+r'} K\left(\frac{2\sqrt{rr'}}{r+r'}\right) \mathrm{d}r', \tag{4.74}$$

where $K(k)$ is the complete elliptic integral of the first kind [40].

Proceeding as in [11], we introduce a smooth bounded function

$$F(t) := e^t u(e^t), \quad t \in \mathbb{R}, \tag{4.75}$$

which satisfies $F(\ln r) = ru(r)$. From (4.50) and the boundedness of u, we conclude that

$$F(t) \sim t^{-1} \quad \text{as } t \to +\infty, \tag{4.76}$$

and $F(t)$ decays exponentially as $t \to -\infty$. In particular, $F \in L^2(\mathbb{R})$. Then, with the substitution $r = e^t$, (4.73) written in terms of $F(t)$ becomes

$$F(t) = \frac{Z}{2\pi\sqrt{1 + d^2 e^{-2t}}} - \frac{2}{\pi}\int_{-\infty}^{\infty} \frac{F^2(t')}{1 + e^{t'-t}} K\left(\frac{1}{\cosh\frac{t'-t}{2}}\right) \mathrm{d}t'. \tag{4.77}$$

We further introduce (with the opposite sign convention to that in [11])

$$\phi(t) := \frac{2K(1/\cosh(t2))}{\pi(1 + e^{-t})} - \theta(t), \tag{4.78}$$

where $\theta(t)$ is the Heaviside step function, and note that $\phi(t)$ is a positive, exponentially decaying function as $t \to \pm\infty$, which is smooth, except for a logarithmic singularity at $t = 0$. Then, since $F(t) \to 0$ as $t \to +\infty$ by (4.76), passing to the limit using the weak convergence of $\phi(t - \cdot) \rightharpoonup 0$ in $L^2(\mathbb{R})$ as $t \to +\infty$ and monotone convergence, we conclude that

$$\int_{-\infty}^{+\infty} F^2(t)\,\mathrm{d}t = \frac{Z}{2\pi}. \tag{4.79}$$

With this (4.77) becomes

$$F(t) = \frac{Z\left(1 - \sqrt{1 + d^2 e^{-2t}}\right)}{2\pi\sqrt{1 + d^2 e^{-2t}}} + \int_t^{\infty} F^2(t')\,\mathrm{d}t' - \int_{-\infty}^{\infty} \phi(t - t')F^2(t')\,\mathrm{d}t'. \tag{4.80}$$

To conclude, we observe that in view of (4.76), we can estimate the last term in (4.80) to be $O(t^{-2})$ as $t \to +\infty$. Similarly, the first term gives an exponentially small contribution for $t \to +\infty$ and can, therefore, be absorbed into the $O(t^{-2})$ term as well. Thus, we have

$$F(t) = G(t) + O(t^{-2}) \quad \text{and} \quad G(t) := \int_t^{\infty} F^2(t')\,\mathrm{d}t', \tag{4.81}$$

and it follows that $G(t)$ satisfies for all t sufficiently large

$$\frac{dG(t)}{\mathrm{d}t} = -(G(t) + O(t^{-2}))^2. \tag{4.82}$$

In particular, using (4.76), we can further estimate for $t \gg 1$

$$\frac{\mathrm{d}G(t)}{\mathrm{d}t} = -G^2(t)(1 + O(t^{-1}))^2. \tag{4.83}$$

Integrating this expression from some sufficiently large t_0 then gives

$$\frac{1}{G(t)} - \frac{1}{G(t_0)} = t - t_0 + O\left(\ln\left(\frac{t}{t_0}\right)\right), \quad t > t_0. \tag{4.84}$$

Finally, solving for $G(t)$ and inserting it into (4.81) results in

$$F(t) = \frac{1}{t + O(\ln t)} \quad \text{as } t \to +\infty, \tag{4.85}$$

which yields the claim after converting back into the original variables. ■

(h) Proof of the main results

We finish this section by concluding the proofs of the results in §2.

Proof of theorem 2.1. The statement of the theorem follows by combining the statements of proposition 3.1, lemma 3.4 and proposition 4.2. ■

Proof of theorem 2.2. The conclusion of this theorem is the consequence of theorem 2.1, together with corollary 4.4 and propositions 4.10, 4.13 and 4.14, taking into account (2.10) and performing a change of variables from u_V to ρ_V. ■

Proof of corollary 2.6. Now that we established proposition 4.14 for the potential $V_{Z,d}$ with $Z > 0$ and $d > 0$, we may proceed to use the comparison principle in lemma 4.3 to establish the sharp estimate in (4.71) for a potential given by (2.4) with all $Z_i > 0$ and $d_i > 0$. In this case by (2.10), we have

$$(-\Delta)^{1/2} V_N(x) = \sum_{i=1}^{N} \frac{Z_i d_i}{2\pi (d_i^2 + |x - x_i|^2)^{3/2}}. \tag{4.86}$$

In particular, V_N satisfies the assumptions of proposition 4.10. Hence, the conclusions of propositions 4.10 and 4.13 are still valid for $V = V_N$.

It remains to establish the sharp decay estimate in (4.71). For that, simply observe that there exist constants $Z_2 > Z_1 > 0$ such that

$$(-\Delta)^{1/2} V_{Z_1,1}(x) \le (-\Delta)^{1/2} V_N(x) \le (-\Delta)^{1/2} V_{Z_2,1}(x) \quad \forall\, x \in \mathbb{R}^2. \tag{4.87}$$

Therefore, by lemma 4.3, we have that $u_{V_{Z_1,1}} \le u_{V_N} \le u_{V_{Z_2,1}}$, and the conclusion follows from proposition 4.14 and a change of variables from u_{V_N} to ρ_{V_N}. ■

Remark 4.15. From the proof above, it is clear that the universal decay estimate (4.71) on the minimizer ρ_V remains valid for any potential $V \in \mathring{H}^{1/2}(\mathbb{R}^2)$ such that $(-\Delta)^{1/2} V$ is non-negative and bounded, and $(-\Delta)^{1/2} V \lesssim |x|^{-3}$ as $|x| \to \infty$.

5. Non-zero background charge

We now turn to the situation in which a net background charge density $\bar\rho \in \mathbb{R}$ is present, which is achieved in graphene via back-gating. This leads to the modified TF energy [14]

$$\begin{aligned}\mathcal{E}^{TF}_{\bar\rho}(\rho) = \frac{2}{3}\int_{\mathbb{R}^2} (|\rho(x)|^{3/2} - |\bar\rho|^{3/2})\, d^2x - \operatorname{sgn}(\bar\rho)|\bar\rho|^{1/2} \int_{\mathbb{R}^2} (\rho(x) - \bar\rho)\, d^2x \\ - \int_{\mathbb{R}^2} (\rho(x) - \bar\rho) V(x)\, d^2x + \frac{1}{4\pi} \iint_{\mathbb{R}^2\times\mathbb{R}^2} \frac{(\rho(x) - \bar\rho)(\rho(y) - \bar\rho)}{|x-y|}\, d^2x\, d^2y,\end{aligned}$$

where $\rho(x) \to \bar\rho$ sufficiently fast as $|x| \to \infty$. Since this energy is invariant with respect to

$$\rho \to -\rho, \quad \bar\rho \to -\bar\rho,\ V \to -V,$$

in the sequel, we assume, without loss of generality, that $\bar\rho > 0$.

(a) A representation of the energy functional

For a given charge density $\rho(x)$ and $\bar\rho > 0$, we define

$$\phi := \rho - \bar\rho. \tag{5.1}$$

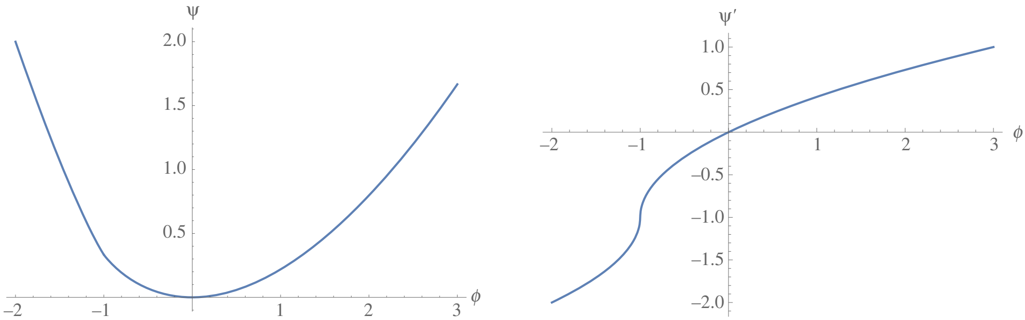

Figure 1. Plot of $\Psi_{\bar\rho}(\phi)$ and $\Psi'_{\bar\rho}(\phi)$ for $\bar\rho = 1$.

Then, for $\phi \in C_c^\infty(\mathbb{R}^2)$, the energy $\mathcal{E}_{\bar\rho}^{TF}(\phi)$ can be written as (with a slight abuse of notation, in what follows, we use the same letter to denote both the energy as a function of ρ and that as a function of ϕ)

$$\mathcal{E}_{\bar\rho}^{TF}(\phi) = \int_{\mathbb{R}^2} \Psi_{\bar\rho}(\phi(x))\,\mathrm{d}^2x - \int_{\mathbb{R}^2} V(x)\phi(x)\,\mathrm{d}^2x + \frac{1}{4\pi}\iint_{\mathbb{R}^2\times\mathbb{R}^2} \frac{\phi(x)\phi(y)}{|x-y|}\,\mathrm{d}^2x\,\mathrm{d}^2y, \tag{5.2}$$

where

$$\Psi_{\bar\rho}(\phi) := \tfrac{2}{3}|\bar\rho + \phi|^{3/2} - \tfrac{2}{3}\bar\rho^{3/2} - \bar\rho^{1/2}\phi. \tag{5.3}$$

Clearly, $\Psi_{\bar\rho} : \mathbb{R} \to \mathbb{R}$ is a convex C^1-function of ϕ with

$$\Psi'_{\bar\rho}(\phi) = |\bar\rho + \phi|^{1/2}\mathrm{sgn}(\bar\rho + \phi) - \bar\rho^{1/2}, \tag{5.4}$$

and $\Psi_{\bar\rho} \in C^\infty(\mathbb{R} \setminus \{-\bar\rho\})$. The graphs of $\Psi_{\bar\rho}(\phi)$ and $\Psi'_{\bar\rho}(\phi)$ for $\bar\rho = 1$ are presented in figure 1.

Using elementary calculus, one can see that

$$\frac{c|\phi|^2}{\sqrt{\bar\rho + |\phi|}} \le \Psi_{\bar\rho}(\phi) \le \frac{C|\phi|^2}{\sqrt{\bar\rho + |\phi|}} \quad (\phi \in \mathbb{R}), \tag{5.5}$$

for some universal $C > c > 0$. This implies that for $\bar\rho > 0$,

$$\{\phi \in L^1_{\mathrm{loc}}(\mathbb{R}^2) : ||\Psi_{\bar\rho}(\phi)||_{L^1(\mathbb{R}^2)} < +\infty\} = L^{3/2}(\mathbb{R}^2) + L^2(\mathbb{R}^2). \tag{5.6}$$

Lemma 5.1. *Let $\bar\rho > 0$. Then $||\Psi_{\bar\rho}(\cdot)||_{L^1(\mathbb{R}^2)} : L^{3/2}(\mathbb{R}^2) + L^2(\mathbb{R}^2) \to \mathbb{R}$ is a strictly convex and weakly lower semi-continuous functional, i.e.*

$$\langle \phi_n, \varphi\rangle \to \langle \phi, \varphi\rangle \quad \forall\,\varphi \in L^3(\mathbb{R}^2) \cap L^2(\mathbb{R}^2) \implies ||\Psi_{\bar\rho}(\phi)||_{L^1(\mathbb{R}^2)} \le \liminf_n ||\Psi_{\bar\rho}(\phi_n)||_{L^1(\mathbb{R}^2)}. \tag{5.7}$$

Proof. The strict convexity of $||\Psi_{\bar\rho}(\cdot)||_{L^1(\mathbb{R}^2)}$ follows from the strict convexity of the function $\Psi_{\bar\rho} : \mathbb{R} \to \mathbb{R}$.

Let $(\phi_n) \subset L^{3/2}(\mathbb{R}^2) + L^2(\mathbb{R}^2)$ be a sequence that converges strongly to ϕ, i.e. there exist representations $\phi_n = f_n + g_n$ and $\phi = f + g$ such that $||f_n - f||_{L^{3/2}(\mathbb{R}^2)} \to 0$ and $||g_n - g||_{L^2(\mathbb{R}^2)} \to 0$. Then, up to a subsequence $\Psi_{\bar\rho}(\phi_n) \to \Psi_{\bar\rho}(\phi)$ a.e. in $\mathbb{R}^2$. By Fatou's lemma,

$$||\Psi_{\bar\rho}(\phi)||_{L^1(\mathbb{R}^2)} \le \liminf_n ||\Psi_{\bar\rho}(\phi_n)||_{L^1(\mathbb{R}^2)}, \tag{5.8}$$

i.e. the sublevel sets of $||\Psi_{\bar\rho}(\cdot)||_{L^1(\mathbb{R}^2)}$ are closed in the norm of $L^{3/2}(\mathbb{R}^2) + L^2(\mathbb{R}^2)$. Using the convexity of $||\Psi_{\bar\rho}(\phi)||_{L^1(\mathbb{R}^2)}$, by Mazur's theorem, we conclude that all sublevels sets are also weakly closed in $L^{3/2}(\mathbb{R}^2) + L^2(\mathbb{R}^2)$, i.e. (5.7) holds. ■

(b) Variational set-up and the main result

In view of lemma 5.1, the natural domain of the total TF energy $\mathcal{E}_{\bar\rho}^{TF}$ is

$$\mathcal{H}_{\bar\rho} := \mathring{H}^{-1/2}(\mathbb{R}^2) \cap (L^{3/2}(\mathbb{R}^2) + L^2(\mathbb{R}^2)), \tag{5.9}$$

and the TF energy is correctly defined on $\mathcal{H}_{\bar\rho}$ in the form

$$\mathcal{E}_{\bar\rho}(\phi) := \int_{\mathbb{R}^2} \Psi_{\bar\rho}(\phi(x))\, \mathrm{d}^2x - \langle \phi, V\rangle + \frac{1}{2}||\phi||^2_{\mathring{H}^{-1/2}(\mathbb{R}^2)}, \tag{5.10}$$

where $\langle\cdot,\cdot\rangle$ denotes the duality pairing between $\mathcal{H}'_{\bar\rho}$ and $\mathcal{H}_{\bar\rho}$. Having in mind the definition of $\mathcal{H}_{\bar\rho}$ in (5.9), we have

$$\mathcal{H}'_{\bar\rho} = \mathring{H}^{1/2}(\mathbb{R}^2) + (L^3(\mathbb{R}^2) \cap L^2(\mathbb{R}^2)). \tag{5.11}$$

Our main result concerning minimizers of $\mathcal{E}_{\bar\rho}$ is the following.

Theorem 5.2. *Let $\bar\rho > 0$ and $V \in \mathcal{H}'_{\bar\rho}$. Then, $\mathcal{E}_{\bar\rho}$ admits a unique minimizer $\phi_{\bar\rho} \in \mathcal{H}_{\bar\rho}$ such that $\mathcal{E}_{\bar\rho}(\phi_{\bar\rho}) = \inf_{\mathcal{H}_{\bar\rho}} \mathcal{E}_{\bar\rho}$. The minimizer $\phi_{\bar\rho}$ satisfies the Euler–Lagrange equation*

$$\int_{\mathbb{R}^2} \Psi'_{\bar\rho}(\phi_{\bar\rho}(x))\varphi(x)\, \mathrm{d}^2x - \langle \varphi, V\rangle + \langle \phi_{\bar\rho}, \varphi\rangle_{\mathring{H}^{-1/2}(\mathbb{R}^2)} = 0 \quad \forall \varphi \in \mathcal{H}_{\bar\rho}. \tag{5.12}$$

Proof. The proofs of the existence and uniqueness of the minimizer (employing lemma 5.1), as well as the derivation of the Euler–Lagrange equations (5.12) are small modifications of the arguments in the proof of proposition 3.1, so we omit the details. For the differentiability of the map $\Psi_{\bar\rho}$, see [14, lemma 6.2]. ■

Remark 5.3. If, for instance, $\phi_{\bar\rho} \in \mathcal{H}_{\bar\rho} \cap L^{4/3}(\mathbb{R}^2)$ then (5.12) can be interpreted pointwise as

$$\Psi'_{\bar\rho}(\phi_{\bar\rho}(x)) + \frac{1}{2\pi}\int_{\mathbb{R}^2} \frac{\phi_{\bar\rho}(y)}{|x-y|}\, \mathrm{d}^2y = V(x) \quad \text{a.e. in } \mathbb{R}^2. \tag{5.13}$$

However, in general, the Euler–Lagrange equation for $\mathcal{E}_{\bar\rho}$ should be understood as

$$\Psi'_{\bar\rho}(\phi_{\bar\rho}) + U_{\phi_{\bar\rho}} = V \quad \text{in } \mathcal{D}'(\mathbb{R}^2), \tag{5.14}$$

where $\phi_{\bar\rho} \in \mathcal{H}_{\bar\rho} \subset L^2(\mathbb{R}^2) + L^{3/2}(\mathbb{R}^2)$ and $U_{\phi_{\bar\rho}} \in \mathring{H}^{1/2}(\mathbb{R}^2)$ is the potential of $\phi_{\bar\rho}$ defined via (3.5).

In the rest of the section, under some additional assumptions on V we will use the equivalent half-Laplacian representation of (5.12) to establish further regularity and decay properties of the minimizer $\phi_{\bar\rho}$ when $\bar\rho > 0$. Our crucial observation is that unlike in the case $\bar\rho = 0$, for $\bar\rho > 0$ the minimizer $\phi_{\bar\rho}$ has the same fast polynomial decay as the Green function of $(-\Delta)^{1/2} + 1$ in $\mathbb{R}^2$, for all reasonably fast decaying potentials V.

Theorem 5.4. *Let $\bar\rho > 0$, $V \in \mathring{H}^{1/2}(\mathbb{R}^2)$ and $\phi_{\bar\rho}$ be the minimizer of $\mathcal{E}_{\bar\rho}$ from theorem 5.2.*

(*i*) *If $(-\Delta)^{1/2}V \in L^\infty(\mathbb{R}^2)$ then $\phi_{\bar\rho} \in H^{1/2}(\mathbb{R}^2) \cap C^{1/2}(\mathbb{R}^2)$.*
(*ii*) *If additionally, $(-\Delta)^{1/2}V \geq 0$, $V \not\equiv 0$, and for some $C > 0$, we have*

$$(-\Delta)^{1/2}V \leq \frac{C}{(1+|x|^2)^{3/2}} \quad \text{in } \mathbb{R}^2, \tag{5.15}$$

then $\phi_{\bar\rho} > 0$ in $\mathbb{R}^2$ and

$$\phi_{\bar\rho}(x) \sim \frac{1}{|x|^3} \quad \text{as } |x| \to \infty. \tag{5.16}$$

In particular, $\phi_{\bar\rho} \in L^1(\mathbb{R}^2)$.

In the rest of this section, we are going to sketch the proof of theorem 5.4. We only emphasize the difference in the asymptotic behaviour, other arguments that are similar to the case $\bar\rho = 0$ will be omitted.

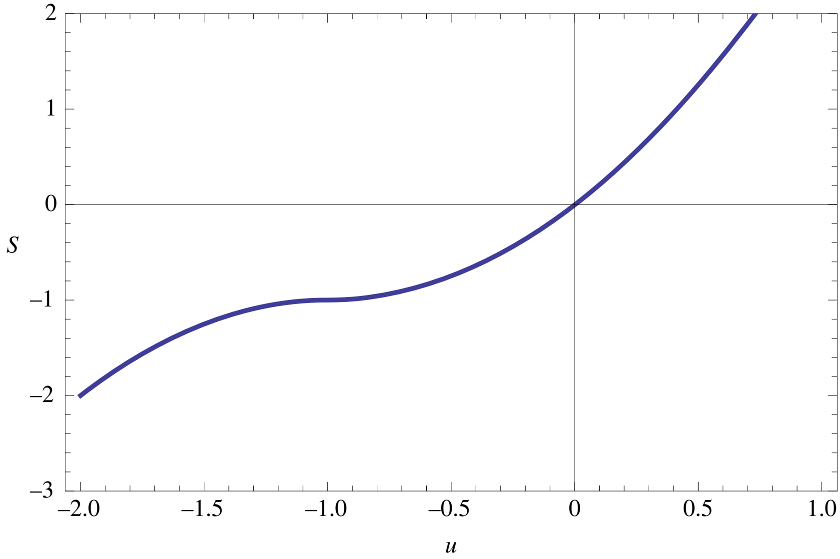

Figure 2. Plot of $S_{\bar\rho}(u)$ for $\bar\rho = 1$.

(c) Half-Laplacian representation, regularity and decay

Let $\bar\rho > 0$ and $\phi_{\bar\rho} \in \mathcal{H}_{\bar\rho}$ be the minimizer of $\mathcal{E}_{\bar\rho}$. Introduce the substitution

$$u_{\bar\rho} := \Psi'_{\bar\rho}(\phi_{\bar\rho}). \tag{5.17}$$

Then (5.12) transforms into

$$\int_{\mathbb{R}^2} u_{\bar\rho}(x)\varphi(x)\,\mathrm{d}^2x - \langle\varphi, V\rangle + \langle U_{S_{\bar\rho}(u_{\bar\rho})}, \varphi\rangle_{\mathring{H}^{1/2}(\mathbb{R}^2)} = 0 \quad \forall\, \varphi \in \mathcal{H}_{\bar\rho}, \tag{5.18}$$

where

$$S_{\bar\rho}(u) := |\bar\rho^{1/2} + u|(\bar\rho^{1/2} + u) - \bar\rho \quad (u \in \mathbb{R}), \tag{5.19}$$

is the inverse function of $\Psi'_{\bar\rho}$, so that $S_{\bar\rho}(\Psi'_{\bar\rho}(\phi)) = \phi$, for all $\phi \in \mathbb{R}$. The graph of $S_{\bar\rho}(u)$ is shown in figure 2.

Proposition 5.5 (Equivalent PDE). *Let $\bar\rho > 0$, $V \in \mathring{H}^{1/2}(\mathbb{R}^2)$ and $u_{\bar\rho}$ be defined by (5.17). Then $u_{\bar\rho} \in \mathring{H}^{1/2}(\mathbb{R}^2)$ and $u_{\bar\rho}$ is the unique solution of the equation*

$$(-\Delta)^{1/2}u + S_{\bar\rho}(u) = (-\Delta)^{1/2}V \quad in\, \mathring{H}^{1/2}(\mathbb{R}^2). \tag{5.20}$$

Moreover,

$$-\,v_- \le u_{\bar\rho} \le v_+, \tag{5.21}$$

where $v_\pm \ge 0$ are solutions of $(-\Delta)^{1/2}v_\pm = ((-\Delta)^{1/2}V)^\pm$ in $\mathring{H}^{1/2}(\mathbb{R}^2)$.

Proof. Similar to the proof of propositions 4.1 and 4.2. The uniqueness of the solution and the bound (5.21) follows from an extension of the comparison principle of lemma 4.3 to the case of a monotone increasing function $S_{\bar\rho}(u)$. ∎

Proposition 5.6. *Let $\bar\rho > 0$ and $V \in \mathring{H}^{1/2}(\mathbb{R}^2)$. Assume that $(-\Delta)^{1/2}V \in L^\infty(\mathbb{R}^2)$, $(-\Delta)^{1/2}V \geq 0$ and $V \neq 0$. Then, $u_{\bar\rho} \in H^{1/2}(\mathbb{R}^2) \cap C^{1/2}(\mathbb{R}^2)$, $u_{\bar\rho} > 0$ in $\mathbb{R}^2$ and*

$$u_{\bar\rho}(x) \gtrsim \frac{1}{|x|^3} \quad \text{as } |x| \to \infty. \tag{5.22}$$

If, in addition, for some $C > 0$,

$$(-\Delta)^{1/2}V \leq \frac{C}{(1+|x|^2)^{3/2}} \quad \text{in } \mathbb{R}^2, \tag{5.23}$$

then

$$u_{\bar\rho}(x) \sim \frac{1}{|x|^3} \quad \text{as } |x| \to \infty. \tag{5.24}$$

In particular, $u_{\bar\rho} \in L^1(\mathbb{R}^2)$.

Proof. Represent (5.20) as

$$((-\Delta)^{1/2} + 2\bar\rho^{1/2})u_{\bar\rho} + s_{\bar\rho}(u_{\bar\rho}) = (-\Delta)^{1/2}V \quad \text{in } \mathcal{D}'(\mathbb{R}^2), \tag{5.25}$$

where $s_{\bar\rho}(t) = S_{\bar\rho}(t) - 2\bar\rho^{1/2}t$ and observe that $s_{\bar\rho}(t) = t^2$ for $|t| < \bar\rho^{1/2}$ small, while $s_{\bar\rho}(t) \sim |t|t$ for t large. In particular, in view of (5.21), we have $u_{\bar\rho} \geq 0$ and $u_{\bar\rho} \in L^\infty(\mathbb{R}^2)$. Then, for a sufficiently large $c > 0$,

$$((-\Delta)^{1/2} + 2\bar\rho^{1/2} + c)u_{\bar\rho} = c - s_{\bar\rho}(u_{\bar\rho}) + (-\Delta)^{1/2}V \geq 0 \quad \text{in } \mathbb{R}^2. \tag{5.26}$$

This implies $u_{\bar\rho} \in H^{1/2}(\mathbb{R}^2) \cap C^{1/2}(\mathbb{R}^2)$, $u_{\bar\rho} > 0$ in $\mathbb{R}^2$ and additionally,

$$u_{\bar\rho}(x) \gtrsim \frac{1}{|x|^3} \quad \text{as } |x| \to \infty, \tag{5.27}$$

cf. [14, lemma 7.1] for a similar argument.

To derive the upper bound on $u_{\bar\rho}$, consider the dipole-type family of barriers

$$W_{Z,\lambda}(|x|) := \frac{Z}{2\pi(1+|\lambda x|^2)^{3/2}},$$

and note that using (4.21), scaling, $s_{\bar\rho}(W_{Z,\lambda}) \geq 0$ and (5.24), we obtain

$$\begin{aligned}((-\Delta)^{1/2} &+ 2\bar\rho^{1/2})W_{Z,\lambda} + s_{\bar\rho}(W_{Z,\lambda}) - (-\Delta)^{1/2}V \\ &\geq \frac{Z\lambda(2-|\lambda x|^2)}{2\pi(1+|\lambda x|^2)^{5/2}} + \frac{2Z\bar\rho^{1/2}(1+|\lambda x|^2)}{2\pi(1+|\lambda x|^2)^{5/2}} - \frac{C}{(1+|x|^2)^{3/2}} \geq 0 \quad \text{in } \mathbb{R}^2,\end{aligned} \tag{5.28}$$

provided that we choose $\lambda = 2\bar\rho^{1/2}$ and $Z \gg 1$ sufficiently large. Then $u_{\bar\rho} \leq W_{Z,2\bar\rho^{1/2}}$ in $\mathbb{R}^2$ by an extension of the comparison principle of lemma 4.3 to equation (5.25). ■

Proof of theorem 5.4. Follows from proposition 5.6 using the explicit representation $\phi_{\bar\rho} = S_{\bar\rho}(u_{\bar\rho}) = 2\bar\rho^{1/2}u_{\bar\rho} + u_{\bar\rho}^2$ in (5.19), which is valid since $u_{\bar\rho} > 0$. ■

Data accessibility. There is no further data available for this study.

Authors' contributions. V.M.: writing—original draft, writing—review and editing; C.B.M.: writing—original draft, writing—review and editing.

All authors gave final approval for publication and agreed to be held accountable for the work performed therein.

Declaration of AI use. We have not used AI-assisted technologies in creating this article.

Conflict of interest declaration. We declare we have no competing interests.

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