SIAM J. MATH. ANAL.
Vol. 47, No. 2, pp. 1001–1021

ON THE CRYSTAL GROUND STATE IN THE SCHRÖDINGER–POISSON MODEL*

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Abstract. A space-periodic ground state is shown to exist for lattices of smeared ions in $\mathbb{R}^3$ coupled to the Schrödinger and scalar fields. The elementary cell is necessarily neutral. The one-dimensional (1D), two-dimensional (2D), and three-dimensional (3D) lattices in $\mathbb{R}^3$ are considered, and a ground state is constructed by minimizing the energy per cell. The case of a 3D lattice is rather standard, because the elementary cell is compact, and the spectrum of the Laplacian is discrete. In the cases of 1D and 2D lattices, the energy functional is differentiable only on a dense set of variations, due to the presence of the continuous spectrum of the Laplacian that causes the infrared divergence of the Coulomb bond. Respectively, the construction of electrostatic potential and the derivation of the Schrödinger equation for the minimizer in these cases require an extra argument. The space-periodic ground states for 1D and 2D lattices give the model of the nanostructures similar to the carbon nanotubes and graphene, respectively.

Key words. crystal, lattice, ion, charge, wave function, potential, Schrödinger equation, Poisson equation, elementary cell, energy, Coulomb energy, minimization, neutrality condition, spectrum, embedding theorems, Fourier transform, infrared divergence, variation, nanostructures

AMS subject classifications. 35L10, 34L25, 47A40, 81U05

DOI. 10.1137/130949932

1. Introduction.

We consider d-dimensional ion lattices in $\mathbb{R}^3$,

$$\Gamma_d := \{\mathbf{x}(\mathbf{n}) = \mathbf{a}_1 n_1 + \cdots + \mathbf{a}_d n_d : \mathbf{n} = (n_1, \dots, n_d) \in \mathbb{Z}^d\}, \tag{1.1}$$

where $d = 1, 2, 3$ and $\mathbf{a}_k \in \mathbb{R}^3$ are linearly independent periods. A two-dimensional (2D) lattice (respectively, one-dimensional (1D) lattice) is a mathematical model of a monomolecular film (a wire).

Born and Oppenheimer [6] developed the quantum dynamical approach to the crystal structure, separating the motion of "light electrons" and of "heavy ions." As an extreme form of this separation, the ions could be considered as classical nonrelativistic particles governed by the Coulomb force, while the electrons could be described by the Schrödinger equation neglecting the electron spin. The scalar potential is the solution to the corresponding Poisson equation.

We consider the crystal with N ions per cell. Let us denote by μ_j the charge density of an ion and by $M_j > 0$ its mass, $j = 1, \dots, N$. Then the coupled equations read

$$i\hbar\dot{\psi}(\mathbf{x},t) = -\frac{\hbar^2}{2\mathrm{m}}\Delta\psi(\mathbf{x},t) + e\phi(\mathbf{x},t)\psi(\mathbf{x},t), \qquad \mathbf{x} \in \mathbb{R}^3, \tag{1.2}$$

$$\left[\frac{1}{c^2}\partial_t^2 - \Delta\right]\phi(\mathbf{x},t) = \rho(\mathbf{x},t)$$

$$:= \sum_{j=1}^{N}\sum_{\mathbf{n}\in\mathbb{Z}^d}\mu_j(\mathbf{x} - \mathbf{x}(\mathbf{n}) - \mathbf{x}_j(\mathbf{n},t)) + e|\psi(\mathbf{x},t)|^2, \qquad \mathbf{x} \in \mathbb{R}^3, \tag{1.3}$$

$$M_j\ddot{\mathbf{x}}_j(\mathbf{n},t) = -(\nabla\phi(\mathbf{x},t), \mu_j(\mathbf{x} - \mathbf{x}(\mathbf{n}) - \mathbf{x}_j(\mathbf{n},t))), \quad \mathbf{n} \in \mathbb{Z}^d, \quad j = 1, \dots, N. \tag{1.4}$$

*Received by the editors December 20, 2013; accepted for publication (in revised form) December 29, 2014; published electronically March 4, 2015. The research of the author was supported partly by the Alexander von Humboldt Research Award, Austrian Science Fund, P22198-N13, and grants of DFG and the Russian Foundation for Basic Research.

http://www.siam.org/journals/sima/47-2/94993.html

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Here, $e < 0$ is the electron charge, m is its mass, $\psi(\mathbf{x}, t)$ denotes the wave function of the electron field, and $\phi(\mathbf{x}, t)$ is the electrostatic potential generated by the ions and the electrons, with $\mathbf{x}_j(\mathbf{n}, t)$ denoting the ions's positions. Further, $(\cdot, \cdot)$ stands for the scalar product in the Hilbert space $L^2(\mathbb{R}^3)$. All derivatives here and below are understood in the sense of distributions. The system is nonlinear and translation invariant, i.e., $\psi(\mathbf{x} - \mathbf{a}, t)$, $\phi(\mathbf{x} - \mathbf{a}, t)$, $\mathbf{x}_j(\mathbf{n}, t) + \mathbf{a}$ is also a solution for any $\mathbf{a} \in \mathbb{R}^3$.

A dynamical quantum description of the solid state as a many-body system is not rigorously established yet (see the introduction of [25] and the preface of [29]). Up-to-date rigorous results concern only the ground state in different models (see below).

The classical "one-electron" theory of Bethe and Sommerfeld, based on the periodic Schrödinger equation, does not take into account oscillations of ions. Moreover, the choice of the periodic potential in this theory is very problematic and corresponds to a fixation of the ion positions which are unknown.

The system (1.2)–(1.4) eliminates these difficulties, though it does not respect the electron spin like the periodic Schrödinger equation. To remedy this deficiency, we should replace the Schrödinger equation by the Hartree–Fock equations as the next step toward a more realistic model. However, we expect that the techniques developed for the system (1.2)–(1.4) will be useful also for more realistic dynamical models of crystals. These goals were our main motivation in writing this paper.

Here, we take the first step toward proving the existence of the ground state, which is a Γ_d-periodic stationary solution $\psi^0(\mathbf{x})e^{-i\omega^0 t}$, $\phi^0(\mathbf{x})$, $\overline{\mathbf{x}} = (\mathbf{x}_1^0, \dots, \mathbf{x}_N^0)$ to the system (1.2)–(1.4):

$$\hbar\omega^0\psi^0(\mathbf{x}) = -\frac{\hbar^2}{2\mathrm{m}}\Delta\psi^0(\mathbf{x}) + e\phi^0(\mathbf{x})\psi^0(\mathbf{x}), \qquad \mathbf{x} \in T_d, \tag{1.5}$$

$$-\Delta\phi^0(\mathbf{x}) = \rho^0(\mathbf{x}) := \sigma^0(\mathbf{x}) + e|\psi^0(\mathbf{x})|^2, \qquad \mathbf{x} \in T_d, \tag{1.6}$$

$$0 = -\langle\nabla\phi^0(\mathbf{x}), \mu_j^{\mathrm{per}}(\mathbf{x} - \mathbf{x}_j^0)\rangle, \qquad j = 1, \dots, N. \tag{1.7}$$

Here, $T_d := \mathbb{R}^3/\Gamma_d$ denotes the "elementary cell" of the crystal, $\langle\cdot, \cdot\rangle$ stands for the scalar product in the Hilbert space $L^2(T_d)$ and its different extensions, and

$$\sigma^0(\mathbf{x}) := \sum_{j=1}^{N} \mu_j^{\mathrm{per}}(\mathbf{x} - \mathbf{x}_j^0), \quad \mu_j^{\mathrm{per}}(\mathbf{x}) := \sum_{\mathbf{n}\in\mathbb{Z}^d} \mu_j(\mathbf{x} - \mathbf{x}(\mathbf{n})), \tag{1.8}$$

where we assume that the series converge in an appropriate sense. More precisely, we will construct a solution to the system (1.5)–(1.7) with $\sigma^0(\mathbf{x})$ given by the first equation of (1.8), where μ_j^{per} satisfy the following condition:

$$\text{Condition I.} \qquad \mu_j^{\mathrm{per}} \in L^1(T_d) \cap L^2(T_d), \qquad j = 1, \dots, N. \tag{1.9}$$

For instance, $\mu_j^{\mathrm{per}} \in L^1(T_d)$ if $\mu_j \in L^1(\mathbb{R}^3)$, so we consider the case of smeared ions. The case of the point ions will be considered elsewhere. In the cases $d = 2$ and $d = 1$, we will assume additional conditions (3.11) and (4.9), respectively.

The elementary cell T_d is isomorphic to the three-dimensional (3D) torus for $d = 3$, to the direct product of the 2D torus by $\mathbb{R}$ for $d = 2$, and to the direct product of the 1D torus (circle) by $\mathbb{R}^2$ for $d = 1$.

The system (1.5)–(1.7) is translation invariant similarly to (1.2)–(1.4). Let us note that ω^0 should be real since $\Im\omega^0 \neq 0$ means an instability of the ground state: the decay as $t \to \infty$ in the case $\Im\omega^0 < 0$ and the explosion if $\Im\omega^0 > 0$.

Let us denote $Z_j := \int_{T_d} \mu_j^{\mathrm{per}}(\mathbf{x})d\mathbf{x}/|e|$. Then

$$\int_{T_d} \sigma^0(\mathbf{x})d\mathbf{x} = Z|e|, \qquad Z := \sum_j Z_j. \tag{1.10}$$

The total charge per cell should be zero (cf. [3]):

$$\int_{T_d} \rho^0(\mathbf{x})d\mathbf{x} = \int_{T_d} [\sigma^0(\mathbf{x}) + e|\psi^0(\mathbf{x})|^2]d\mathbf{x} = 0. \tag{1.11}$$

For $d = 3$, this neutrality condition follows directly from (1.6) by integration using Γ_3-periodicity of $\phi^0(\mathbf{x})$. For $d = 1$ and $d = 2$, it follows from the finiteness of energy per cell. Equivalently, the neutrality condition can be written as the normalization

$$\int_{T_d} |\psi^0(\mathbf{x})|^2 d\mathbf{x} = Z. \tag{1.12}$$

We allow arbitrary $Z_j \in \mathbb{R}$, but we assume that $Z > 0$; otherwise, the theory is trivial.

Let us comment on our approach. The neutrality condition (1.12) defines the submanifold $\mathcal{M}$ in the space $H^1(T_d) \times T_d^N$ of space-periodic configurations $(\psi^0, \overline{\mathbf{x}}^0)$. We construct a ground state as a minimizer over $\mathcal{M}$ of the energy per cell (2.3), (3.1), (4.1).

Our technique in the case of a 3D lattice is rather standard, and we use it as an "Ariadne's thread" to manage the more complicated cases of 2D and 1D lattices, because the corresponding elementary cells are unbounded.

Namely, the derivation of (1.5)–(1.7) for the minimizer in the cases of 2D and 1D lattices is not straightforward. The difficulty is that the energy per cell is finite only on a dense subset of $\mathcal{M}$ due to the infrared divergence of the Coulomb bond. In these cases, we restrict ourselves by one ion per cell, i.e., by $N = 1$. Then $\overline{\mathbf{x}}^0 = \mathbf{x}_1^0$ can be chosen arbitrarily because of the translation invariance of the system (1.5)–(1.7). Respectively, now the energy per cell should be minimized over $\psi \in M$, where M is the submanifold of $H^1(T_d)$ defined by the neutrality condition (1.12).

The main novelties of our approach behind the technical proofs for 2D and 1D lattices are as follows:

I. The energy per cell consists of two contributions: the kinetic energy and the Coulomb bond. Generally, the Coulomb bond for 2D and 1D lattices is infinite due to the infrared divergence which is caused by the continuous spectrum of the Laplace operator on the corresponding elementary cells. The spectrum is continuous since the elementary cells are unbounded in the case of 2D and 1D lattices in $\mathbb{R}^3$. Let us note that the continuous spectrum and the infrared singularity also appear in the Schrödinger–Poisson molecular systems in $\mathbb{R}^3$ studied in [2, 16, 28], where the singularity is summable, contrary to the space-periodic case.

We indicate suitable conditions (3.11), (4.9), which provide the finiteness of the Coulomb bond for a dense set of the fields in the case of 2D and 1D lattice, respectively.

Both contributions to the energy per cell (the kinetic energy and the Coulomb bond) are nonnegative. Hence, for any minimizing sequence, both contributions are bounded. The bound for the kinetic energy ensures the compactness in each finite region of a cell by the Sobolev embedding theorem. However, this bound cannot prevent the decay of the electron field, i.e., its escape to infinity. Nevertheless, the Coulomb interaction prevents even the partial escape to infinity, as we show in Lemma 3.4. Physically, this means that the electrostatic potential of the remaining positive charge becomes confining.

II. We construct the solution to the Poisson equation (1.6) as the contour integral, providing the continuity and a bound for the electrostatic potential. The main difficulty is a verification of the Schrödinger equation (1.5) for the minimizer. Namely, the Lagrange method of multipliers is not applicable because the energy per cell is infinite outside the submanifold $M \subset H^1(T_d)$ due to the infrared divergence of the Coulomb bond. Moreover, the Coulomb bond is infinite for a dense set of $\psi \in M$. Hence, to differentiate the energy functional, we should construct the smooth paths in M lying outside this dense set.

III. Finally, the proof that ω^0 is real (which is the stability condition for the ground state) is not straightforward for 2D and 1D lattices, since the potential $\phi^0(\mathbf{x})$ a priori can grow at infinity. The correponding bounds for the potentials are given by (3.15) and (4.12).

The minimization strategy ensures the existence of a ground state for any lattice (1.1). One could expect that a stable lattice should provide a local minimum of the energy per cell for fixed d, N and functions ρ_j, but this is still an open problem.

Let us comment on related works. For atomic systems in $\mathbb{R}^3$, a ground state was constructed by Lieb, Simon, and Lions in the case of the Hartree and Hartree–Fock models [24, 26, 27], and by Nier for the Schrödinger–Poisson model [28]. The Hartree–Fock dynamics for molecular systems in $\mathbb{R}^3$ has been constructed by Cancès and Le Bris [7].

A mathematical theory of the stability of matter started from the pioneering works of Dyson, Lebowitz, Lenard, Lieb, and others for the Schrödinger many body model [14, 20, 21, 23]; see the survey in [17]. Recently, the theory was extended to the quantized Maxwell field [22].

These results and methods were developed in the last two decades by Blanc, Le Bris, Catto, Lions, and others to justify the thermodynamic limit for the Thomas–Fermi and Hartree–Fock models with space-periodic ion arrangement [4, 10, 11, 12] and to construct the corresponding space-periodic ground states [13]; see the survey and further references in [5].

Recently, Giuliani, Lebowitz, and Lieb have established the periodicity of the thermodynamic limit in the 1D local mean field model without the assumption of periodicity of the ion arrangement [15].

Cancès and others studied short-range perturbations of the Hartree–Fock model and proved that the density matrices of the perturbed and unperturbed ground states differ by a compact operator [8, 9].

The Hartree–Fock dynamics for infinite particle systems were considered recently by Cancès and Stoltz [9] and Lewin and Sabin [18]. In [9], the well-posedness is established for local perturbations of the periodic ground state density matrix in an infinite crystal. However, the space-periodic nuclear potential in [9, equation (3)] does not depend on time that corresponds to the fixed nuclei positions. Thus the back reaction of the electrons onto the nuclei is neglected. In [18], the well-posedness is established for the von Neumann equation with density matrices of infinite trace for pairwise interaction potentials $w \in L^1(\mathbb{R}^3)$. Moreover, the authors prove the asymptotic stability of the ground state in the 2D case [19]. Nevertheless, the case of the Coulomb potential for infinite particle systems remains open since the corresponding generator is infinite.

Let us note that 2D and 1D crystals in $\mathbb{R}^3$ were not considered previously. The space-periodic ground states for 1D and 2D lattices give the model of the nanostructures similar to the carbon nanotubes and graphene, respectively.

The plan of our paper is as follows. In section 2, we consider the 3D lattice. In section 3, we construct a ground state, derive (1.5)–(1.7), and study smoothness properties of a ground state for the 2D lattice. In section 4, we consider the 1D lattice. Finally, in the appendix we construct and estimate the potential for the 1D lattice.

2. 3D lattice. We consider the system (1.5)–(1.7) for the corresponding functions on the torus $T_3 = \mathbb{R}^3/\Gamma_3$ with $\mathbf{x}_j^0 \bmod \Gamma_3 \in T_3$. For $s \in \mathbb{R}$, we denote by H^s the complex Sobolev space on the torus T_3, and for $1 \le p \le \infty$, we denote by L^p the complex Lebesgue space of functions on T_3.

2.1. Energy per cell. The ground state will be constructed by minimizing the energy in the cell T_3. To this aim, we will minimize the energy with respect to $\overline{\mathbf{x}} := (\mathbf{x}_1, \dots, \mathbf{x}_N) \in (T_3)^N$ and $\psi \in H^1$ satisfying the neutrality condition (1.11):

$$\int_{T_3} \rho(\mathbf{x}) d\mathbf{x} = 0, \qquad \rho(\mathbf{x}) := \sigma(\mathbf{x}) + e|\psi(\mathbf{x})|^2, \tag{2.1}$$

where we set

$$\sigma(\mathbf{x}) := \sum_j \mu_j^{\mathrm{per}}(\mathbf{x} - \mathbf{x}_j), \tag{2.2}$$

similarly to (1.8). Let us note that $\rho \in L^2$ for $\psi \in H^1$ by our condition (1.9) since $\psi \in L^6$ by the Sobolev embedding theorem.

We define the energy in the periodic cell for $\psi \in H^1$ by

$$E(\psi, \overline{\mathbf{x}}) := \int_{T_3} \left[\frac{\hbar^2}{2\mathrm{m}} |\nabla \psi(\mathbf{x})|^2 + \frac{1}{2} \phi(\mathbf{x}) \rho(\mathbf{x}) \right] d\mathbf{x}, \qquad \phi(\mathbf{x}) := (-\Delta)^{-1} \rho, \tag{2.3}$$

where $(-\Delta)^{-1}\rho$ is well defined by (2.1). Namely, consider the dual lattice

$$\Gamma_3^* = \{ \mathbf{k}(\mathbf{n}) = \mathbf{b}_1 n_1 + \mathbf{b}_2 n_2 + \mathbf{b}_3 n_3 : \mathbf{n} = (n_1, n_2, n_3) \in \mathbb{Z}^3 \}, \tag{2.4}$$

where $\mathbf{b}_k \mathbf{a}_{k'} = 2\pi \delta_{kk'}$. Every function $\rho \in L^2$ admits the Fourier representation

$$\rho(\mathbf{x}) = \frac{1}{\sqrt{|T_3|}} \sum_{\mathbf{k} \in \Gamma_3^*} \hat{\rho}(\mathbf{k}) e^{-i\mathbf{k}\mathbf{x}}, \qquad \hat{\rho}(\mathbf{k}) = \frac{1}{\sqrt{|T_3|}} \int e^{i\mathbf{k}\mathbf{x}} \rho(\mathbf{x}) d\mathbf{x}. \tag{2.5}$$

Respectively, we set

$$\phi(\mathbf{x}) = (-\Delta)^{-1} \rho(\mathbf{x}) := \frac{1}{\sqrt{|T_3|}} \sum_{\mathbf{k} \in \Gamma_3^* \setminus 0} \frac{\hat{\rho}(\mathbf{k})}{\mathbf{k}^2} e^{-i\mathbf{k}\mathbf{x}}. \tag{2.6}$$

This function $\phi \in H^2$ and satisfies the Poisson equation $-\Delta \phi = \rho$, since $\hat{\rho}(0) = 0$ due to the neutrality condition (2.1). Finally,

$$\int_{T_3} \phi(\mathbf{x}) d\mathbf{x} = 0. \tag{2.7}$$

Now it is clear that the energy (2.3) is finite for $\psi \in H^1$. Let us rewrite the energy as

$$E(\psi, \overline{\mathbf{x}}) = I_1 + I_2, \tag{2.8}$$

where

$$I_1(\psi) := \frac{\hbar^2}{2\mathrm{m}} \int_{T_3} |\nabla\psi(\mathbf{x})|^2 d\mathbf{x} \geq 0, \tag{2.9}$$

$$I_2(\phi) := \frac{1}{2} \int_{T_3} (-\Delta)^{-1} \rho(\mathbf{x}) \cdot \rho(\mathbf{x}) d\mathbf{x} = \frac{1}{2} \int_{T_3} |\nabla\phi(\mathbf{x})|^2 d\mathbf{x} \geq 0. \tag{2.10}$$

The functional (2.3) is chosen because

$$\frac{\delta E}{\delta \mathbf{x}_j} = -\langle (-\Delta)^{-1} \rho(\mathbf{x}), \nabla \rho_j^{\text{per}}(\mathbf{x} - \mathbf{x}_j) \rangle = \langle \nabla\phi(\mathbf{x}), \rho_j^{\text{per}}(\mathbf{x} - \mathbf{x}_j) \rangle, \tag{2.11}$$

and the variational derivatives *formally* read

$$\frac{\delta E}{\delta \Psi(\mathbf{x})} = -2\frac{\hbar^2}{2\mathrm{m}} \Delta\psi + 2e(-\Delta)^{-1} \rho(\mathbf{x})\psi(\mathbf{x}) = -2\frac{\hbar^2}{2\mathrm{m}} \Delta\psi + 2e\phi(\mathbf{x})\psi(\mathbf{x}). \tag{2.12}$$

The variation in (2.12) is taken over $\Psi(\mathbf{x}) = (\psi_1(\mathbf{x}), \psi_2(\mathbf{x})) \in L^2(T_3, \mathbb{R}^2)$, where $\psi_1(\mathbf{x}) = \Re\psi(x)$ and $\psi_2(\mathbf{x}) = \Im\psi(x)$. Respectively, all the terms in (2.12) are identified with the corresponding $\mathbb{R}^2$-valued distributions.

2.2. Compactness of minimizing sequence. Our purpose here is to minimize the energy with respect to

$$(\psi, \overline{\mathbf{x}}) \in \mathcal{M} := M \times T_3^N,$$

where M denotes the manifold (cf. (1.12))

$$M = \left\{ \psi \in H^1 : \int_{T_3} |\psi(\mathbf{x})|^2 d\mathbf{x} = Z \right\}. \tag{2.13}$$

The energy is bounded from below since $E(\psi, \overline{\mathbf{x}}) \geq 0$ by (2.8)–(2.10). We choose a minimizing sequence $(\psi_n, \overline{\mathbf{x}}_n) \in \mathcal{M}$ such that

$$E(\psi_n, \overline{\mathbf{x}}_n) \to E^0 := \inf_{\mathcal{M}} E(\psi, \overline{\mathbf{x}}), \qquad n \to \infty. \tag{2.14}$$

Our main result for a 3D lattice is the following.

THEOREM 2.1. *Let condition* (1.9) *hold. Then*

(i) *there exists* $(\psi^0, \overline{\mathbf{x}}^0) \in \mathcal{M}$ *with*

$$E(\psi^0, \overline{\mathbf{x}}^0) = E^0; \tag{2.15}$$

(ii) *moreover,* $\psi^0 \in H^2$ *and satisfies* (1.5)–(1.7) *with* $d = 3$*, where the potential* $\phi^0 \in H^2$ *is real, and* $\omega^0 \in \mathbb{R}$.

To prove item (i), let us denote

$$\rho_n(\mathbf{x}) := \sigma_n(\mathbf{x}) + e|\psi_n(\mathbf{x})|^2, \qquad \sigma_n(\mathbf{x}) := \sum_j \mu_j^{\text{per}}(\mathbf{x} - \mathbf{x}_{jn}). \tag{2.16}$$

Now the sequence ψ_n and the corresponding sequence $\phi_n := (-\Delta)^{-1}\rho_n$ are bounded in H^1 by (2.8)–(2.10), (2.7), and (2.13)–(2.14). Hence, both sequences are precompact in L^p for any $p \in [1,6)$ by the Sobolev embedding theorem [1, 30]. Therefore, the sequence ρ_n is precompact in L^2 by our assumption (1.9), and respectively, the sequence ϕ_n is precompact in H^2. As a result, there exist a subsequence $n' \to \infty$ for which

$$\psi_{n'} \xrightarrow{L^p} \psi^0, \qquad \phi_{n'} \xrightarrow{H^2} \phi^0, \qquad \overline{\mathbf{x}}_{n'} \to \overline{\mathbf{x}}^0, \qquad n' \to \infty \tag{2.17}$$

with any $p \in [1,6)$. Respectively,

$$\sigma_{n'} \xrightarrow{L^2} \sigma^0, \qquad \rho_{n'} \xrightarrow{L^2} \rho^0, \qquad n' \to \infty, \tag{2.18}$$

where $\sigma^0(\mathbf{x})$ and $\rho^0(\mathbf{x})$ are defined by (1.8) and (1.6). Hence, the neutrality condition (1.11) holds, $(\psi^0, \overline{\mathbf{x}}^0) \in \mathcal{M}$, $\phi^0 \in H^2$, and for these limit functions we have

$$-\Delta\phi^0 = \rho^0, \qquad \int_{T_3} \phi^0(\mathbf{x}) d\mathbf{x} = 0. \tag{2.19}$$

To prove identity (2.15), we take into account that $I_1(\psi)$ is lower semicontinuous on L^2, while $I_2(\phi)$ is continuous on H^2, i.e.,

$$I_1(\psi^0) \le \liminf_{n' \to \infty} I_1(\psi_{n'}), \qquad I_2(\phi^0) = \lim_{n' \to \infty} I_2(\phi_{n'}). \tag{2.20}$$

These limits, together with (2.14), imply that

$$E(\psi^0, \overline{\mathbf{x}}^0) = I_1(\psi^0) + I_2(\phi^0) \le E^0. \tag{2.21}$$

Now (2.15) follows from the definition of E^0, since $(\psi^0, \overline{\mathbf{x}}^0) \in \mathcal{M}$. Thus Theorem 2.1 (i) is proved.

We will prove item (ii) in the next sections.

2.3. Variation of the energy. Theorem 2.1(ii) follows from the next proposition.

PROPOSITION 2.2. *The limit functions* (2.17) *satisfy* (1.5)–(1.7) *with* $d = 3$ *and* $\omega^0 \in \mathbb{R}$.

Equation (1.6) is proved in (2.19), and (1.7) follows from (2.11) and (2.15). It remains to prove the Schrödinger equation (1.5). Let us denote $\mathcal{E}(\psi) := E(\psi, \overline{\mathbf{x}}^0)$. We derive (1.5) in the next sections, equating the variation of $\mathcal{E}(\cdot)|_M$ to zero at $\psi = \psi^0$. In this section we calculate the corresponding Gâteaux variational derivative.

We should work directly on M, introducing an atlas in a neighborhood of ψ^0 in M. We define the atlas as the stereographic projection from the tangent plane $TM(\psi^0) = (\psi^0)^\perp := \{\psi \in H^1 : \langle \psi, \psi^0 \rangle = 0\}$ to the sphere (2.13):

$$\psi_\tau = \frac{\psi^0 + \tau}{\|\psi^0 + \tau\|_{L^2}} \sqrt{Z}, \qquad \tau \in (\psi^0)^\perp. \tag{2.22}$$

Obviously,

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \psi_{\varepsilon\tau} = \tau, \qquad \tau \in (\psi^0)^\perp, \tag{2.23}$$

where the derivative exists in H^1. We define the “Gâteaux derivative” of $\mathcal{E}(\cdot)|_M$ as

$$D_\tau \mathcal{E}(\psi^0) := \lim_{\varepsilon \to 0} \frac{\mathcal{E}(\psi_{\varepsilon\tau}) - \mathcal{E}(\psi^0)}{\varepsilon} \tag{2.24}$$

if this limit exists. We should restrict the set of allowed tangent vectors τ.

Definition 2.3. *$\mathcal{T}^0$ is the space of test functions $\tau \in (\psi^0)^\perp \cap C^\infty(T_3)$.*

Obviously, $\mathcal{T}^0$ is dense in $(\psi^0)^\perp$ in the norm of H^1. Let us rewrite the energy (2.3) as

$$\mathcal{E}(\psi) := \int_{T_3} \left[\frac{\hbar^2}{2\mathrm{m}} |\nabla\psi(\mathbf{x})|^2 + \frac{1}{2}|\Lambda\rho(\mathbf{x})|^2 \right] d\mathbf{x}, \qquad \rho(\mathbf{x}) := \sigma(\mathbf{x}) + e|\psi(\mathbf{x})|^2, \tag{2.25}$$

where $\Lambda := (-\Delta)^{-1/2}$ is defined similarly to (2.6):

$$\Lambda\rho(\mathbf{x}) := \frac{1}{\sqrt{|T_3|}} \sum_{\mathbf{k}\in\Gamma_3^*\setminus 0} \frac{\hat{\rho}(\mathbf{k})}{|\mathbf{k}|} e^{-i\mathbf{k}\mathbf{x}} \in L^2 \qquad \text{for} \qquad \rho \in L^2. \tag{2.26}$$

Lemma 2.4. *Let $\tau \in \mathcal{T}^0$. Then the derivative (2.24) exists, and (cf. (2.12))*

$$D_\tau \mathcal{E}(\psi^0) = \int_{T_3} \left[\frac{\hbar^2}{2\mathrm{m}} (\nabla\tau\overline{\nabla\psi^0} + \nabla\psi^0\overline{\nabla\tau}) + e\Lambda\rho^0\Lambda(\tau\overline{\psi^0} + \psi^0\overline{\tau}) \right] d\mathbf{x}. \tag{2.27}$$

Proof. Let us denote $\rho_{\varepsilon\tau}(\mathbf{x}) := \sigma^0(\mathbf{x}) + e|\psi_{\varepsilon\tau}(\mathbf{x})|^2$.

Lemma 2.5. *For $\tau \in \mathcal{T}^0$, we have*

$$D_\tau\Lambda\rho := \lim_{\varepsilon\to 0} \frac{\Lambda\rho_{\varepsilon\tau} - \Lambda\rho^0}{\varepsilon} = e\Lambda(\tau\overline{\psi^0} + \psi^0\overline{\tau}), \tag{2.28}$$

where the limit converges in L^2.

Proof. In the polar coordinates,

$$\psi_{\varepsilon\tau} = (\psi^0 + \varepsilon\tau)\cos\alpha, \qquad \alpha = \alpha(\varepsilon) = \arctan \frac{\varepsilon\|\tau\|_{L^2}}{\|\psi^0\|_{L^2}}. \tag{2.29}$$

Hence,

$$\begin{aligned} \Lambda\rho_{\varepsilon\tau} &= \Lambda\sigma^0 + e\cos^2\alpha\Lambda|\psi^0 + \varepsilon\tau|^2 \\ &= \Lambda\rho^0 + e\varepsilon\cos^2\alpha\Lambda(\tau\overline{\psi^0} + \psi^0\overline{\tau}) + e\Lambda[\varepsilon^2|\tau|^2\cos^2\alpha - |\psi^0|^2\sin^2\alpha]. \end{aligned} \tag{2.30}$$

Here, $\Lambda\rho^0 \in L^2$ since $\rho^0 \in L^2$, and similarly $\Lambda[\psi^0\overline{\tau}] \in L^2$ since $\psi^0\overline{\tau} \in L^2$. It remains to estimate the last term of (2.30),

$$R_\varepsilon := \Lambda[\varepsilon^2|\tau|^2\cos^2\alpha - |\psi^0|^2\sin^2\alpha]. \tag{2.31}$$

Here, $|\psi^0|^2 \in L^2$ since $\psi^0 \in H^1 \subset L^6$. Finally, $|\tau|^2 \in L^2$ and $\sin^2\alpha \sim \varepsilon^2$. Hence, the convergence (2.28) holds in L^2. ∎

Now (2.27) follows by differentiation in ε of (2.25) with $\psi = \psi_{\varepsilon\tau}$ and $\rho = \rho_{\varepsilon\tau}$. ∎

2.4. The variational identity. Since ψ^0 is a minimal point, the Gâteaux derivative (2.27) vanishes:

$$\int_{T_2} \left[\frac{\hbar^2}{2\mathrm{m}} (\nabla\tau\overline{\nabla\psi^0} + \nabla\psi^0\overline{\nabla\tau}) + e\Lambda\rho^0\Lambda(\tau\overline{\psi^0} + \psi^0\overline{\tau}) \right] d\mathbf{x} = 0. \tag{2.32}$$

Substituting $i\tau$ instead of τ in this identity and subtracting, we obtain

$$-\frac{\hbar^2}{2\mathrm{m}} \langle \Delta\psi^0, \tau\rangle + e\langle \Lambda\rho^0, \Lambda(\overline{\psi^0}\tau)\rangle = 0. \tag{2.33}$$

In the next step, we should evaluate the "nonlinear" term.

LEMMA 2.6. *For the limit functions* (2.17)–(2.18), *we have*

$$\langle \Lambda\rho^0, \Lambda(\overline{\psi^0}\tau)\rangle = \langle \phi^0\psi^0, \tau\rangle, \qquad \tau \in \mathcal{T}^0. \tag{2.34}$$

Proof. Let us substitute $\rho^0 = -\Delta\phi^0$. Then, by the Parseval–Plancherel identity,

$$\langle \Lambda\rho^0, \Lambda(\overline{\psi^0}\tau)\rangle = \sum_{\mathbf{k}\in\Gamma_3^*\setminus 0} \frac{\mathbf{k}^2\hat{\phi}^0(\mathbf{k})}{|\mathbf{k}|} \cdot \frac{\widehat{\overline{\psi^0}\tau}(\mathbf{k})}{|\mathbf{k}|} = \langle \hat{\phi}^0, \widehat{\overline{\psi^0}\tau}\rangle = \langle \phi^0, \overline{\psi^0}\tau\rangle = \langle \phi^0\psi^0, \tau\rangle, \tag{2.35}$$

which proves (2.34). ∎

Using (2.34), we can rewrite (2.33) as the variational identity (cf. (2.12))

$$\left\langle -\frac{\hbar^2}{2\mathrm{m}}\Delta\psi^0 + e\phi^0\psi^0, \tau \right\rangle = 0, \qquad \tau \in \mathcal{T}^0. \tag{2.36}$$

2.5. The Schrödinger equation. Now we prove the Schrödinger equation (1.5) with $d = 3$.

LEMMA 2.7. ψ^0 *is the eigenfunction of the Schrödinger operator* $H = -\frac{\hbar^2}{2\mathrm{m}}\Delta + e\phi^0$*:*

$$H\psi^0 = \lambda\psi^0, \tag{2.37}$$

where $\lambda \in \mathbb{R}$.

Proof. First, $H\psi^0$ is a well-defined distribution since $\phi^0 \in H^2 \subset C(T_3)$ by (2.17). Second, $\psi^0 \neq 0$ since $\psi^0 \in M$ and $Z > 0$. Hence, there exists a test function $\theta \in C^\infty(T_3) \setminus \mathcal{T}^0$, i.e.,

$$\langle \psi^0, \theta\rangle \neq 0. \tag{2.38}$$

Then

$$\langle (H - \lambda)\psi^0, \theta\rangle = 0 \tag{2.39}$$

for an appropriate $\lambda \in \mathbb{C}$. However, $(H - \lambda)\psi^0$ also annihilates $\mathcal{T}^0$ by (2.36), and hence it annihilates the whole space $C^\infty(T_3)$. This implies (2.37) in the sense of distributions with a $\lambda \in \mathbb{C}$. Finally, the potential is real, and $\phi^0 \in C(T_3)$. Hence, $\lambda \in \mathbb{R}$. ∎

This lemma implies (1.5) with $\hbar\omega^0 = \lambda$. Hence, $\psi^0 \in H^2$ since $\phi^0 \in C(T_3)$. Now Theorem 2.1(ii) is proved.

2.6. Smoothness of the ground state. We have proved that $\psi^0 \in H^2$ under condition (1.9). Using the Schrödinger equation (2.37), we can improve further the smoothness of ψ^0, strengthening the condition (1.9). Namely, let us assume that

$$\mu_j^{\mathrm{per}} \in C^\infty(T_3), \qquad j = 1, \ldots, N. \tag{2.40}$$

Then also

$$\sigma^0(\mathbf{x}) := \sum_{j=1}^{N} \mu_j^{\mathrm{per}}(\mathbf{x} - \mathbf{x}_j^0) \in C^\infty(T_3). \tag{2.41}$$

For example, (2.40) and (2.41) hold if $\mu_j \in \mathcal{S}(\mathbb{R}^3)$, where $\mathcal{S}(\mathbb{R}^3)$ is the Schwartz space of test functions.

LEMMA 2.8. *Let condition* (2.40) *hold, and* $\psi^0 \in H^2$, $\phi^0 \in H^2$ *be a solution to* (1.5)–(1.6) *with* $d = 3$. *Then the functions* ψ^0 *and* ϕ^0 *are smooth.*

Proof. First, $\phi^0\psi^0 \in H^2$ since H^s is the algebra for $s > 3/2$. Hence, (1.5) implies that

$$\psi^0 \in H^4 \subset C^2(T_3). \tag{2.42}$$

Now $\rho^0 := \sigma^0 + e|\psi^0|^2 \in H^4$ by (2.40). Then (1.6) implies that $\phi^0 \in H^6 \subset C^4(T_3)$. Hence, $\phi^0\psi^0 \in H^4$, $\psi^0 \in H^6$, $\rho^0 \in H^6$, etc. □

3. 2D lattice. For simplicity of notation, we will consider the 2D lattice $\Gamma_2 = \mathbb{Z}^2$ and construct a solution to system (1.5)–(1.7) for the corresponding functions on the "cylindrical cell" $T_2 := \mathbb{R}^3/\Gamma_2 = \mathbb{T}^2 \times \mathbb{R}$ with the coordinates $\mathbf{x} = (x_1, x_2, x_3)$, where $(x_1, x_2) \in \mathbb{T}^2$ and $x_3 \in \mathbb{R}$. Now we denote by H^s the complex Sobolev space on T_2, and by L^p, the complex Lebesgue space of functions on T_2.

We will construct a ground state by minimizing the energy (2.3), where the integral is extended over T_2 instead of T_3. The neutrality condition of type (2.1) holds for Γ_2-periodic states with finite energy, as we show below.

3.1. The energy per cell. We restrict ourselves by $N = 1$, so $\overline{\mathbf{x}}^0 = \mathbf{x}_1^0$ can be chosen arbitrarily because of the translation invariance of the system (1.5)–(1.7). For example, we can set $\mathbf{x}_1^0 = 0$.

The energy in the cylindrical cell T_2 is defined similarly to (2.3), which we rewrite as (2.25)

$$\mathcal{E}(\psi) := \int_{T_2} \left[\frac{\hbar^2}{2\mathrm{m}}|\nabla\psi(\mathbf{x})|^2 + \frac{1}{2}|\Lambda\rho(\mathbf{x})|^2\right] d\mathbf{x}, \qquad \rho(\mathbf{x}) := \sigma^0(\mathbf{x}) + e|\psi(\mathbf{x})|^2. \tag{3.1}$$

Here, $\sigma^0(\mathbf{x})$ is defined by (2.2) with $N = 1$ and $\mathbf{x}_1^0 = 0$,

$$\sigma^0 = \mu_1^{\mathrm{per}} \in L^1 \cap L^2 \tag{3.2}$$

according to our condition (1.9). Hence, we have

$$\int_{T_2} \sigma^0(\mathbf{x}) d\mathbf{x} = Z_1|e|, \qquad Z_1 > 0. \tag{3.3}$$

Further, Λ is the operator $(-\Delta)^{-1/2}$ defined by the Fourier transform. Namely, we denote $\Gamma_2^* = 2\pi\Gamma_2$ and define the Fourier representation for the test functions $\varphi \in C_0^\infty(T_2)$ by

$$\varphi(\mathbf{x}) = \frac{1}{\sqrt{2\pi}} \sum_{\mathbf{k}\in\Gamma_2^*} e^{-i(\mathbf{k}_1x_1+\mathbf{k}_2x_2)} \int_{\mathbb{R}} e^{-i\xi x_3}\hat{\varphi}(\mathbf{k}, \xi) d\xi, \qquad \mathbf{x} \in T_2, \tag{3.4}$$

where

$$\hat{\varphi}(\mathbf{k}, \xi) = F\varphi(\mathbf{k}, \xi) = \frac{1}{\sqrt{2\pi}} \int_{T_2} e^{i(\mathbf{k}_1x_1+\mathbf{k}_2x_2+\xi x_3)}\varphi(\mathbf{x}) d\mathbf{x}, \qquad (\mathbf{k}, \xi) \in \Sigma_2 := \Gamma_2^* \times \mathbb{R}. \tag{3.5}$$

The operator Λ is defined for $\varphi \in L^1 \cap L^2$ by

$$\Lambda\varphi = F^{-1}\frac{\hat{\varphi}(\mathbf{k}, \xi)}{\sqrt{\mathbf{k}^2 + \xi^2}} \tag{3.6}$$

provided that the quotient belongs to $L^2(\Sigma_2)$. In this case,

$$\hat{\varphi}(0, 0) = 0. \tag{3.7}$$

Let us note that $\rho \in L^1 \cap L^2$ for $\psi \in H^1$ by our condition (1.9) since $\psi \in L^p$ with $p \in [2,6]$ by the Sobolev embedding theorem. For $\psi \in H^1$ with finite energy (3.1), we have $\Lambda\rho \in L^2(\Sigma_2)$. Therefore, (3.7) with $\varphi = \rho$ implies the neutrality condition (2.1) with T_2 instead of T_3:

$$\hat{\rho}(0,0) = \int_{T_2} \rho(\mathbf{x}) d\mathbf{x} = \int_{T_2} [\sigma^0(\mathbf{x}) + e|\psi(\mathbf{x})|^2] d\mathbf{x} = 0. \tag{3.8}$$

Now (3.3) gives

$$\int_{T_2} |\psi(\mathbf{x})|^2 d\mathbf{x} = Z_1. \tag{3.9}$$

In other words, the finiteness of the Coulomb energy $\|\Lambda\rho\|^2$ prevents the electron charge from escaping to infinity, as mentioned in the introduction.

DEFINITION 3.1. *M_2 denotes the set of $\psi \in H^1$ satisfying the neutrality condition* (3.9).

It is important that the energy be finite for a nonempty set of $\psi \in H^1$. To find the corresponding condition, let us rewrite the energy (3.1) using the Parseval–Plancherel identity:

$$\mathcal{E}(\psi) = \sum_{\mathbf{k}\in\Gamma_2^*} \frac{\hbar^2}{2\mathrm{m}} \int_{\mathbb{R}} (\mathbf{k}^2 + \xi^2)|\hat{\psi}(\mathbf{k},\xi)|^2 d\xi + \frac{1}{2} \sum_{\mathbf{k}\in\Gamma_2^*} \int_{\mathbb{R}} \frac{|\hat{\rho}(\mathbf{k},\xi)|^2}{\mathbf{k}^2 + \xi^2} d\xi. \tag{3.10}$$

Here, the first term on the right-hand side is finite for all $\psi \in H^1$. The second term is finite up to the infrared divergence at the point $(\mathbf{k},\xi) = (0,0)$ since $\rho \in L^2(\Sigma_2)$ for $\psi \in H^1$.

We note that (3.3) can be written as $\hat{\mu}_1^{\mathrm{per}}(0) + eZ_1 = 0$. We will assume that, moreover,

$$\text{Condition II.} \qquad \frac{\hat{\mu}_1^{\mathrm{per}}(0,\xi) + eZ_1}{|\xi|} \in L^2(-1,1). \tag{3.11}$$

For example, this condition holds, provided that

$$\int_{T_2} |x^3||\mu_1^{\mathrm{per}}(\mathbf{x})| d\mathbf{x} < \infty. \tag{3.12}$$

LEMMA 3.2. *Let conditions* (1.9) *and* (3.11) *hold, $N = 1$, and $\mathbf{x}_1^0 \in T_2$. Then the energy* (3.10) *is finite for a dense set of $\psi \in H^1$.*

Proof. By definition, $\hat{\rho}(0,\xi) = \hat{\mu}_1^{\mathrm{per}}(0,\xi) + e\hat{P}(0,\xi)$, where $P(\mathbf{x}) := |\psi(\mathbf{x})|^2$. Hence, (3.11) implies that the energy (3.10) is finite for $\psi \in M_2$ with finite momenta $\int_{T_2} |x^3|\, |\psi(\mathbf{x})|^2 d\mathbf{x} < \infty$. ∎

3.2. Compactness of minimizing sequence. Similarly to the 3D case, the energy is nonnegative, and we choose a minimizing sequence $\psi_n \in M_2$ such that

$$\mathcal{E}(\psi_n) \to \mathcal{E}^0 := \inf_{M_2} \mathcal{E}(\psi), \qquad n \to \infty. \tag{3.13}$$

The second main result of the present paper is the following.

THEOREM 3.3. *Let conditions* (1.9) *and* (3.11) *hold, and* $N = 1$. *Then*

(i) *there exists* $\psi^0 \in M_2$ *with*

$$\mathcal{E}(\psi^0) = \mathcal{E}^0; \tag{3.14}$$

(ii) *moreover,* $\psi^0 \in H^2_{\rm loc}(T_2)$ *and satisfies* (1.5)–(1.7) *with* $d = 2$, *where the potential* $\phi^0 \in H^2_{\rm loc}(T_2)$ *is real,* $\mathbf{x}^0_1 = 0$, *and* $\omega^0 \in \mathbb{R}$;

(iii) *the following bound holds:*

$$|\phi^0(\mathbf{x})| \le C(1 + |x_3|)^{1/2}, \qquad \mathbf{x} \in T_2. \tag{3.15}$$

To prove item (i), let us note that the sequence ψ_n is bounded in H^1 due to (3.1), (3.9), and (3.13). Hence, by the Sobolev embedding theorem [1, 30], the sequence ψ_n is bounded in L^p with each $p \in [2, 6)$ and compact in $L^p_R := L^p(T_2(R))$ for any $R > 0$, where $T_2(R) = \{\mathbf{x} \in T_2 : \ |x_3| < R\}$. Therefore, there exists a subsequence

$$\psi_{n'} \xrightarrow{L^p_R} \psi^0, \qquad \rho_{n'} := \mu_1^{\rm per} + e|\psi_{n'}|^2 \xrightarrow{L^2_R} \rho^0, \qquad n' \to \infty \quad \forall R > 0, \tag{3.16}$$

since $\mu_1^{\rm per} \in L^1 \cap L^2$ by (1.9). Hence, $\psi^0 \in H^1 \cap L^p$, and

$$\rho^0(\mathbf{x}) = \mu_1^{\rm per}(\mathbf{x}) + e|\psi^0(\mathbf{x})|^2 \in L^1 \cap L^2. \tag{3.17}$$

The next problem is to check the neutrality condition (3.9) for the limit charge density ρ^0 since the convergence (3.16) itself is not sufficient.

LEMMA 3.4. *The limit function* $\psi^0 \in M_2$, *and the energy* (3.1) *for* ψ^0 *is finite.*

Proof. Let us prove that

$$\mathcal{E}(\psi^0) \le \mathcal{E}^0. \tag{3.18}$$

Indeed, (3.10) with $\psi = \psi_{n'}$ reads

$$\mathcal{E}(\psi_{n'}) := \left\langle \frac{\hbar^2}{2\mathrm{m}} |f_{n'}(\mathbf{k}, \xi)|^2 + \frac{1}{2} |g_{n'}(\mathbf{k}, \xi)|^2 \right\rangle_{\Sigma_2}, \tag{3.19}$$

where $\langle \dots \rangle_{\Sigma_2}$ stands for $\displaystyle\sum_{\mathbf{k} \in \Gamma_2^*} \int_{\mathbb{R}} \dots \, d\xi$ and

$$f_{n'}(\mathbf{k}, \xi) := \sqrt{\mathbf{k}^2 + \xi^2}\, \hat{\psi}_{n'}(\mathbf{k}, \xi), \qquad g_{n'}(\mathbf{k}, \xi) := \frac{\hat{\rho}_{n'}(\mathbf{k}, \xi)}{\sqrt{\mathbf{k}^2 + \xi^2}}.$$

The functions $\hat{\psi}_{n'}$ and $\hat{\rho}_{n'}$ are bounded in $L^2(\Sigma_2)$ and are converging in the sense of distributions due to (3.16). Hence,

$$\hat{\psi}_{n'} \xrightarrow{L^2_w} \hat{\psi}^0, \qquad \hat{\rho}_{n'} \xrightarrow{L^2_w} \hat{\rho}^0, \qquad n' \to \infty. \tag{3.20}$$

Similarly, the functions $f_{n'}$ and $g_{n'}$ are bounded in $L^2(\Sigma_2)$ by (3.19), (3.13) and are converging in the sense of distributions due to (3.20). Therefore,

$$f_{n'} \xrightarrow{L^2_w} f^0, \qquad g_{n'} \xrightarrow{L^2_w} g^0, \qquad n' \to \infty. \tag{3.21}$$

Hence, for the limit functions,

$$f^0(\mathbf{k},\xi)=\sqrt{\mathbf{k}^2+\xi^2}\hat{\psi}^0(\mathbf{k},\xi), \qquad g^0(\mathbf{k},\xi)=\frac{\hat{\rho}^0(\mathbf{k},\xi)}{\sqrt{\mathbf{k}^2+\xi^2}}, \qquad \text{a.a. } (\mathbf{k},\xi)\in\Sigma_2.$$

Therefore, (3.18) holds since

$$\mathcal{E}(\psi^0)=\left\langle \frac{\hbar^2}{2\mathrm{m}}|f^0(\mathbf{k},\xi)|^2+\frac{1}{2}|g^0(\mathbf{k},\xi)|^2\right\rangle_{\Sigma_2}\le \mathcal{E}^0 \tag{3.22}$$

by the weak convergence (3.21) and the lower semicontinuity. In particular,

$$\Lambda\rho^0\in L^2. \tag{3.23}$$

Therefore, $\hat{\rho}^0(0,0)=0$ as in (3.8) since $\rho^0\in L^1$ by (3.17). Hence, $\psi^0\in M_2$. ∎

Now (3.18) implies (3.14). Thus, Theorem 3.3(i) is proved.

3.3. The Poisson equation. Our aim here is to construct the potential which is the solution to the Poisson equation (1.6) with $d=2$. It suffices to solve the equation

$$\nabla\phi^0(\mathbf{x})=G^0(\mathbf{x}), \qquad \mathbf{x}\in T_2, \tag{3.24}$$

where $G^0(\mathbf{x}):=-iF^{-1}\frac{(\mathbf{k},\xi)}{\mathbf{k}^2+\xi^2}\hat{\rho}^0(\mathbf{k},\xi)$ is a real vector field, $G^0\in L^2\otimes\mathbb{R}^3$ by (3.23), and $\operatorname{rot} G^0(\mathbf{x})\equiv 0$.

LEMMA 3.5. *Equation* (3.24) *admits real solution* $\phi^0\in H^2_{\mathrm{loc}}(T_2)$, *which is unique up to an additive constant and satisfies the bound* (3.15).

Proof. The uniqueness up to constant is obvious. If the solution exists, then $\phi^0\in H^2_{\mathrm{loc}}(T_2)$ by (3.17). Local solutions exist since $\operatorname{rot} G^0(\mathbf{x})\equiv 0$. However, the existence of the global solution is not obvious since the cell T_2 is not 1-connected.

We will prove the existence using the following arguments. Formally, $\phi^0(x)=F^{-1}\frac{\hat{\rho}^0(\mathbf{k},\xi)}{\mathbf{k}^2+\xi^2}$. However, the last expression is not correctly defined distribution in the neighborhood of the point $(0,0)$. To avoid this infrared divergence, we split $\hat{\rho}^0=\hat{\rho}_1+\hat{\rho}_2$, where

$$\hat{\rho}_1(\mathbf{k},\xi)=\begin{cases}\hat{\rho}^0(0,\xi), & \mathbf{k}=0,\ |\xi|<1,\\ 0 & \text{otherwise.}\end{cases} \tag{3.25}$$

Respectively, $G^0=G_1+G_2$, and the solution $\phi^0=\phi_1+\phi_2$. Obviously,

$$G_1(\mathbf{x})=-iF^{-1}\frac{(0,\xi)}{\xi^2}\hat{\rho}_1(0,\xi)=\mathbf{e}_3 g_1(x_3), \qquad \mathbf{e}_3:=(0,0,1), \tag{3.26}$$

and $g_1(x_3)$ is a smooth function. Moreover, (3.17) implies that $g_1\in L^2(\mathbb{R})$ since $G^0\in L^2\otimes\mathbb{R}^3$. Hence, the term $\phi_1(\mathbf{x})=\int_0^{x_3}g_1(s)ds$ is smooth and depends on x_3 only. The bound (3.15) for ϕ_1 follows by the Cauchy–Schwarz inequality.

The second term is given by $\phi_2(\mathbf{x})=F^{-1}\frac{\hat{\rho}_2(\mathbf{k},\xi)}{\mathbf{k}^2+\xi^2}$, where $\hat{\rho}_2\in L^2(\Sigma_2)$ by (3.17). Moreover, $\hat{\rho}_2(0,\xi)=0$ for $|\xi|<1$, and hence $\phi_2\in H^2$. ∎

Remark 3.6.

(i) The function $\phi^0(\mathbf{x}) = (1 + |x_3|)^{1/2-\varepsilon}$ with $\varepsilon > 0$ shows that the bound (3.15) is exact under the condition $\nabla\phi^0 \in L^2$. Note that the potential of a uniformly charged plane grows linearly with the distance.

(ii) In the Fourier transform, (3.24) implies that

$$(\mathbf{k}, \xi)\hat{\phi}^0(\mathbf{k}, \xi) \in L^2(\Sigma_2) \otimes \mathbb{C}^3. \tag{3.27}$$

3.4. Variation of the energy. Theorem 3.3(ii) follows from next proposition.

PROPOSITION 3.7. *The functions ψ^0, ϕ^0 satisfy* (1.5)–(1.7) *with $d = 2$ and $\omega^0 \in \mathbb{R}$.*

Equation (1.6) is proved above, and (1.7) follows from (2.11) and (3.14) by the translation invariance of the energy. It remains to prove the Schrödinger equation (1.5). We are going to derive (1.5), equating the variation of $\mathcal{E}(\psi)|_{M_2}$ to zero at $\psi = \psi^0$. In this section, we calculate the corresponding Gâteaux variational derivative.

Similarly to (2.22), we define the atlas in a neighborhood of ψ^0 in M_2 as the stereographic projection from the tangent plane $TM_2(\psi^0) = (\psi^0)^\perp := \{\psi \in H^1 : \langle\psi, \psi^0\rangle = 0\}$ to the sphere (3.9):

$$\psi_\tau = \frac{\psi^0 + \tau}{\|\psi^0 + \tau\|_{L^2}}\sqrt{Z_1}, \qquad \tau \in (\psi^0)^\perp. \tag{3.28}$$

DEFINITION 3.8. *$\mathcal{T}^0$ is the space of test functions $\tau \in (\psi^0)^\perp \cap C_0^\infty(T_2)$.*

Obviously, $\mathcal{T}^0$ is dense in $(\psi^0)^\perp$ in the norm of H^1.

LEMMA 3.9. *Let $\tau \in \mathcal{T}^0$. Then*

(i) *the energy $\mathcal{E}(\psi_{\varepsilon\tau})$ is finite for $\varepsilon \in \mathbb{R}$;*

(ii) *the Gâteaux derivative* (2.24) *exists, and similarly to* (2.27),

$$D_\tau\mathcal{E}(\psi^0) = \int_{T_2}\left[\frac{\hbar^2}{2\mathrm{m}}(\nabla\tau\overline{\nabla\psi^0} + \nabla\psi^0\overline{\nabla\tau}) + e\Lambda\rho^0\Lambda(\tau\overline{\psi^0} + \psi^0\overline{\tau})\right]d\mathbf{x}. \tag{3.29}$$

Proof. (i) We should prove the bound

$$\mathcal{E}(\psi_{\varepsilon\tau}) := \frac{\hbar^2}{2\mathrm{m}}\int_{T_2}|\nabla\psi_{\varepsilon\tau}(\mathbf{x})|^2 d\mathbf{x} + \frac{1}{2}\int_{T_2}|\Lambda\rho_{\varepsilon\tau}(\mathbf{x})|^2 d\mathbf{x} < \infty, \tag{3.30}$$

where $\rho_{\varepsilon\tau}(\mathbf{x}) := \sigma^0(\mathbf{x}) + e|\psi_{\varepsilon\tau}(\mathbf{x})|^2$. The first integral in (3.30) is finite, since $\psi_{\varepsilon\tau} \in H^1$.

LEMMA 3.10. *$\Lambda\rho_{\varepsilon\tau} \in L^2$ for $\tau \in \mathcal{T}^0$ and $\varepsilon \in \mathbb{R}$, and*

$$D_\tau\Lambda\rho := \lim_{\varepsilon\to 0}\frac{\Lambda\rho_{\varepsilon\tau} - \Lambda\rho^0}{\varepsilon} = e\Lambda(\tau\overline{\psi^0} + \psi^0\overline{\tau}), \tag{3.31}$$

where the limit converges in L^2.

Proof. We use the polar coordinates (2.29) and the corresponding representation (2.30):

$$\Lambda\rho_{\varepsilon\tau} = \Lambda\rho^0 + e\varepsilon\cos^2\alpha\Lambda(\tau\overline{\psi^0} + \psi^0\overline{\tau}) + e\Lambda[\varepsilon^2|\tau|^2\cos^2\alpha - |\psi^0|^2\sin^2\alpha]. \tag{3.32}$$

Now, $\Lambda\rho^0 \in L^2$ according to (3.23). Further, $\Lambda[\tau\overline{\psi^0}] \in L^2$ by the following arguments:

(a) $\tau\overline{\psi^0} \in L^2$,

(b) $\widehat{\tau\overline{\psi^0}}$ is the smooth function on Σ_2, and

(c) the orthogonality $\tau \perp \psi^0$ implies that

$$\widehat{\tau\overline{\psi^0}}(0,0) = 0. \tag{3.33}$$

It remains to estimate the last term of (3.32). Let us denote $T(\mathbf{x}) := |\tau(\mathbf{x})|^2$ and $P(\mathbf{x}) := |\psi^0(\mathbf{x})|^2$. Then the last term (up to a constant factor) reads

$$R_\varepsilon(\mathbf{x}) := \Lambda[\varepsilon^2 T(\mathbf{x}) \cos^2\alpha - P(\mathbf{x}) \sin^2\alpha]. \tag{3.34}$$

LEMMA 3.11. *$R_\varepsilon \in L^2$ for $\varepsilon \in \mathbb{R}$, and*

$$\|R_\varepsilon\|_{L^2} = \mathcal{O}(\varepsilon^2), \qquad \varepsilon \to 0. \tag{3.35}$$

Proof.
(i) It suffices to check that

$$\begin{aligned} &\frac{\varepsilon^2 \hat{T}(0,\xi)\cos^2\alpha - \hat{P}(0,\xi)\sin^2\alpha}{|\xi|} \\ &= \frac{(\varepsilon^2 \hat{T}(0,\xi) - Z_1 \tan^2\alpha)\cos^2\alpha}{|\xi|} - \frac{(\hat{P}(0,\xi) - Z_1)\sin^2\alpha}{|\xi|} \in L^2(-1,1). \end{aligned} \tag{3.36}$$

Let us consider each term of the last line of (3.36) separately.

(1) The first quotient belongs to $L^2(-1,1)$, since

$$\varepsilon^2 \hat{T}(0,0) - Z_1 \tan^2\alpha = \int_{T_2} \varepsilon^2 |\tau|^2 d\mathbf{x} - Z_1 \tan^2\alpha = 0 \tag{3.37}$$

by the definition of α in (2.29) since $\|\psi^0\| = \sqrt{Z_1}$.

(2) The second quotient belongs to $L^2(-1,1)$, since

$$\frac{\hat{\rho}^0}{|\xi|} = \frac{\hat{\mu}_1^{\text{per}}}{|\xi|} + e\frac{\hat{P}}{|\xi|} = \frac{\hat{\mu}_1^{\text{per}} + eZ_1}{|\xi|} + e\frac{\hat{P} - Z_1}{|\xi|}, \tag{3.38}$$

where all the functions are taken at the point $(0,\xi)$. Here, the left-hand side belongs to $L^2(-1,1)$, since $\Lambda\rho^0 \in L^2$, while the first term on the right belongs to $L^2(-1,1)$ by our assumption (3.11).

(ii) The bound (3.35) holds for both terms of (3.36) by the arguments above since $\tan\alpha \sim \sin\alpha \sim \varepsilon$ as $\varepsilon \to 0$. ∎

Formula (3.32) implies (3.31), where the limit converges in L^2 by (3.35). ∎

(ii) Lemma 3.10 implies the bound (3.30). Formula (3.29) follows by differentiation of (3.30) in ε. ∎

3.5. The variational identity. Since ψ^0 is a minimal point, the Gâteaux derivative (3.29) vanishes:

$$\int_{T_2} \left[\frac{\hbar^2}{2\mathrm{m}} (\nabla\tau \overline{\nabla\psi^0} + \nabla\psi^0 \overline{\nabla\tau}) + e\Lambda\rho^0 \Lambda(\tau\overline{\psi^0} + \psi^0\overline{\tau}) \right] d\mathbf{x} = 0. \tag{3.39}$$

Substituting $i\tau$ instead of τ in this identity and subtracting, we obtain

$$-\frac{\hbar^2}{2\mathrm{m}} \langle \Delta\psi^0, \tau \rangle + e\langle \Lambda\rho^0, \Lambda(\tau\overline{\psi^0}) \rangle = 0. \tag{3.40}$$

In the next step, we should evaluate the "nonlinear" term.

LEMMA 3.12. *For the limit functions* (3.16), *we have*

$$\langle \Lambda\rho^0, \Lambda(\tau\overline{\psi^0})\rangle = \langle \phi^0\psi^0, \tau\rangle, \qquad \tau \in \mathcal{T}^0, \tag{3.41}$$

where ϕ^0 *is any potential satisfying* (3.24).

Proof. First we note that $\Lambda\rho^0 \in L^2$ by 3.23), and $\Lambda(\tau\overline{\psi^0}) \in L^2$ as we have established in the proof of Lemma 3.10. Moreover, $\rho^0 = -\Delta\phi^0$. Then, by the Parseval–Plancherel identity,

(3.42)
$$\langle \Lambda\rho^0, \Lambda(\tau\overline{\psi^0})\rangle = \sum_{\mathbf{k}\in\Gamma_2^*\setminus 0}\int \hat\phi^0(\mathbf{k},\xi)\overline{\widehat{\tau\overline{\psi^0}}(\mathbf{k},\xi)}d\xi + \lim_{\varepsilon\to 0+}\int_{|\xi|>\varepsilon}\hat\phi^0(0,\xi)\overline{\widehat{\tau\overline{\psi^0}}(0,\xi)}d\xi$$
$$= \langle \hat\phi^0, \widehat{\tau\overline{\psi^0}}\rangle,$$

where $\hat\phi^0$ is the distribution on Σ_2. The last identity holds (and the right-hand side is well defined) by (3.33) since $\xi\hat\phi^0(0,\xi) \in L^2(-1,1)$ due to (3.24) with $G^0 \in L^2 \otimes \mathbb{R}^3$. Finally,

$$\langle \hat\phi^0, \widehat{\tau\overline{\psi^0}}\rangle = \langle \phi^0, \tau\overline{\psi^0}\rangle = \int \phi^0(\mathbf{x})\overline{\tau}(\mathbf{x})\psi^0(\mathbf{x})d\mathbf{x} \tag{3.43}$$

by an obvious extension of the Parseval–Plancherel identity. ∎

Using (3.41), we can rewrite (3.40) as the variational identity similar to (2.36):

$$\left\langle -\frac{\hbar^2}{2\mathrm{m}}\Delta\psi^0 + e\phi^0\psi^0, \tau\right\rangle = 0, \qquad \tau \in \mathcal{T}^0. \tag{3.44}$$

3.6. The Schrödinger equation. Now we prove the Schrödinger equation (1.5) with $d = 2$.

LEMMA 3.13. ψ^0 *is the eigenfunction of the Schrödinger operator:*

$$H\psi^0 = \lambda\psi^0, \tag{3.45}$$

where $\lambda \in \mathbb{R}$.

Proof. This equation with $\lambda \in \mathbb{C}$ follows as in Lemma 2.7. It remains to verify that λ is real. Our plan is standard: to multiply (3.45) by ψ^0 and to integrate. Formally, we would obtain

$$\langle H\psi^0, \psi^0\rangle = \lambda\langle \psi^0, \psi^0\rangle. \tag{3.46}$$

However, it is not clear that the left-hand side is well defined and real since the potential $\phi^0(\mathbf{x})$ can grow by (3.15).

To avoid this problem, we multiply by a function $\psi_\varepsilon \in H^1$ with compact support, where $\varepsilon > 0$ and $\|\psi_\varepsilon - \psi^0\|_{H^1} \to 0$ as $\varepsilon \to 0$. Then

$$\langle H\psi^0, \psi_\varepsilon\rangle = \lambda\langle \psi^0, \psi_\varepsilon\rangle, \tag{3.47}$$

and the right-hand side converges to the one of (3.46) as $\varepsilon \to 0$. Hence, the left-hand sides also converge. In detail,

$$\langle H\psi^0, \psi_\varepsilon\rangle = -\frac{\hbar^2}{2\mathrm{m}}\langle \Delta\psi^0, \psi_\varepsilon\rangle + \langle \phi^0\psi^0, \psi_\varepsilon\rangle. \tag{3.48}$$

For the middle term, the limit exists and is real. Therefore, identity (3.47) implies that the last term is also converging, and hence it remains to make its limit real by a suitable choice of approximations ψ_ε. We note that

$$\langle \phi^0\psi^0, \psi_\varepsilon\rangle = \lim_{\delta\to 0}\langle \phi^0\psi_\delta, \psi_\varepsilon\rangle = \lim_{\delta\to 0}\langle \phi^0, \overline{\psi}_\delta\psi_\varepsilon\rangle, \tag{3.49}$$

since $\phi^0 \in H^2_{\rm loc}(T_2) \subset C(T_2)$. Hence, we can set

$$\psi_\varepsilon(\mathbf{x}) = \chi(\varepsilon x_3)\psi^0(\mathbf{x}), \tag{3.50}$$

where χ is a real function from $C_0^\infty(\mathbb{R}^3)$ with $\psi(0) = 1$. Now the functions $\overline{\psi}_\delta(\mathbf{x})\psi_\varepsilon(\mathbf{x})$ are real for all $\varepsilon, \delta > 0$. It remains to note that the potential $\phi^0(\mathbf{x})$ is also real by Lemma 3.5. ∎

This lemma implies (1.5). Therefore, $\psi^0 \in H^2_{\rm loc}(T_2)$ since $\phi^0 \in C(T_2)$. Theorem 3.3(ii) is proved.

3.7. Smoothness of the ground state. We have proved that $\psi^0 \in H^2_{\rm loc}(T_2)$ under conditions (1.9) and (3.11). Using the Schrödinger equation (1.5), we can improve the smoothness of ψ^0 strengthening the condition (1.9). Namely, let us assume that

$$\mu_1^{\rm per} \in C^\infty(T_2). \tag{3.51}$$

For example, (3.51) holds if $\mu_1 \in \mathcal{S}(\mathbb{R}^3)$, where $\mathcal{S}(\mathbb{R}^3)$ is the Schwartz space of test functions.

LEMMA 3.14. *Let condition* (3.51) *hold, and* $\psi^0 \in H^2_{\rm loc}(T_2)$, $\phi^0 \in H^2_{\rm loc}(T_2)$ *is a solution to* (1.5)–(1.6) *with* $d = 2$. *Then the functions* ψ^0, ϕ^0 *are smooth.*

The proof is similar to the one of Lemma 2.8.

4. 1D lattice. The case of a 1D lattice Γ_1 is very similar to the 2D case, though some of our constructions and arguments require suitable modifications. For $d = 1$, we can assume $\Gamma_1 = \mathbb{Z}$ without loss of generality and construct a solution to system (1.5)–(1.7) for the corresponding functions on the "slab" $T_1 := \mathbb{R}^3/\Gamma_1 = \mathbb{T}^1 \times \mathbb{R}^2$ with coordinates $\mathbf{x} = (x_1, x_2, x_3)$, where $x_1 \in \mathbb{T}^1$, and $(x_2, x_3) \in \mathbb{R}^2$. Now, we denote by H^s the complex Sobolev space on T_1, and by L^p, the complex Lebesgue space of functions on T_1.

The existence of the ground state follows by minimizing the energy (2.3), where the integral is extended over T_1 instead of T_3. The neutrality condition of type (2.1) holds for Γ_1-periodic states with finite energy, as for $d = 2$.

Again, we restrict ourselves by $N = 1$, so $\overline{\mathbf{x}}^0 = \mathbf{x}_1^0$ can be chosen arbitrarily, and we set $\mathbf{x}_1^0 = 0$.

The energy in the slab T_1 is defined by an expression similar to (3.1):

$$\mathcal{E}(\psi) := \int_{T_1}\left[\frac{\hbar^2}{2\mathrm{m}}|\nabla\psi(\mathbf{x})|^2 + \frac{1}{2}|\Lambda\rho(\mathbf{x})|^2\right]d\mathbf{x}, \qquad \rho(\mathbf{x}) := \sigma^0(\mathbf{x}) + e|\psi(\mathbf{x})|^2. \tag{4.1}$$

Here, $\sigma^0 = \mu_i^{\rm per} \in L^1 \cap L^2$ as in (3.2). Hence,

$$\int_{T_1}\sigma^0(\mathbf{x})d\mathbf{x} = Z_1|e|, \qquad Z_1 > 0. \tag{4.2}$$

Now the Fourier representation for the test functions $\varphi(x) \in C_0^\infty(T_1)$ is defined by

$$\varphi(\mathbf{x}) = \frac{1}{2\pi}\sum_{\mathbf{k}\in\Gamma_1^*} e^{-i\mathbf{k}x_1}\int_{\mathbb{R}^2} e^{-i(\xi_1x_2+\xi_2x_3)}\hat{\varphi}(\mathbf{k},\xi)d\xi, \tag{4.3}$$

where $\Gamma_1^* = 2\pi\Gamma_1$ and
(4.4)
$$\hat{\varphi}(\mathbf{k},\xi) = F\varphi(\mathbf{k},\xi) = \frac{1}{2\pi}\int_{T_1} e^{i(\mathbf{k}x_1+\xi_1x_2+\xi_2x_3)}\varphi(\mathbf{x})d\mathbf{x}, \qquad (\mathbf{k},\xi)\in\Sigma_1 := \Gamma_1^*\times\mathbb{R}^2.$$

The operator $\Lambda = (-\Delta)^{1/2}$ is defined for $\varphi \in L^1 \cap L^2$ by the same formula (3.6) provided the quotient belongs to $L^2(\Sigma_1)$. This implies

$$\hat{\varphi}(0,0) = 0. \tag{4.5}$$

For $\psi \in H^1$ with finite energy (4.1), we have $\Lambda\rho \in L^2(\Sigma_1)$, and hence (4.5) with $\varphi = \rho$ implies the neutrality condition (3.8) with T_1 instead of T_2:

$$\hat{\rho}(0,0) = \int_{T_1}\rho(\mathbf{x})d\mathbf{x} = \int_{T_1}[\sigma^0(\mathbf{x}) + e|\psi(\mathbf{x})|^2]d\mathbf{x} = 0. \tag{4.6}$$

Now, (4.2) gives

$$\int |\psi(\mathbf{x})|^2 d\mathbf{x} = Z_1. \tag{4.7}$$

Thus, the finiteness of the Coulomb energy $\|\Lambda\rho\|^2$ prevents the electron charge from escaping to infinity, as in the 2D case.

Finally, the Fourier transform $F : \psi \mapsto \hat{\psi}$ is a unitary operator from $L^2(T_1)$ to $L^2(\Sigma_1)$. Hence, energy (3.1) reads

$$\mathcal{E}(\psi) = \sum_{\mathbf{k}\in\Gamma_1^*}\int_{\mathbb{R}^2}\Big[\frac{\hbar^2}{2\mathrm{m}}(\mathbf{k}^2+\xi^2)|\hat{\psi}(\mathbf{k},\xi)|^2 + \frac{1}{2}\frac{|\hat{\rho}(\mathbf{k},\xi)|^2}{\mathbf{k}^2+\xi^2}\Big]d\xi. \tag{4.8}$$

Definition 4.1. *M_1 denotes the set of $\psi \in H^1$ satisfying the neutrality condition* (4.7).

We note that (4.2) can be written as $\hat{\mu}_1^{\mathrm{per}}(0) + eZ_1 = 0$. We assume, moreover,

(4.9) Condition III. $$\frac{\hat{\mu}_1^{\mathrm{per}}(0,\xi) + eZ_1}{|\xi|} \in L^2(D), \qquad D := \{\xi \in \mathbb{R}^2 : |\xi| \le 1\}$$

similarly to (3.11). For example, this condition holds, provided that

$$\int_{\mathbb{R}^3}(1 + |x_2| + |x_3|)|\mu_1(\mathbf{x})|d\mathbf{x} < \infty. \tag{4.10}$$

The third main result of the present paper is the following.

Theorem 4.2. *Let conditions* (1.9) *and* (4.9) *hold, and $N = 1$. Then*

(i) *there exists $\psi^0 \in M_1$ with*

$$\mathcal{E}(\psi^0) = \inf_{\psi\in M_1}\mathcal{E}(\psi); \tag{4.11}$$

(ii) *moreover, $\psi^0 \in H^2_{\mathrm{loc}}(T_1)$ and satisfies* (1.5)–(1.7) *with $d = 1$, where the potential $\phi^0 \in H^2_{\mathrm{loc}}(T_1)$ is real, $\mathbf{x}_1^0 = 0$, and $\omega^0 \in \mathbb{R}$;*

(iii) *the following bound holds:*

$$|\phi^0(\mathbf{x})| \le C(1 + |x_2| + |x_3|)^{1/2}, \qquad \mathbf{x} \in T_2. \tag{4.12}$$

The proof is similar to the one of Theorem 3.3. As in the 2D case, we obtain $\psi^0 \in M_1$ as a minimizer for the energy (4.1). The potential ϕ^0 can be constructed by a modification of Lemma 3.5; see the appendix below.

Finally, the next lemma follows similarly to Lemma 2.8.

LEMMA 4.3. *The functions ψ^0, ϕ^0 are smooth under condition*

$$\mu_1^{\text{per}} \in C^\infty(T_1). \tag{4.13}$$

Appendix A. The potential of the 1D lattice. We start with obvious modifications of the proof of Lemma 3.5. Namely, the potential $\phi^0(\mathbf{x})$ for the 1D lattice satisfies the equation of type (3.24) with

$$G^0 := -iF^{-1}\frac{(\mathbf{k},\xi)}{\mathbf{k}^2+\xi^2}\hat{\rho}^0(\mathbf{k},\xi) \in L^2(T_1), \qquad \text{rot}\, G^0(\mathbf{x}) \equiv 0. \tag{A.1}$$

We use the splitting of type (3.25), and, respectively, the solution splits as $\phi^0 = \phi_1 + \phi_2$. The second term $\phi_2 \in H^2$ as in the proof of Lemma 3.5. Hence, ϕ_2 is bounded continuous function on T_1 by the Sobolev embedding theorem.

On the other hand, the analysis of the first term needs some modifications. Now, $G_1(\mathbf{x}) = g_1(x_2, x_3) \in L^2(\mathbb{R}^2) \otimes \mathbb{R}^2$ is the real vector field, and $\text{supp}\, \hat{g}_1 \subset \{\xi \in \mathbb{R}^2 : |\xi| \le 1\}$. Therefore, g_1 is the smooth function, and

$$\Delta\phi_1 = \nabla \cdot g_1 \in L^2(\mathbb{R}^2), \qquad \text{rot}\, g_1(\mathbf{x}) \equiv 0. \tag{A.2}$$

Respectively, the solution to $\nabla\phi_1 = g_1$ is given by the contour integral

$$\phi_1(\mathbf{x}) = \int_0^{\mathbf{x}} g_1(\mathbf{y})d\mathbf{y} + C, \qquad \mathbf{x} \in \mathbb{R}^2, \tag{A.3}$$

which does not depend on the path in $\mathbb{R}^2$. This solution is real and smooth.

We still should prove the estimate (4.12). We will deduce it from the corresponding estimate "in the mean." Let us denote the circle $B := \{\mathbf{x} \in \mathbb{R}^2 : |\mathbf{x}| < 1\}$.

LEMMA A.1. *For any unit vector $\mathbf{e} \in \mathbb{R}^2$*

$$\|\phi_1\|_{L^2(B+\mathbf{e}R)} \le C(1+R)^{1/2}, \qquad R > 0. \tag{A.4}$$

Proof. First, (A.3) implies that

$$\phi_1(\mathbf{x}+\mathbf{e}R) - \phi_1(\mathbf{x}) = \int_0^R g_1(\mathbf{x}+\mathbf{e}t)dt, \qquad \mathbf{x} \in \mathbb{R}^2 \tag{A.5}$$

for any $R \in \mathbb{R}$. Now the Cauchy–Schwarz inequality implies that

$$|\phi_1(\mathbf{x}+\mathbf{e}R)|^2 \le C_1 + 2R\int_0^R |g_1(\mathbf{x}+\mathbf{e}t)|^2 dt, \qquad \mathbf{x} \in B \tag{A.6}$$

since the function ϕ_1 is bounded in B. Finally, averaging over $\mathbf{x} \in B$, we get

$$\int_B |\phi_1(\mathbf{x}+\mathbf{e}R)|^2 d\mathbf{x} \le C_1|B| + 2R\int_0^R \int_B |g_1(\mathbf{x}+\mathbf{e}t)|^2 d\mathbf{x}\, dt \le C_1 + C_2 R\|g_1\|^2_{L^2(\mathbb{R}^2)}. \tag{A.7}$$

Hence, (A.4) is proved. ∎

Now (4.12) follows from the Sobolev embedding theorem:

$$\max_{\mathbf{x}\in B+\mathbf{e}R} |\phi_1(\mathbf{x})| \le C_3\|\phi_1\|_{H^2(B+\mathbf{e}R)}$$
$$\le C_4[\|\Delta\phi_1\|_{L^2(B+\mathbf{e}R)} + \|\phi_1\|_{L^2(B+\mathbf{e}R)})] \le C(1+R)^{1/2}$$

since $\Delta\phi_1 \in L^2(\mathbb{R}^2)$ by (A.2).

Remark A.2. Our estimate (4.12) seems to be far from optimal since the potential of uniformly charged line grows logarithmically with the distance. One could expect an optimal estimate

$$|\phi^0(\mathbf{x})| \le C[\log(2+|x_2|+|x_3|)]^{1/2}$$

in the case $\nabla\phi^0 \in L^2$ due to the example $\phi(\mathbf{x}) = [\log(2+|x_2|+|x_3|)]^{1/2-\varepsilon}$ with $\nabla\phi(\mathbf{x}) \in L^2$ for $\varepsilon > 0$.

Acknowledgments. The author thanks H. Spohn for useful remarks and E. Kopylova for helpful discussions.

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