On orbital stability of ground states for finite crystals in fermionic Schrödinger–Poisson model

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Abstract

We consider the Schrödinger–Poisson–Newton equations for finite crystals under periodic boundary conditions with one ion per cell of a lattice. The electron field is described by the N-particle Schrödinger equation with antisymmetric wave function.

Our main results are i) the global dynamics with moving ions, and ii) the orbital stability of periodic ground state under a novel Jellium and Wiener-type conditions on the ion charge density. Under Jellium condition both ionic and electronic charge densities for the ground state are uniform.

Key words and phrases: crystal; lattice; Schrödinger–Poisson equations; Pauli exclusion principle; antisymmetric wave function; ground state; orbital stability; Hamilton structure; energy conservation; charge conservation; symmetry group; Hessian; Fourier transform.

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1 Introduction

First mathematical results on the stability of matter were obtained by Dyson and Lenard in [11, 12] where the energy bound from below was established. The thermodynamic limit for the Coulomb systems was first studied by Lebowitz and Lieb [22, 23], see the survey and further development in [26]. These results were extended by Catto, Le Bris, Lions, and others to the Thomas–Fermi and Hartree–Fock models [7, 8, 9]. Further results in this direction are due to Cancés, Lahbabi, Lewin, Sabin, Stoltz, and others [5, 6, 21, 24, 25]. All these results concern either the convergence of the ground state of finite particle systems in the thermodynamic limit or the existence of the ground state for infinite particle systems.

However, no attention was paid to the dynamical stability of crystals with moving ions. This stability is necessary for a rigorous analysis of fundamental quantum phenomena in the solid state physics: heat conductivity, electric conductivity, thermoelectronic emission, photoelectric effect, Compton effect, etc., see [3].

In present paper we consider the coupled Schrödinger–Poisson–Newton equations for finite crystals under periodic boundary conditions with one ion per cell of a lattice. The electrons are described by the N-particle Schrödinger equation with antisymmetric wave function. We construct the global dynamics of crystals with moving ions and prove the conservation of energy and charge.

Our main result is the orbital stability of every ground state with periodic arrangement of ions under the novel 'Jellium' and Wiener-type conditions on the ion charge density.

The electron field is described by the many-particle Schrödinger equation in the space of antisymmetric wave functions which corresponds to the Pauli exclusion principle. The ions are described as classical particles corresponding to the Born and Oppenheimer approximation. The ions interact with the electron field via the scalar potential, which is a solution to the corresponding Poisson equation. We find a novel stability criterion (3.1), (3.3).

We consider crystals which occupy the finite torus $\mathbb{T} := \mathbb{R}^3/N\mathbb{Z}^3$ and have one ion per cell of the cubic lattice $\Gamma := \mathbb{Z}^3/N\mathbb{Z}^3$, where $N \in \mathbb{N}$. The cubic lattice is chosen for the simplicity of notation. We denote by $\sigma(x)$ the charge density of one ion,

$$\sigma \in C^2(\mathbb{T}), \qquad \int_{\mathbb{T}} \sigma(x)dx = eZ > 0, \tag{1.1}$$

where $e > 0$ is the elementary charge. Let us denote

$$\overline{\mathbb{T}} := \mathbb{T}^{\overline{N}} := \{\overline{x} = (x_1, ..., x_{\overline{N}}) : x_j \in \mathbb{T}, \quad j = 1, ..., \overline{N}\}, \qquad \overline{N} := N^3. \tag{1.2}$$

Definition 1.1. *$\mathscr{F}$ is the 'fermionic' Hilbert space of complex antisymmetric functions $\psi(x_1, ..., x_{\overline{N}})$ on $\overline{\mathbb{T}}$ with the norm*

$$\|\psi\|^2_{\mathscr{F}} := \|\nabla^{\otimes}\psi\|^2_{L^2(\overline{\mathbb{T}})} + \|\psi\|^2_{L^2(\overline{\mathbb{T}})}, \tag{1.3}$$

where $\nabla^{\otimes}$ denotes the gradient with respect to $\overline{x} \in \overline{\mathbb{T}}$.

Let $\psi(\cdot, t) \in \mathscr{F}$ for $t \in \mathbb{R}$ be the antisymmetric wave function of the fermionic electron field, $q(n,t)$ denotes the ion displacement from the reference position $n \in \Gamma$, and $\Phi(x,t)$ be the electrostatic potential generated by the ions and electrons. We assume $\hbar = c = \mathrm{m} = 1$, where c is the speed of light and m is the electron mass. Let us denote the 'second quantized' operators on $\mathscr{F}$,

$$\Delta^{\otimes} := \sum_{j=1}^{\overline{N}} \Delta_{x_j}; \qquad \Phi^{\otimes}(\overline{x}, t) := \sum_{j=1}^{\overline{N}} \Phi(x_j, t). \tag{1.4}$$

The coupled Schrödinger-Poisson-Newton equations read as follows

$$i\dot{\psi}(\overline{x},t) = -\frac{1}{2}\Delta^{\otimes}\psi(\overline{x},t) - e\Phi^{\otimes}(\overline{x},t)\psi(\overline{x},t), \qquad \overline{x}\in\overline{\mathbb{T}}, \tag{1.5}$$

$$-\Delta\Phi(x,t) = \rho(x,t) := \sum_{n\in\Gamma}\sigma(x-n-q(n,t)) + \rho^{e}(x,t), \qquad x\in\mathbb{T}, \tag{1.6}$$

$$M\ddot{q}(n,t) = -(\nabla\Phi(x,t),\sigma(x-n-q(n,t))), \qquad n\in\Gamma. \tag{1.7}$$

Here the brackets $(\cdot,\cdot)$ stand for the scalar product on the real Hilbert space $L^2(\mathbb{T})$ and for its different extensions, $M>0$ is the mass of one ion, and the electronic charge density is defined by

$$\rho^{e}(x,t) := -e\int_{\overline{\mathbb{T}}}\sum_{j=1}^{\overline{N}}\delta(x-x_j)|\psi(\overline{x},t)|^2\,d\overline{x}, \quad x\in\mathbb{T}. \tag{1.8}$$

Similar finite periodic approximations of crystals are treated in all textbooks on quantum theory of solid state [4, 16, 30]. However, the stability of ground states in this model was newer discussed.

The total electronic charge (up to a factor) is defined by

$$Q(\psi,q,p) := \int_{\overline{\mathbb{T}}}|\psi(\overline{x})|^2 d\overline{x} = \|\psi\|^2_{L^2(\overline{\mathbb{T}})}. \tag{1.9}$$

The Poisson equation (1.6) implies that

$$\int_{\mathbb{T}}\rho(x,t)dx = 0. \tag{1.10}$$

Hence, the potential $\Phi(x,t)$ can be eliminated from the system (1.5)–(1.7) using the operator $G := (-\Delta)^{-1}$, see (2.1) for a more precise definition. Then the system (1.5)–(1.7) can be written in the Hamilton form

$$i\dot{\psi}(\overline{x},t) = \frac{1}{2}\partial_{\overline{\psi}}E, \qquad \dot{q}(n,t) = \partial_{p(n)}E, \quad \dot{p}(n,t) = -\partial_{q(n)}E. \tag{1.11}$$

Here $\partial_{\overline{\psi}} := \frac{1}{2}[\partial_{\psi_1} - i\partial_{\psi_2}]$, where $\psi_1 := \operatorname{Re}\psi$ and $\psi_2 := \operatorname{Im}\psi$, and the Hamilton functional (energy) reads

$$E(\psi,q,p) = \frac{1}{2}\int_{\overline{\mathbb{T}}}|\nabla^{\otimes}\psi(\overline{x})|^2\,d\overline{x} + \frac{1}{2}(\rho,G\rho) + \sum_{n\in\Gamma}\frac{p^2(n)}{2M}. \tag{1.12}$$

Here $q := (q(n): \ n\in\Gamma)\in\overline{\mathbb{T}}$, $p := (p(n): \ n\in\Gamma)\in\mathbb{R}^{3\overline{N}}$, and the total charge density $\rho(x)$ is the sum of the ion and electronic charge densities,

$$\rho(x) := \rho^{i}(x) + \rho^{e}(x), \quad \rho^{i}(x) := \sum_{n\in\Gamma}\sigma(x-n-q(n)), \qquad x\in\mathbb{T}, \tag{1.13}$$

in accordance with (1.6) and (1.8). The identity (1.10) implies the normalization

$$\|\psi(\cdot,t)\|^2_{L^2(\overline{\mathbb{T}})} = Z, \qquad t\in\mathbb{R}. \tag{1.14}$$

We denote the Hilbert manifolds

$$\mathscr{V} := H^1(\overline{\mathbb{T}})\otimes\overline{\mathbb{T}}\otimes\mathbb{R}^{3\overline{N}}, \qquad \mathscr{M} := \{X\in\mathscr{V} : Q(X) = Z\}. \tag{1.15}$$

We prove the the global well-posedness of the dynamics: for any $X(0) \in \mathscr{M}$ there exists a unique solution $X(t) \in C(\mathbb{R}, \mathscr{V})$ to (1.11), and the energy and charge conservations hold:

$$E(X(t)) = E(X(0)), \quad Q(X(t)) = Q(X(0)), \qquad t \in \mathbb{R}. \tag{1.16}$$

The charge conservation formally follows by the Noether theory [2, 14, 17] due to the $U(1)$-invariance of the Hamilton functional:

$$E(e^{i\alpha}\psi, q, p) = E(\psi, q, p), \qquad \alpha \in \mathbb{R}. \tag{1.17}$$

Our main goal is the stability of ground states, i.e., solutions to (1.11) with minimal energy (1.12). We consider only ground states with Γ-periodic arrangement of ions (nonperiodic arrangements exist for some degenerate densities σ, see Remark 1.3 iii) below).

We impose two special Jellium and the Wiener conditions (3.1) and (3.3) onto the ion densities $\sigma(x)$. The Wiener condition is a suitable version of the Fermi Golden Rule for crystals. The Jellium condition implies that total density of ions is uniform when $q(n,t) \equiv 0$, see (3.2).

The energy (1.12) is nonnegative, and its minimum is zero. We show that under the Jellium condition all ground states with Γ-periodic arrangement of ions have the form

$$S(t) := (\psi_0 e^{-i\omega_0 t}, \overline{r}, 0), \quad r \in \mathbb{T}. \tag{1.18}$$

Here

$$\overline{r} \in \overline{\mathbb{T}}: \quad \overline{r}(n) = r,\ n \in \Gamma, \tag{1.19}$$

while ψ_0 is an eigenfunction

$$-\frac{1}{2}\Delta^{\otimes}\psi_0(\overline{x}) = \omega_0\psi_0(\overline{x}), \qquad \overline{x} \in \overline{\mathbb{T}}, \tag{1.20}$$

corresponding to the minimal eigenvalue $\omega_0 := \min \operatorname{Spec}(-\frac{1}{2}\Delta^{\otimes})$.

We establish the stability of the real 4-dimensional 'solitary manifold'

$$\mathscr{S} = \{S_{\alpha,r} = (\psi_\alpha, \overline{r}, 0):\ \psi_\alpha(\overline{x}) \equiv e^{i\alpha}\psi_0(\overline{x}),\ \ \alpha \in [0, 2\pi];\ \ r \in \mathbb{T}\}, \tag{1.21}$$

where ψ_0 is a fixed eigenfunction, satisfying the additional restriction (3.7). The normalization (1.14) and the identity (1.20) imply that

$$E(S) = \omega_0 Z, \qquad S \in \mathscr{S}. \tag{1.22}$$

Our main result is the following theorem.

Theorem 1.2. *Let the Jellium and Wiener conditions (3.1) and (3.3) hold as well as (3.7). Then for any $\varepsilon > 0$ there exists $\delta = \delta(\varepsilon) > 0$ such that for $X(0) \in \mathscr{M}$ with $d_{\mathscr{V}}(X(0), \mathscr{S}) < \delta$ we have*

$$d_{\mathscr{V}}(X(t), \mathscr{S}) < \varepsilon, \qquad t \in \mathbb{R}, \tag{1.23}$$

where $X \in C(\mathbb{R}, \mathscr{V})$ is the corresponding solution to (1.11).

This theorem means the 'orbital stability' in the sense of [14], since the manifold $\mathscr{S} = S^1 \times \mathbb{T}$ is an orbit of the symmetry group $U(1) \times \mathbb{T}$.

Let us comment on our approach. We prove the local well-posedness for the system (1.11) by the contraction mapping principle. The global well-posedness we deduce from the energy conservation which follows by the Galerkin approximations.

The orbital stability of the solitary manifold $\mathscr{S}$ is deduced from the lower energy estimate

$$E(X) - \omega_0 Z \geq \nu\, d^2(X, \mathscr{S}) \qquad \text{if} \qquad d(X, \mathscr{S}) \leq \delta, \qquad X \in \mathscr{M}, \tag{1.24}$$

where $\nu, \delta > 0$ and 'd' is the distance in the 'energy norm'. We deduce this estimate from the positivity of the Hessian $E''(S)$ for $S \in \mathscr{S}$ in the orthogonal directions to $\mathscr{S}$ on the manifold $\mathscr{M}$. We show that the Wiener condition (3.3) is necessary for this positivity under the Jellium condition (3.1). The last condition cancels the negative energy which is provided by the electrostatic instability ('Earnshaw's Theorem' [29], see [20, Remark 10.2]). We expect that this condition is also necessary for the positivity of $E''(S)$; however, this is still an open challenging problem. Anyway, the positivity of $E''(S)$ can break down when condition (3.1) fails. We have shown this in [20, Lemma 10.1] in the context of infinite crystals; the proof however extends directly to the finite crystals.

Remarks 1.3. i) In the case of infinite crystal, corresponding to $N = \infty$, the orbital stability seems impossible. Namely, for $N = \infty$ the estimates (A.8), (A.9), (5.34) and (5.37) break down, as well as the estimate of type (1.24) which is due to the discrete spectrum of the energy Hessian $E''(S)$ on the compact torus.

ii) The identity (3.8) generically breaks down for the eigenfunctions (3.6) if the condition (3.7) fails. Respectively, the orbital stability of these 'mixed states' is an open problem.

Let us comment on previous works in this field.

The ground state for crystals in the Schrödinger–Poisson model was constructed in [18, 19]; its linear stability was proved in [20].

In the Hartree–Fock model the crystal ground state was constructed for the first time by Catto, Le Bris, and Lions [8, 9]. For the Thomas–Fermi model, see [7].

In [6], Cancés and Stoltz have established the well-posedness for the dynamics of local perturbations of the ground state density matrix in the *random phase approximation* for the reduced Hartree–Fock equations with the Coulomb pairwise interaction potential $w(x-y) = 1/|x-y|$. However, the space-periodic nuclear potential in the equation [6, (3)] does not depend on time that corresponds to the fixed nuclei positions.

The nonlinear Hartree–Fock dynamics with the Coulomb potential and without the random phase approximation was not studied previously, see the discussion in [21] and in the Introductions of [5, 6].

In [5] E. Cancès, S. Lahbabi, and M. Lewin have considered the random reduced HF model of crystal when the ions charge density and the electron density matrix are random processes, and the action of the lattice translations on the probability space is ergodic. The authors obtained suitable generalizations of the Hoffmann–Ostenhof and Lieb–Thirring inequalities for ergodic density matrices, and construct a random potential which is a solution to the Poisson equation with the corresponding stationary stochastic charge density. The main result is the coincidence of this model with the thermodynamic limit in the case of the short-range Yukawa interaction.

In [24], Lewin and Sabin have established the well-posedness for the reduced von Neumann equation, describing the Fermi gas, with density matrices of infinite trace and pair-wise interaction potentials $w \in L^1(\mathbb{R}^3)$. Moreover, they proved the asymptotic stability of translation-invariant stationary states for 2D Fermi gas [25].

The paper is organized as follows. In Section 2 we introduce function spaces. In Section 3 we collect all our assumptions. In Section 4 we describe all fermionic jellium ground states and give basic examples. In Section 5 we prove the stability of the solitary manifold $\mathscr{S}$ establishing the positivity the energy Hessian. In Appendices we construct the global dynamics.

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2 Function spaces and integral equation

The operator $G := (-\Delta)^{-1}$ is well defined in the Fourier series:

$$\rho(x) = \sum_{\xi \in \Xi} \tilde{\rho}(\xi) e^{i\xi x}, \quad G\rho := \sum_{\xi \in \Xi \setminus 0} \frac{\tilde{\rho}(\xi)}{\xi^2} e^{i\xi x}, \qquad x \in \mathbb{T}. \tag{2.1}$$

Here $\tilde{\rho}(0,t) = 0$ by (1.10). Hence, $\Phi(\cdot,t) = G\rho(\cdot,t)$ up to an additive constant $C(t)$, which can be offset by a gauge transform $\psi(\overline{x},t) \mapsto \psi(\overline{x},t)\exp(ie\int_0^t C(s)ds)$. Substituting $\Phi(\cdot,t) = G\rho(\cdot,t)$ into the remaining equations (1.5) and (1.7) we can write these equations as

$$\dot{X}(t) = F(X(t)), \qquad t \in \mathbb{R}, \tag{2.2}$$

where $X(t) = (\psi(\cdot,t), q(\cdot,t), p(\cdot,t))$ with $p(\cdot,t) := \dot{q}(\cdot,t)$. Equation (2.2) with the normalization (1.14) is equivalent, up to a gauge transform, to the system (1.5)–(1.7). Finally, the equation (2.2) can be written in the Hamilton form (1.11), which is equivalent to

$$\dot{X}(t) = JE'(X(t)), \tag{2.3}$$

where

$$J = \begin{pmatrix} -i/2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}. \tag{2.4}$$

We will use the following function spaces with $s = 0, \pm 1$. Let us define the Sobolev space $H^s(\overline{\mathbb{T}})$ as the real Hilbert space of complex-valued functions with the scalar product

$$(\psi, \varphi)_s := \mathrm{Re} \int_{\overline{\mathbb{T}}} \sum_{|\alpha| \le s} \partial^\alpha \psi(\overline{x}) \partial^\alpha \overline{\varphi}(\overline{x}) d\overline{x}, \qquad s = 0, 1. \tag{2.5}$$

By definition, $H^{-1}(\overline{\mathbb{T}})$ is the dual space to $H^1(\overline{\mathbb{T}})$, which will be identified with distributions by means of the scalar product in $H^0(\overline{\mathbb{T}})$.

Definition 2.1. *i) Let us denote the real Hilbert space* $\mathscr{W}^s := H^s(\overline{\mathbb{T}}) \oplus \mathbb{R}^{3\overline{N}} \oplus \mathbb{R}^{3\overline{N}}$ *for* $s = 0, \pm 1$.

ii) $\mathscr{V}^s := H^s(\overline{\mathbb{T}}) \otimes \overline{\mathbb{T}} \otimes \mathbb{R}^{3\overline{N}}$ *is the real Hilbert manifold endowed with the metric*

$$d_{\mathscr{V}^s}(X, X') := \|\psi - \psi'\|_{H^s(\mathbb{T})} + |q - q'| + |p - p'|, \qquad X = (\psi, q, p), \quad X' = (\psi', q', p') \tag{2.6}$$

and with the 'quasinorm'

$$|X|_{\mathscr{V}^s} := \|\psi\|_{H^s(\overline{\mathbb{T}})} + |p|, \qquad X = (\psi, q, p). \tag{2.7}$$

The linear space $\mathscr{W}^s$ is the tangent space to the Hilbert manifold $\mathscr{V}^s$ in each point $X \in \mathscr{V}^s$. We will write $\mathscr{X} := \mathscr{V}^0$, $\mathscr{V} := \mathscr{V}^1$, $\mathscr{W} := \mathscr{W}^1$, and $(\cdot,\cdot)_0 = (\cdot,\cdot)$, which agrees with the definition of the scalar product on the real Hilbert space $L^2(\mathbb{T})$. In particular,

$$(1, i) = 0. \tag{2.8}$$

Denote by the brackets $\langle\cdot,\cdot\rangle$ the scalar product on $\mathscr{X}$ and also the duality between $\mathscr{W}^{-1}$ and $\mathscr{W}^1$:

$$\langle Y, Y'\rangle := (\varphi, \varphi') + \varkappa\varkappa' + \pi\pi', \qquad Y = (\varphi, \varkappa, \pi), \quad Y' = (\varphi', \varkappa', \pi'). \tag{2.9}$$

Obviously,

$$|X|^2_{\mathscr{V}} \le C[E(X) + Q(X)], \qquad X \in \mathscr{V}. \tag{2.10}$$

We construct global dynamics for the system (2.3). This system is a nonlinear infinite-dimensional perturbation of the free Schrödinger equation. We rewrite it in the integral form

$$\left\{\begin{array}{lcl} \psi(t) & = & e^{\frac{i}{2}t\Delta^{\otimes}}\psi(0) + ie\displaystyle\int_0^t e^{\frac{i}{2}(t-s)\Delta^{\otimes}}[\Phi^{\otimes}(s)\psi(s)]ds, \\ q(n,t) & = & q(n,0) + \frac{1}{M}\displaystyle\int_0^t p(n,s)ds \mod N\mathbb{Z}^3, \\ p(n,t) & = & p(n,0) - \displaystyle\int_0^t (\nabla\Phi(s), \sigma(\cdot - n - q(n,s)))ds, \end{array}\right. \tag{2.11}$$

where $\Phi(s) := G\rho(s)$. In the vector form (2.11) reads

$$X(t) = e^{-tA}X(0) + \int_0^t e^{-(t-s)A}N(X(s))ds \mod \begin{pmatrix} 0 \\ N\mathbb{Z}^3 \\ 0 \end{pmatrix}. \tag{2.12}$$

Here

$$\begin{array}{rcl} A & = & \begin{pmatrix} -\frac{i}{2}\Delta^{\otimes} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ N(X) & = & (ie\Phi^{\otimes}\psi\,, p,\, f),\ f(n) := -(\nabla\Phi, \sigma(\cdot - n - q(n))),\ \Phi := G\rho, \end{array} \tag{2.13}$$

where ρ is defined by (1.13).

3 Main assumptions

Our main result concerns the orbital stability of the ground states (1.18). We will see that the ground states can be stable depending on the choice of the ion density σ. We study densities σ satisfying the following two conditions. First, we will assume

The Jellium Condition: $\quad \tilde{\sigma}(\xi) := \displaystyle\int_{\mathbb{T}} e^{i\xi x}\sigma(x)dx = 0, \quad \xi \in \gamma^* \setminus 0,$ (3.1)

where $\gamma^* := 2\pi\mathbb{Z}^3$. This condition implies that total density of ions is uniform when $q(n,t) \equiv 0$,

$$\sum_{n\in\Gamma} \sigma(x-n) \equiv eZ, \qquad x \in \mathbb{T}. \tag{3.2}$$

The simplest example of such a σ is a constant over the unit cell of a given lattice, which is what physicists usually call Jellium [13]. Moreover, this condition holds for a broad class of functions σ, see Section 4.3. Here we study this model in the rigorous context of the Schrödinger–Poisson equations.

Furthermore, we will assume the Wiener type spectral property

$$\textbf{The Wiener Condition:} \quad \Sigma(\theta) := \sum_{m\in\mathbb{Z}^3} \Big[\frac{\xi\otimes\xi}{|\xi|^2}|\tilde{\sigma}(\xi)|^2\Big]_{\xi=\theta+2\pi m} > 0, \quad \theta \in \Pi^* \setminus \gamma^*, \tag{3.3}$$

where the Brillouin zone Π^* is defined by

$$\Pi^* := \{\xi = (\xi^1,\xi^2,\xi^3) \in \Xi : 0 \le \xi^j \le 2\pi, \ \ j = 1,2,3\}, \quad \Xi := \frac{2\pi}{N}\mathbb{Z}^3. \tag{3.4}$$

This condition is an analogue of the Fermi Golden Rule for crystals. It is independent of (3.1). We have introduced conditions of type (3.1) and (3.3) in [20] in the framework of infinite crystals.

Remark 3.1. i) The series (3.3) converges for $\theta \in \Xi \setminus \gamma^*$ by the Parseval identity since $\sigma \in L^2(\mathbb{T})$ by (1.1).

ii) The matrix $\Sigma(\theta)$ is γ^*-periodic outside γ^*. Thus, (3.3) means that $\Sigma(\theta)$ is a positive matrix for $\theta \in \overline{\Pi}^* \setminus 0$, where $\overline{\Pi}^*$ is the 'discrete torus' Ξ/γ^*.

The series (3.3) is a nonnegative matrix. Hence, the Wiener condition holds 'generically'. For example it holds if

$$\tilde{\sigma}(\xi) \neq 0, \qquad \xi \in \Xi \setminus \gamma^*, \tag{3.5}$$

i.e., (3.1) are the only zeros of $\tilde{\sigma}(\xi)$. However, (3.3) does not hold for the simplest Jellium model, when σ is constant on the unit cell, see (4.8) and (4.9).

Finally, we need an additional condition for the orbital stability of the ground state (1.18). Namely, every eigenfunction (1.20) admits an expansion in exterior products (see (B.1)),

$$\psi_0(\overline{x}) = \sum_{\overline{k}} C(\overline{k}) \Lambda_{j=1}^{\overline{N}} e^{ik_j x_j}. \qquad k_j \in \Xi := \frac{2\pi}{N}\mathbb{Z}^3. \tag{3.6}$$

Here $\overline{k} := \{k_1,...,k_{\overline{N}}\}$, where k_j are different for distinct j, and $\frac{1}{2}\sum_{j=1}^{\overline{N}} k_j^2 = \omega_0$. We will consider the eigenfunctions (3.6) with the additional restriction

$$\#(\overline{k} \setminus \overline{k}') \ge 2 \quad \text{if} \quad \overline{k} \neq \overline{k}'. \tag{3.7}$$

This condition implies that the corresponding electronic charge density is uniform (see Lemma 4.1),

$$\rho^e(x) \equiv -eZ, \qquad x \in \mathbb{T}. \tag{3.8}$$

This identity plays a crucial role in our approach. It implies that the corresponding total charge density (1.13) identically vanishes by (3.2). Let us emphasize that both ionic and electronic charge densities are uniform for the ground state under the Jellium condition together with (3.7).

4 Fermionic jellium ground states

Here we check the key identity (3.8) and construct all solutions to (2.3) with minimal energy (1.12). Furthermore we give examples illustrating the Jellium and the Wiener conditions.

4.1 Uniform electronic charge density

Let us establish the identity (3.8).

Lemma 4.1. *Let the condition (3.7) hold for an eigenfunction (3.6), and*

$$\int_{\overline{\mathbb{T}}} |\psi_0(\overline{x})|^2 d\overline{x} = Z. \tag{4.1}$$

Then the identity (3.8) holds.

Proof. By the antisymmetry of $\psi_0(x_1,...,x_{\overline{N}})$ it remains to prove that

$$\int_{\overline{\mathbb{T}}} \delta(x-x_1)|\psi_0(\overline{x})|^2 d\overline{x} = Z/\overline{N}, \qquad x \in \mathbb{T}. \tag{4.2}$$

Let us use the expansion (3.6). The normalization condition (4.1) gives

$$\sum_{\overline{k}} |C(\overline{k})|^2 \overline{N}^{\overline{N}} = Z. \tag{4.3}$$

Further,

$$\int_{\overline{\mathbb{T}}} \delta(x-x_1)|\psi_0(\overline{x})|^2 d\overline{x} = \frac{1}{\overline{N}!}\sum_{\overline{k}} \Big\{ |C(\overline{k})|^2 \int_{\overline{\mathbb{T}}} \delta(x-x_1)\Big[\sum_{\pi,\pi' \in S_{\overline{N}}} (-1)^{|\pi|+|\pi'|} \prod_{j=1}^{\overline{N}} e^{i[k_{\pi(j)}-k_{\pi'(j)}]x_j}\Big] d\overline{x}\Big\}$$

$$+ \quad \frac{1}{\overline{N}!}\mathrm{Re}\sum_{\overline{k}\neq\overline{k}'} \Big\{ C(\overline{k})\overline{C}(\overline{k}')\Big[\sum_{\pi,\pi' \in S_{\overline{N}}} (-1)^{|\pi|+|\pi'|} \int_{\overline{\mathbb{T}}} \delta(x-x_1) \prod_{j=1}^{\overline{N}} e^{i[k_{\pi(j)}-k'_{\pi'(j)}]x_j} d\overline{x}\Big]\Big\}. \tag{4.4}$$

The integrals in the last line vanish since $k_{\pi(j)} - k'_{\pi'(j)} \neq 0$ at least for one $j \neq 1$ by (3.7). On the other hand, the integrals in the first line do not vanish only in the case when $k_{\pi(j)} \equiv k_{\pi'(j)}$ for $j \neq 1$, i.e., when $\pi = \pi'$. Hence,

$$\int_{\overline{\mathbb{T}}} \delta(x-x_1)|\psi_0(\overline{x})|^2 d\overline{x} = \overline{N}^{\overline{N}-1}\sum_{\overline{k}} |C(\overline{k})|^2 \int_{\mathbb{T}} \delta(x-x_1)dx_1 = \overline{N}^{\overline{N}-1}\sum_{\overline{k}} |C(\overline{k})|^2 = Z/\overline{N} \tag{4.5}$$

by (4.3).

□

Remark 4.2. *Similar calculations show that the uniformity (4.2) can break down for the wave functions (3.6) if the condition (3.7) fails.*

4.2 Description of ground states

The following lemma describe all ground states with Γ-periodic arrangement of ions.

Lemma 4.3. *All solutions to (2.3) of minimal energy with Γ-periodic arrangement of ions are given by (1.18), where ψ_0 is an eigenfunction (1.20) with the normalization (1.14).*

Proof. It suffices to construct all solutions $(\psi(t), q(t), p(t))$ which minimize the first integral on the right hand side of (1.12) under the normalization condition (1.14), with zero second and the third terms and with Γ-periodic arrangement of ions.

First, the solutions (1.18) have all these properties when ψ_0 is the eigenfunction (3.6) satisfying the condition (3.7). Namely, the first integral on the right hand side of (1.12) takes the minimal value for the eigenfunctions under the normalization condition (1.14). The second and the third terms on the right hand side vanish since the corresponding total charge density $\rho(x) \equiv 0$ by (3.2) and (3.8).

Similarly, for general solution $(\psi(t), q(t), p(t))$ the first integral, under the normalization condition (1.14), takes the minimal value for the eigenfunctions (1.20). Then

$$-\frac{1}{2}\Delta^{\otimes}\psi(\overline{x},t) = \omega_0\psi(\overline{x},t), \qquad \overline{x} \in \overline{\mathbb{T}}, \quad t \in \mathbb{R}. \tag{4.6}$$

The second summand of (1.12) vanishes only for $\rho(x) \equiv 0$. Then, up to a gauge transformation, $\Phi(\cdot,t) = G\rho(\cdot,t) = 0$. Now the equation (1.5) implies that $\psi(\overline{x},t) = e^{i\omega_0 t}\psi_0(\overline{x})$ by (4.6). Finally, the third summand of (1.12) vanishes only for $\dot{q}(n,t) = p(n,t) \equiv 0$. Hence, by the Γ-periodicity,

$$q(n,t) \equiv r, \qquad n \in \Gamma, \quad t \in \mathbb{R}, \tag{4.7}$$

where $r \in \mathbb{T}$. □

4.3 The Jellium and Wiener conditions. Examples

The Wiener condition (3.3) for the ground states (1.18) holds under the generic assumption (3.5). On the other hand, (3.3) does not hold for the simplest Jellium model, when $\sigma(x)$ is the function

$$\sigma_1(x) := eZ\chi_1(x)\chi_1(x)\chi_1(x), \qquad x \in \mathbb{T}, \tag{4.8}$$

where χ_1 is the characteristic function of the interval $[0,1] \bmod N$. In this case the Fourier transform

$$\tilde{\sigma}_1(\xi) = eZ\tilde{\chi}_1(\xi_1)\tilde{\chi}_1(\xi_2)\tilde{\chi}_1(\xi_3), \qquad \xi \in \Xi, \tag{4.9}$$

where

$$\tilde{\chi}_1(s) = \frac{2\sin s/2}{s}, \quad s \in \frac{2\pi}{N}\mathbb{Z} \setminus 0. \tag{4.10}$$

Now for $\theta = (0, \theta_2, \theta_3)$ we have

$$\Sigma(\theta) = \sum_{m \in \mathbb{Z}^3 : m_1 = 0} \Big[\frac{\xi \otimes \xi}{|\xi|^2}|\tilde{\sigma}(\xi)|^2\Big]_{\xi = \theta + 2\pi m}, \qquad \theta \in \Pi^* \setminus \gamma^*, \tag{4.11}$$

which is a degenerate matrix since $\xi_1 = 0$ in each summand. Hence, (3.3) fails. Similarly, the Wiener condition fails for $\sigma_k(x) = eZ\chi_k(x_1)\chi_k(x_2)\chi_k(x_3)$, where $\chi_k = \chi_1 * ... * \chi_1$ (k times) with $k = 2, 3, ...$, since in this case

$$\tilde{\sigma}_k(\xi) = eZ\tilde{\chi}_k(\xi_1)\tilde{\chi}_k(\xi_2)\tilde{\chi}_k(\xi_3); \qquad \tilde{\chi}_k(s) = \Big[\frac{2\sin s/2}{s}\Big]^k, \quad s \in \frac{2\pi}{N}\mathbb{Z} \setminus 0. \tag{4.12}$$

5 The orbital stability of the ground state

In this section we expand the energy into the Taylor series and prove the orbital stability checking the positivity of the energy Hessian.

5.1 The Taylor expansion of energy functional

We will deduce the lower estimate (1.24) using the Taylor expansion of $E(S+Y)$ for $S = S_{\alpha,r} = (\psi_\alpha, \overline{r}, 0) \in \mathscr{S}$ and $Y = (\varphi, \varkappa, p) \in \mathscr{W} = H^1(\overline{\mathbb{T}}) \oplus \mathbb{R}^{3\overline{N}} \oplus \mathbb{R}^{3\overline{N}}$:

$$E(S+Y) = E(S) + \langle E'(S), Y\rangle + \frac{1}{2}\langle Y, E''(S)Y\rangle + R(S,Y) = \omega_0 Z + \frac{1}{2}\langle Y, E''(S)Y\rangle + R(S,Y) \qquad (5.1)$$

since $E(S) = \omega_0 Z$ by (1.22), and $E'(S) = 0$. Here $E'(S)$ and $E''(S)$ stand for the Gâteaux differentials. Let us recall that $\psi_\alpha = e^{i\alpha}\psi_0(x)$ where $\psi_0(x)$ is given by (3.6) and the condition (3.7) holds.

First, we expand the charge density (1.13) corresponding to $S+Y = (\psi_\alpha + \varphi, \overline{r} + \varkappa, p)$:

$$\rho(x) = \rho^{(0)}(x) + \rho^{(1)}(x) + \rho^{(2)}(x), \qquad x \in \mathbb{T}, \qquad (5.2)$$

where $\rho^{(0)}$ and $\rho^{(1)}$ are respectively the terms of zero and first order in Y, while $\rho^{(2)}$ is the remainder. However, $\rho^{(0)}(x)$ is the total charge density of the ground state which is identically zero by (3.2) and (3.8):

$$\rho^{(0)}(x) = \rho_0^i(x) - e|\psi_\alpha(x)|^2 \equiv 0, \qquad x \in \mathbb{T}. \qquad (5.3)$$

Thus, $\rho = \rho^{(1)} + \rho^{(2)}$. Expanding (1.13) further, we obtain

$$\rho^{(1)}(x) = \sigma^{(1)}(x) - 2e\sum_{j=1}^{\overline{N}} \mathrm{Re}\,(\psi_\alpha, \varphi)_j(x), \quad \sigma^{(1)}(x) = -\sum_{n\in\Gamma} \varkappa(n)\cdot\nabla\sigma(x-n-r), \qquad (5.4)$$

$$\rho^{(2)}(x) = \sigma^{(2)}(x) - e\sum_{j=1}^{\overline{N}} (\varphi,\varphi)_j(x),\ \sigma^{(2)}(x) = \frac{1}{2}\sum_{n\in\Gamma}\int_0^1 (1-s)[\varkappa(n)\cdot\nabla]^2\sigma(x-n-r-s\varkappa(n))ds, \qquad (5.5)$$

where we denote

$$(\psi_\alpha, \varphi)_j(x) := \int_{\overline{\mathbb{T}}} \delta(x-x_j)\psi_\alpha(\overline{x})\overline{\varphi}(\overline{x})\,d\overline{x}, \qquad x \in \mathbb{T}. \qquad (5.6)$$

Substituting $\psi = \psi_\alpha + \varphi$ and $\rho = \rho^{(1)} + \rho^{(2)}$ into (1.12), we obtain that the quadratic part of (5.1) reads

$$\frac{1}{2}\langle Y, E''(S)Y\rangle = \frac{1}{2}\int_{\overline{\mathbb{T}}} |\nabla\varphi(\overline{x})|^2]d\overline{x} + \frac{1}{2}(\rho^{(1)}, G\rho^{(1)}) + K(p), \qquad K(p) := \sum_n \frac{p^2(n)}{2M} \qquad (5.7)$$

and the remainder equals

$$R(S,Y) = \frac{1}{2}(2\rho^{(1)} + \rho^{(2)}, G\rho^{(2)}). \qquad (5.8)$$

5.2 The null space of Hessian

In this section we calculate the null space

$$\mathscr{K}(S) := \mathrm{Ker}\left[E''(S)\Big|_{\mathscr{W}}\right], \qquad S \in \mathscr{S}. \tag{5.9}$$

Lemma 5.1. *Let the Jellium condition (3.1) and the Wiener condition (3.3) hold, and $S \in \mathscr{S}$. Then*

$$\mathscr{K}(S) = \{(0,\overline{s},0): \ \ s \in \mathbb{R}^3\}, \tag{5.10}$$

where $\overline{s} \in \mathbb{R}^{3\overline{N}}$ is defined similarly to (1.19): $\overline{s}(n) \equiv s$.

Proof. All the summands of the energy (5.7) are nonnegative. Hence, this expression is zero if and only if all the summands vanish: in the notation (5.4)

$$\varphi(\overline{x}) \equiv C, \quad (\rho^{(1)}, G\rho^{(1)}) = \|\sqrt{G}[\sigma^{(1)} - 2e\sum_{j=1}^{\overline{N}} \mathrm{Re}\,(\psi,\varphi)_j(x)]\|^2_{L^2(\mathbb{T})} = 0, \quad p = 0. \tag{5.11}$$

Here $C = 0$ by the antisymmetry of φ. Therefore, $(\psi,\varphi)_k(x) \equiv 0$, and hence, (5.11) implies that

$$\sqrt{G}\sigma^{(1)} = 0. \tag{5.12}$$

On the other hand, in the Fourier transform (5.4) reads

$$\tilde{\sigma}^{(1)}(\xi) = \tilde{\sigma}(\xi)\xi \cdot \sum_{n\in\Gamma} ie^{i\xi[n+r]}\varkappa(n) = i\tilde{\sigma}(\xi)\xi \cdot e^{i\xi r}\hat{\varkappa}(\xi), \qquad \xi \in \Xi, \tag{5.13}$$

where $\hat{\varkappa}(\xi) := \sum_{n\in\Gamma} e^{i\xi n}\varkappa(n)$ is a $2\pi\mathbb{Z}^3$-periodic function on Ξ. Hence, Definition (2.1) and the Jellium condition (3.1) imply that

$$\begin{aligned} 0 = \|\sqrt{G}\sigma^{(1)}\|^2_{L^2(\mathbb{T})} &= N^{-3}\sum_{\Xi\setminus\gamma^*} |\tilde{\sigma}(\xi)\frac{\xi\hat{\varkappa}(\xi)}{|\xi|}|^2 \\ &= N^{-3}\sum_{\theta\in\Pi^*\setminus\gamma^*} \langle\hat{\varkappa}(\theta), \sum_{m\in\mathbb{Z}^3}\Big[\frac{\xi\otimes\xi}{|\xi|^2}|\tilde{\sigma}(\xi)|^2\Big]_{\xi=\theta+2\pi m}\hat{\varkappa}(\theta)\rangle \\ &= N^{-3}\sum_{\theta\in\Pi^*\setminus\gamma^*} \langle\hat{\varkappa}(\theta), \Sigma(\theta)\hat{\varkappa}(\theta)\rangle. \end{aligned} \tag{5.14}$$

As a result,

$$\hat{\varkappa}(\theta) = 0, \qquad \theta \in \Pi^* \setminus \gamma^* \tag{5.15}$$

by the Wiener condition (3.3). On the other hand, $\hat{\varkappa}(0) \in \mathbb{R}^3$ remains arbitrary, see Remark 3.1 ii). Respectively, $\varkappa = \overline{s}$ with an arbitrary $s \in \mathbb{R}^3$. □

Remark 5.2. The key point of the proof is the explicit calculation (5.13) in the Fourier transform. This calculation relies on the invariance of the Hessian $E''(S)$ with respect to Γ-translations which is due to the periodicity of the ions arrangement of the ground state.

Remark 5.3. *Beyond the Wiener condition* If the Wiener condition (3.3) fails, the dimension of the space

$$V := \{v \in \mathbb{R}^{3\overline{N}} : \ v(n) = \sum_{\theta \in \Pi^* \setminus \gamma^*} e^{-i\theta n} \hat{v}(\theta), \qquad \hat{v}(\theta) \in \mathbb{C}^3, \ \Sigma(\theta)\hat{v}(\theta) = 0\} \tag{5.16}$$

is positive. The above calculations show that in this case

$$\mathscr{K}(S) = \{(0, \overline{s} + v, 0) : \ s \in \mathbb{R}^3, \ v \in V\}. \tag{5.17}$$

The subspace $V \subset \mathbb{R}^{3\overline{N}}$ is orthogonal to the $3D$ subspace $\{\overline{s} : s \in \mathbb{R}^3\} \subset \mathbb{R}^{3\overline{N}}$ by the Parseval theorem. Hence, $\dim \mathscr{K}(S) = 3 + d$, where $d := \dim V > 0$. Thus, $\dim \mathscr{K}(S) > 3$. Under the Wiener condition $V = 0$, and (5.17) coincides with (5.10).

5.3 The positivity of Hessian

Denote by $N_S\mathscr{S}$ the normal subspace to $\mathscr{S}$ at a point S:

$$N_S\mathscr{S} := \{Y \in \mathscr{W} = H^1(\overline{\mathbb{T}}) \oplus \mathbb{R}^{3\overline{N}} \oplus \mathbb{R}^{3\overline{N}} : \langle Y, \tau \rangle = 0, \ \ \tau \in T_S\mathscr{S}\}, \tag{5.18}$$

where $T_S\mathscr{S}$ is the tangent space to $\mathscr{S}$ at the point S and $\langle \cdot, \cdot \rangle$ stands for the scalar product (2.9). Obviously, $\mathscr{S} \subset \mathscr{M}$ and the tangent space to $\mathscr{M}$ at a point $S = (\psi_\alpha, \overline{r}, 0)$ is given by

$$T_S\mathscr{M} = \{(\varphi, \varkappa, \pi) \in \mathscr{W} : \varphi \perp \psi_\alpha, \ \ \varkappa \in \mathbb{R}^{3\overline{N}}, \ \ \pi \in \mathbb{R}^{3\overline{N}}\}, \tag{5.19}$$

since $DQ(\psi_\alpha, \overline{r}, 0) = 2(\psi_\alpha, 0, 0)$.

Lemma 5.4. *Let the Jellium condition (3.1) hold, and $S = S_{\alpha,r} \in \mathscr{S}$. Then the Wiener condition (3.3) is necessary and sufficient for the positivity of the Hessian $E''(S)$ in the orthogonal directions to $\mathscr{S}$ on $\mathscr{M}$, i.e.,*

$$E''(S)\Big|_{N_S\mathscr{S} \cap T_S\mathscr{M}} > 0. \tag{5.20}$$

Proof. i) Sufficiency. Differentiating $S_{\alpha,r} = (e^{i\alpha}\psi_0, \overline{r}, 0) \in \mathscr{S}$ in the parameters $\alpha \in [0, 2\pi]$ and $r \in \mathbb{T}$, we obtain

$$T_S\mathscr{S} = \{(iC\psi_\alpha, \overline{s}, 0) : \ C \in \mathbb{R}, \ \ s \in \mathbb{R}^3\}. \tag{5.21}$$

Hence, (5.10) implies that

$$\mathscr{K}(S) \cap N_S\mathscr{S} = (0, 0, 0) \tag{5.22}$$

Now (5.20) follows since $E''(S) \geq 0$ by (5.7).

ii) Necessity. If the Wiener condition (3.3) fails, the space $\mathscr{K}(S)$ is given by (5.17), and hence, (5.21) implies that now

$$\mathscr{K}(S) \cap N_S\mathscr{S} = \{0, v, 0) : \ C \in \mathbb{R}, \ \ v \in V\} \subset T_S\mathscr{M}. \tag{5.23}$$

Therefore, the Hessian $E''(S)$ vanishes on the nontrivial space $\mathscr{K}(S) \cap N_S\mathscr{S} \subset T_S\mathscr{M}$ of the dimension $d > 0$. Respectively, the positivity (5.20) breaks down. □

Remark 5.5. The positivity of type (5.20) breaks down for the submanifold $\mathscr{S}(r) := \{S_{\alpha,r} : \ \alpha \in [0, 2\pi]\}$ with a fixed $r \in \mathbb{T}$ instead of the solitary manifold $\mathscr{S}$. Indeed, then the corresponding tangent space is smaller:

$$T_S\mathscr{S}(r) = \{(iC\psi_\alpha, 0, 0) : \ C \in \mathbb{R}\}. \tag{5.24}$$

Hence, the normal subspace $N_S\mathscr{S}(r)$ is larger, in particular containing all the vectors $(0, \overline{s}, 0)$ generating the shifts of the torus. However, all these vectors also belong to the null space (5.10) and to $T_S\mathscr{M}$. Respectively, the null space of the Hessian $E''(S)$ in $T_S\mathscr{M} \cap N_S\mathscr{S}(r)$ is at least 3-dimensional.

5.4 The orbital stability

Here we prove Theorem 1.2 which is our main result. For the proof is suffices to check the lower energy estimate (1.24):

$$E(X)-\omega_0 Z \geq \nu\, d^2_{\mathscr{Y}}(X,\mathscr{S}) \quad \text{if} \quad d_{\mathscr{Y}}(X,\mathscr{S})\leq \delta, \quad X\in\mathscr{M} \tag{5.25}$$

with some $\nu,\delta>0$. This estimate implies Theorem 1.2 since the energy is conserved along all trajectories. First, we prove similar lower bound for the energy Hessian.

Lemma 5.6. *Let conditions of Theorem 1.2 hold. Then for each $S\in\mathscr{S}$*

$$\langle Y, E''(S)Y\rangle > \nu\|Y\|^2_{\mathscr{W}}, \qquad Y\in N_S\mathscr{S}\cap T_S\mathscr{M}, \tag{5.26}$$

where $\nu>0$.

Proof. It suffices to prove this estimate for $S=(\psi_0,0,0)$. First, we note that $E''(S)$ is not complex linear due to the integral in (1.12). Hence, we should express the action of $E''(S)$ in $\psi_1(x):=\operatorname{Re}\psi(x)$ and $\psi_1(x):=\operatorname{Im}\psi(x)$: by the formula (1.15) of [20],

$$E''(S)Y=\begin{pmatrix} -\Delta^{\otimes}+4e^2\psi_0 G\psi_0 & 0 & 2L & 0\\ 0 & -\Delta^{\otimes} & 0 & 0\\ 2L^* & 0 & T & 0\\ 0 & 0 & 0 & M^{-1}\end{pmatrix} Y \qquad \text{for} \quad Y=\begin{pmatrix}\psi_1\\ \psi_2\\ q\\ p\end{pmatrix}, \tag{5.27}$$

where ψ_0 denotes the operators of multiplication by the real function $\psi_0(x)\equiv\sqrt{Z}$. The operators L correspond to the matrix

$$L(x,n):=e\psi_0(x)G\nabla\sigma(x-n): \quad x\in\mathbb{R}^3,\ n\in\Gamma \tag{5.28}$$

by formula (3.3) of [20] and T corresponds to the real matrix with entries

$$T(n-n'):=-\langle G\nabla\otimes\nabla\sigma(x-n'),\sigma(x-n)\rangle, \qquad n,n'\in\Gamma \tag{5.29}$$

by formula (3.4) of [20] since the corresponding potential $\Phi_0=0$. Hence, $E''(S)$ is a finite-rank perturbation of the operator with the discrete spectrum on the torus $\mathbb{T}$. Finally, (5.20) implies that the minimal eigenvalue of $E''(S)$ is positive. Therefore, (5.26) follows. □

The positivity (5.26) implies the lower energy estimate (5.25) since the higher-order terms in (5.1) are negligible by the following lemma.

Lemma 5.7. *Let $\sigma(x)$ satisfy (1.1). Then the remainder (5.8) admits the bound*

$$|R(S,Y)|\leq C\|Y\|^3_{\mathscr{W}} \quad \text{for} \quad \|Y\|_{\mathscr{W}}\leq 1. \tag{5.30}$$

Proof. Due to (5.8) it suffices to prove the estimates

$$\|\sqrt{G}\rho^{(1)}\|_{L^2(\mathbb{T})}\leq C_1\|Y\|_{\mathscr{W}}, \quad \|\sqrt{G}\rho^{(2)}\|_{L^2(\mathbb{T})}\leq C_2\|Y\|^2_{\mathscr{W}} \quad \text{for} \quad \|Y\|_{\mathscr{W}}\leq 1. \tag{5.31}$$

i) By (5.4) we have for $Y=(\varphi,\varkappa,p)$

$$\sqrt{G}\rho^{(1)}=\sqrt{G}\sigma^{(1)}-2e\sqrt{G}\sum_{j=1}^{\overline{N}}\mathrm{Re}\,(\psi,\varphi)_j(x). \tag{5.32}$$

in the notation (5.6). The operator $\sqrt{G}$ is bounded in $L^2(\mathbb{R}^3)$ by (2.1). Hence, (5.4) implies that

$$\|\sqrt{G}\sigma^{(1)}\|_{L^2(\mathbb{T})}\le C|\varkappa|. \tag{5.33}$$

Applying the Cauchy–Schwarz and Hausdorff–Young inequalities to the second term on the RHS of (5.32), we obtain

$$\begin{aligned}\|\sqrt{G}(\psi,\varphi)_j\|_{L^2(\mathbb{T})} &\le C\Big[\sum_{\xi\in\Xi\setminus 0}\frac{|\tilde{\varphi}(\xi)|^2}{|\xi|^2}\Big]^{1/2}\le C\|\tilde{\varphi}\|_{L^4(\Xi)}\Big[\sum_{\xi\in\Xi\setminus 0}|\xi|^{-4}\Big]^{1/2}\\ &\le C_1\|\varphi\|_{L^{4/3}(\mathbb{T})}\le C_2\|\varphi\|^2_{H^1(\mathbb{T})}\end{aligned} \tag{5.34}$$

by the Sobolev embedding theorem. Hence, the first inequality (5.31) is proved.

ii) Now we prove the second inequality (5.31). According to (5.5),

$$\sqrt{G}\rho^{(2)}(x)=\sqrt{G}\sigma^{(2)}(x)-e\sqrt{G}\sum_{j=1}^{\overline{N}}(\varphi,\varphi)_j(x). \tag{5.35}$$

Similarly to (5.33)

$$\|\sqrt{G}\sigma^{(2)}\|_{L^2(\mathbb{T})}\le C|\varkappa|^2. \tag{5.36}$$

At last, denoting $\beta(x):=(\varphi,\varphi)_j(x)$, we obtain similarly to (5.34)

$$\|\sqrt{G}(\varphi,\varphi)_k\|_{L^2(\mathbb{T})}\le C\Big[\sum_{\xi\in\Xi\setminus 0}\frac{|\tilde{\beta}(\xi)|^2}{|\xi|^2}\Big]^{1/2}\le C_1\|\beta\|_{L^{4/3}(\mathbb{T})}. \tag{5.37}$$

Finally, applying the triangle inequality and the Sobolev embedding theorem, we obtain

$$\begin{aligned}\|\beta\|_{L^{4/3}(\mathbb{T})} &\le \int_{\mathbb{T}^{\overline{N}-1}}[\int_{\mathbb{T}}|\varphi(\overline{x})|^{8/3}dx_j]^{3/4}\,dx_1\ldots\widehat{dx_j}\ldots dx_{\overline{N}}\\ &\le \int_{\mathbb{T}^{\overline{N}-1}}[\int_{\mathbb{T}}|\nabla_{x_j}\varphi(\overline{x})|^2dx_j]\,dx_1\ldots\widehat{dx_j}\ldots dx_{\overline{N}}\le C\|\varphi\|^2_{H^1(\mathbb{T})}.\end{aligned} \tag{5.38}$$

Now the lemma is proved. □

A Global dynamics

Here we prove the global well-posedness of the system (2.3).

Theorem A.1. *Let (1.1) hold and $X(0)\in\mathscr{M}$. Then*

i) There exists a unique solution $X(t)\in C(\mathbb{R},\mathscr{V})$ to (2.3).

ii) The energy and charge conservations (1.16) hold.

First we construct the local solutions by contraction arguments. To construct the global solutions we prove in Appendix B energy conservation using the Galerkin approximations.

Let us prove the local well-posedness.

Theorem A.2. *(Local well-posedness). Let (1.1) hold and* $X(0)=(\psi_0,q_0,p_0)\in\mathscr{V}=H^1(\overline{\mathbb{T}})\otimes\overline{\mathbb{T}}\otimes\mathbb{R}^{3\overline{N}}$ *with* $|X(0)|_{\mathscr{V}}:=\|\psi_0\|_{H^1(\overline{\mathbb{T}})}+|p_0|\le R$. *Then there exists* $\tau=\tau(R)>0$ *such that equation (2.3) has a unique solution* $X\in C([-\tau,\tau],\mathscr{V})$, *and the maps* $U(t):X(0)\mapsto X(t)$ *are continuous in* $\mathscr{V}$ *for* $t\in[-\tau,\tau]$.

In the next two propositions we prove the boundedness and the local Lipschitz continuity of the nonlinearity $N:\mathscr{V}\to\mathscr{W}=H^1(\overline{\mathbb{T}})\oplus\mathbb{R}^{3\overline{N}}\oplus\mathbb{R}^{3\overline{N}}$ defined in (2.13). With this proviso Theorem A.2 follows from the integral form (2.12) of the equation (2.3) by the contraction mapping principle, since e^{-At} is an isometry of $\mathscr{W}$. First, we prove the boundedness of N.

Proposition A.3. *For any* $R>0$ *and* $X=(\psi,q,p)\in\mathscr{V}$

$$\|N(X)\|_{\mathscr{W}}\le C(R)\qquad\text{for}\quad|X|_{\mathscr{V}}\le R. \tag{A.1}$$

Proof. We need appropriate bounds for the charge density ρ and for the corresponding potential Φ.

Lemma A.4. *The charge density (1.13) admits the bounds*

$$\|\rho\|_{L^3(\mathbb{T})}+\|\nabla\rho\|_{L^{3/2}(\mathbb{T})}\le C(1+\|\psi\|_{\mathscr{F}}^2). \tag{A.2}$$

Proof. We split $\rho(x)$ as $\rho(x)=\rho^i(x)+\rho^e(x)$, where

$$\rho^i(x,t)=\sum_{n\in\Gamma}\sigma(x-n-q(n,t)),$$

while ρ^e is defined by (1.8). The bound (A.2) for ρ^i holds by (1.1). It remains to prove the bound for ρ^e. Definition (1.8) implies that

$$\rho^e(x)=-e\sum_{j=1}^{\overline{N}}\int_{\mathbb{T}^{\overline{N}-1}}|\psi(\overline{x})|^2\Big|_{x_j=x}dx_1...\widehat{dx_j}...dx_{\overline{N}},\quad x\in\mathbb{T}, \tag{A.3}$$

where the hat means that this differential is omitted. Differentiating, we obtain that

$$\nabla\rho^e(x)=-e\sum_{j=1}^{\overline{N}}\int_{\mathbb{T}^{\overline{N}-1}}\nabla_{x_j}|\psi(\overline{x})|^2\Big|_{x_j=x}dx_1...\widehat{dx_j}...dx_{\overline{N}},\quad x\in\mathbb{T}. \tag{A.4}$$

Applying the triangle inequality to (A.3), we get

$$\begin{aligned}\|\rho^e(x)\|_{L^3(\mathbb{T})}&\le C\sum_{j=1}^{\overline{N}}\int_{\mathbb{T}^{\overline{N}-1}}[\int_{\mathbb{T}}|\psi(\overline{x})|^6dx_j]^{1/3}dx_1...\widehat{dx_j}...dx_{\overline{N}}\\&\le\int_{\mathbb{T}^{\overline{N}-1}}[\int_{\mathbb{T}}|\nabla_{x_j}\psi(\overline{x})|^2dx_j]dx_1...\widehat{dx_j}...dx_{\overline{N}}\le C\|\psi\|^2_{H^1(\overline{\mathbb{T}})}.\end{aligned} \tag{A.5}$$

by the Sobolev embedding theorem [1, Theorem 5.4, Part I]. Similarly, (A.4) implies that

$$\begin{aligned}\|\nabla\rho^e(x)\|_{L^{3/2}(\mathbb{T})} &\le C\sum_{j=1}^{\overline{N}}\int_{\mathbb{T}^{\overline{N}-1}}[\int_{\mathbb{T}}|\psi(\overline{x})\nabla_{x_j}\overline{\psi}(\overline{x})|^{3/2}dx_j]^{2/3}\,dx_1\ldots\widehat{dx_j}\ldots dx_{\overline{N}}\\ &\le \int_{\mathbb{T}^{\overline{N}-1}}[\int_{\mathbb{T}}|\psi(\overline{x})|^6dx_j]^{1/6}[\int_{\mathbb{T}}|\nabla_{x_j}\psi(\overline{x})|^2dx_j]^{1/2}\,dx_1\ldots\widehat{dx_j}\ldots dx_{\overline{N}}\\ &\le \int_{\mathbb{T}^{\overline{N}-1}}[\int_{\mathbb{T}}|\nabla_{x_j}\psi(\overline{x})|^2dx_j]\,dx_1\ldots\widehat{dx_j}\ldots dx_{\overline{N}}\le C\|\psi\|^2_{H^1(\overline{\mathbb{T}})}\end{aligned}\tag{A.6}$$

by the Hölder inequality and the Sobolev embedding theorem. □

Lemma A.5. *The potential $\Phi := G\rho$ admits the bound*

$$\|\Phi\|_{C(\mathbb{T})}+\|\nabla\Phi\|_{L^3(\mathbb{T})}\le C(1+\|\psi\|^2_{\mathscr{F}}).\tag{A.7}$$

Proof. Applying the Hölder and Hausdorff–Young inequalities to (2.1), we obtain that

$$\|\Phi\|_{C(\mathbb{T})}\le C\|\frac{\tilde\rho(\xi)}{\xi^2}\|_{L^1(\Xi\setminus 0)}\le C_1\|\xi\tilde\rho\|_{L^3(\Xi)}\Big[\sum_{\xi\in\Xi\setminus 0}|\xi|^{-9/2}\Big]^{2/3}\le C_2\|\nabla\rho\|_{L^{3/2}(\mathbb{T})}.\tag{A.8}$$

Similarly,

$$\|\nabla\Phi\|_{L^3(\mathbb{T})}\le C\|\frac{\tilde\rho(\xi)}{|\xi|}\|_{L^{3/2}(\Xi\setminus 0)}\le C_1\|\xi\tilde\rho\|_{L^3(\Xi)}\Big[\sum_{\xi\in\Xi\setminus 0}|\xi|^{-6}\Big]^{1/3}\le C_2\|\nabla\rho\|_{L^{3/2}(\mathbb{T})}.\tag{A.9}$$

Now the bound (A.7) follows from (A.2). □

Now we can prove the estimate (A.1). First, we will prove

$$\|\Phi^{\otimes}\,\psi\|_{\mathscr{F}}\le C(1+\|\psi\|^3_{\mathscr{F}})\tag{A.10}$$

in the notation (1.4). According to definition (1.3) it suffices to check that

$$\|\Phi^{\otimes}\,\psi\|_{L^2(\overline{\mathbb{T}})}+\|\Phi^{\otimes}\,\nabla^{\otimes}\,\psi\|_{L^2(\overline{\mathbb{T}})}+\|\psi\nabla^{\otimes}\,\Phi^{\otimes}\|_{L^2(\overline{\mathbb{T}})}\le C(1+\|\psi\|^3_{\mathscr{F}}).\tag{A.11}$$

The first two summands admit the needed estimate by (A.7). The third summand requires some additional argument. Namely,

$$\begin{aligned}\|\,\psi\nabla^{\otimes}\,\Phi^{\otimes}\,\|^2_{L^2(\overline{\mathbb{T}})} &= \int_{\overline{\mathbb{T}}}|\sum_{j=1}^{\overline{N}}\nabla\Phi(x_j)\,\psi(\overline{x})|^2\,d\overline{x}\le C\sum_{1}^{\overline{N}}\int_{\overline{\mathbb{T}}}|\nabla\Phi(x_j)\,\psi(\overline{x})|^2\,d\overline{x}\\ &= C\sum_{j=1}^{\overline{N}}\int_{\mathbb{T}^{\overline{N}-1}}\Big[\int_{\mathbb{T}}|\nabla\Phi(x_j)\,\psi(\overline{x})|^2\,dx_j\Big]dx_1\ldots\widehat{dx_j}\ldots dx_{\overline{N}}.\end{aligned}\tag{A.12}$$

The inner integral is estimated as follows

$$\int_{\mathbb{T}}|\nabla\Phi(x_j)\,\psi(\overline{x})|^2\,dx_j\le\|\nabla\Phi\|^2_{L^3(\mathbb{T})}\Big[\int_{\mathbb{T}}|\psi(\overline{x})|^6\,dx_j\Big]^{1/3}\le C\|\nabla\Phi\|^2_{L^3(\mathbb{T})}\int_{\mathbb{T}}|\nabla_{x_j}\psi(\overline{x})|^2\,dx_j\tag{A.13}$$

by the Hölder inequality and the Sobolev embedding theorem. Substituting this estimate into (A.12), we obtain

$$\|\psi\nabla^{\otimes}\Phi^{\otimes}\|_{L^2(\overline{\mathbb{T}})} \le C\|\nabla\Phi\|_{L^3(\mathbb{T})}\|\psi\|_{\mathscr{F}}. \tag{A.14}$$

This and (A.7) imply (A.11) for the third summand. Finally, using (2.13), (A.7) and (1.1),

$$|f(n)| \le \|\Phi\|_{C(\mathbb{T})}\|\nabla\sigma\|_{L^1(\mathbb{T})} \le C(1+\|\psi\|^2_{\mathscr{F}}), \qquad n\in\Gamma. \tag{A.15}$$

Hence, (A.10) and (A.15) imply (A.1). Proposition A.3 is proved. □

It remains to prove that the nonlinearity is locally Lipschitz.

Proposition A.6. *For any $R>0$ and $X_1,X_2\in\mathscr{V}=H^1(\overline{\mathbb{T}})\otimes\overline{\mathbb{T}}\otimes\mathbb{R}^{3\overline{N}}$ with $|X_1|_{\mathscr{V}},|X_2|_{\mathscr{V}}\le R$*

$$\|N(X_1)-N(X_2)\|_{\mathscr{W}} \le C(R)d_{\mathscr{V}}(X_1,X_2). \tag{A.16}$$

Proof. Writing $X_k=(\psi_k,q_k,p_k)$ and $\Phi_k=G\rho_k$, we obtain that

$$\|\Phi_1^{\otimes}\psi_1-\Phi_2^{\otimes}\psi_2\|_{\mathscr{F}} \le \|(\Phi_1^{\otimes}-\Phi_2^{\otimes})\psi_1\|_{\mathscr{F}} + \|\Phi_2^{\otimes}(\psi_1-\psi_2)\|_{\mathscr{F}}. \tag{A.17}$$

Using (A.14) and (A.7), we obtain

$$\begin{aligned}\|\Phi_2^{\otimes}(\psi_1-\psi_2)\|_{\mathscr{F}} &\le (\|\Phi_2\|_{C(\mathbb{T})}+\|\nabla\Phi_2\|_{L^3(\mathbb{T})})\|\psi_1-\psi_2\|_{\mathscr{F}}\\ &\le C(1+R^2)\|\psi_1-\psi_2\|_{\mathscr{F}} \le C(R)d_{\mathscr{V}}(X_1,X_2).\end{aligned} \tag{A.18}$$

Further, (A.8) and (A.9) give that

$$\|\Phi_1-\Phi_2\|_{C(\mathbb{T})}+\|\nabla\Phi_1-\nabla\Phi_2\|_{L^3(\mathbb{T})} \le \|\nabla\rho_1-\nabla\rho_2\|_{L^{3/2}(\mathbb{T})} \tag{A.19}$$

However, $|\sigma(x)-\sigma(x-a)|\le C|a|$, where $|a|:=\min_{r\in a}|r|$ for $a\in\mathbb{T}$ (by definition, $a\subset\mathbb{R}^3$ is a class of equivalence mod $N\mathbb{Z}^3$). Therefore, as in (A.2),

$$\|\nabla(\rho_1-\rho_2)\|_{L^{3/2}(\mathbb{T})} \le CR(|q_1-q_2|+\|\psi_1-\psi_2\|_{\mathscr{F}}). \tag{A.20}$$

Hence,

$$\begin{aligned}\|(\Phi_1^{\otimes}-\Phi_2^{\otimes})\psi_1\|_{\mathscr{F}} &\le (\|\Phi_1-\Phi_2\|_{C(\mathbb{T})}+\|\nabla(\Phi_1-\Phi_2)\|_{L^3(\mathbb{T})})\|\psi_1\|_{\mathscr{F}}\\ &\le CR\|\nabla(\rho_1-\rho_2)\|_{L^{3/2}(\mathbb{T})}\|\psi_1\|_{\mathscr{F}} \le C(R)d_{\mathscr{V}}(X_1,X_2).\end{aligned} \tag{A.21}$$

Now (A.17)–(A.21) give

$$\|\Phi_1^{\otimes}\psi_1-\Phi_2^{\otimes}\psi_2\|_{H^1(\mathbb{T})} \le C(R)d_{\mathscr{V}}(X_1,X_2). \tag{A.22}$$

Similarly, (A.19), (A.20) and (A.7) imply

$$\begin{aligned}&\|\langle\nabla\Phi_1,\sigma(\cdot-n-q_1(n))\rangle-\langle\nabla\Phi_2,\sigma(\cdot-n-q_2(n))\rangle\|\\ &\le \|\langle\nabla(\Phi_1-\Phi_2),\sigma(\cdot-n-q_1(n))\rangle\|+\|\langle\nabla\Phi_2,\sigma(\cdot-n-q_1(n))-\sigma(\cdot-n-q_2(n))\rangle\|\\ &\le C(\|\Phi_1-\Phi_2\|_{C(\mathbb{T})}+\|\Phi_2\|_{C(\mathbb{T})})|q_1-q_2|) \le C(R)d_{\mathscr{V}}(X_1,X_2).\end{aligned} \tag{A.23}$$

This estimate together with (A.22) prove (A.16). □

Now Theorem A.2 follows from Propositions A.3 and A.6.

Proof of Theorem A.1. The local solution $X \in C([-\tau,\tau],\mathscr{V})$ to (2.3) exists and is unique by Theorem A.2. On the other hand, the conservation laws (1.16) (proved in Proposition B.2 iii)) together with (2.10) imply a priori bound

$$|X(t)|^2_{\mathscr{V}} \le C[E(X(0))+Q(X(0))], \qquad t \in [-\tau,\tau] \tag{A.24}$$

by (2.10). Hence, the local solution admits an extension to the global one $X \in C(\mathbb{R},\mathscr{V})$. □

Remark A.7. *The condition $X(0) \in \mathscr{M}$ implies that $X(t) \in \mathscr{M}$ for all $t \in \mathbb{R}$ by the charge conservation (1.16). Hence, (2.3) implies (1.5)–(1.7) with the potential $\Phi(\cdot,t) = G\rho(\cdot,t)$.*

B Conservation laws

We deduce the conservation laws (1.16) by the Galerkin approximations [27]. Let us recall that the exterior product of functions $f_j \in L^2(\mathbb{T})$ is defined by

$$[\Lambda_{j=1}^{\overline{N}} f_j](\overline{x}) := \frac{1}{\sqrt{\overline{N}!}} \sum_{\pi \in S_{\overline{N}}} (-1)^{|\pi|} \prod_{j=1}^{\overline{N}} f_j(x_{\pi(j)}), \qquad \overline{x} = (x_1,...,x_{\overline{N}}) \in \overline{\mathbb{T}}, \tag{B.1}$$

where $S_{\overline{N}}$ is the symmetric group and $|\pi|$ denotes the sign (or parity) of a transposition π.

Definition B.1. *i)$\mathscr{V}_m$ with $m \in \mathbb{N}$ denotes the finite-dimensional submanifold of the Hilbert manifold $\mathscr{V} = H^1(\overline{\mathbb{T}}) \otimes \overline{\mathbb{T}} \otimes \mathbb{R}^{3\overline{N}}$*

$$\mathscr{V}_m := \{(\sum_{\overline{k}} C(\overline{k}) \Lambda_{j=1}^{\overline{N}} e^{ik_j x_j}, q, p) : k_j \in \Xi,\ C(\overline{k}) \in \mathbb{C},\ \sum_{j=1}^{\overline{N}} k_j^2 \le m,\ q \in \overline{\mathbb{T}},\ p \in \mathbb{R}^{3\overline{N}}\}, \tag{B.2}$$

where $\overline{k} := (k_1,...,k_{\overline{N}})$.

ii) $\mathscr{W}_m$ with $m \in \mathbb{N}$ denotes the finite-dimensional linear subspace of the Hilbert space $\mathscr{W} = H^1(\overline{\mathbb{T}}) \oplus \mathbb{R}^{3\overline{N}} \oplus \mathbb{R}^{3\overline{N}}$

$$\mathscr{W}_m := \{(\sum_{\overline{k}} C(\overline{k}) \Lambda_{j=1}^{\overline{N}} e^{ik_j x_j}, \varkappa, v) : k_j \in \Xi,\ C(\overline{k}) \in \mathbb{C},\ \sum_{j=1}^{\overline{N}} k_j^2 \le m,\ \varkappa \in \mathbb{R}^{3\overline{N}},\ v \in \mathbb{R}^{3\overline{N}}\}. \tag{B.3}$$

Obviously, $\mathscr{V}_1 \subset \mathscr{V}_2 \subset ...$, the union $\cup_m \mathscr{V}_m$ is dense in $\mathscr{V}$, and $\mathscr{W}_m$ are invariant with respect to H and J. Let us denote by P_m the orthogonal projector $\mathscr{X} \to \mathscr{W}_m$. This projector is also orthogonal in the Hilbert space $\mathscr{W}$. Let us approximate the system (2.3) by finite-dimensional Hamilton systems on the manifold $\mathscr{V}_m$,

$$\dot{X}_m(t) = JE'_m(X_m(t)), \qquad t \in \mathbb{R}, \tag{B.4}$$

where $E_m := E|_{\mathscr{V}_m}$ and $X_m(t) = (\psi_m(t), q_m(t), p_m(t)) \in C(\mathbb{R},\mathscr{V}_m)$. The equation (B.4) can be also written as

$$\langle \dot{X}_m(t), Y\rangle = -\langle E'(X_m(t)), JY\rangle, \qquad Y \in \mathscr{W}_m. \tag{B.5}$$

This form of the equation (B.4) holds since $E_m := E|_{\mathscr{V}_m}$ and $\mathscr{W}_m$ is invariant with respect to J. Equivalently,

$$\dot{X}_m(t) = HX_m(t) + P_m N(X_m(t)). \tag{B.6}$$

The Hamiltonian form guarantees the energy and charge conservation (1.16):

$$E(X_m(t)) = E(X_m(0)), \quad Q(X_m(t)) = Q(X_m(0)), \qquad t \in \mathbb{R}. \tag{B.7}$$

Indeed, the energy conservation holds by the Hamiltonian form (B.4), while the charge conservation holds by the Noether theory [2, 14, 17] due to the $U(1)$-invariance of E_m, see (1.17).

The equation (B.6) admits a unique local solution for every initial state $X_m(0) \in \mathscr{V}_m$ since the right hand side is locally bounded and Lipschitz continuous. The global solutions exist by (2.10) and the energy and charge conservation (B.7).

Finally, we take any $X(0) \in \mathscr{V}$ and choose a sequence

$$X_m(0) \to X(0), \qquad m \to \infty, \tag{B.8}$$

where the convergence holds in the metric of $\mathscr{V}$. Therefore,

$$E(X_m(0)) \to E(X(0)), \qquad Q(X_m(0)) \to Q(X(0)). \tag{B.9}$$

Hence, (B.7) and (2.10) imply the basic uniform bound

$$R := \sup_{m\in\mathbb{N}} \sup_{t\in\mathbb{R}} |X_m(t)|_{\mathscr{V}} < \infty. \tag{B.10}$$

Therefore, (B.6) and Proposition A.3 imply the second basic uniform bound

$$\sup_{m\in\mathbb{N}} \sup_{t\in\mathbb{R}} \|\dot{X}_m(t)\|_{\mathscr{W}^{-1}} < C(R), \tag{B.11}$$

since the operator $H : \mathscr{W} \to \mathscr{W}^{-1}$ is bounded, and the projector P_m is also a bounded operator in $\mathscr{W} \subset \mathscr{W}^{-1}$. Hence, the Galerkin approximations $X_m(t)$ are uniformly Lipschitz-continuous with values in $\mathscr{V}^{-1}$:

$$\sup_{m\in\mathbb{N}} d_{\mathscr{V}^{-1}}(X_m(t), X_m(s)) \le C(R)|t-s|, \qquad s,t \in \mathbb{R}. \tag{B.12}$$

Let us show that the uniform estimates (B.10) and (B.12) imply a compactness of the Galerkin approximations and the conservation laws. Let us recall that $\mathscr{X} := \mathscr{V}^0$ and $\mathscr{V} := \mathscr{V}^1$.

Proposition B.2. *Let (1.1) hold and $X(0) \in \mathscr{V}$. Then*

i) There exists a subsequence $m' \to \infty$ such that

$$X_{m'}(t) \xrightarrow{\mathscr{X}} X(t), \qquad m' \to \infty, \qquad t \in \mathbb{R}, \tag{B.13}$$

where $X(\cdot) \in C(\mathbb{R}, \mathscr{X})$.

ii) Every limit function $X(\cdot)$ is a solution to (2.3), and $X(\cdot) \in C(\mathbb{R}, \mathscr{V})$.

iii) The conservation laws (1.16) hold.

Proof. i) The convergence (B.13) follows from (B.10) and (B.11) by the Dubinsky 'theorem on three spaces' [10] (Theorem 5.1 of [27]). Namely, the embedding $\mathscr{V} \subset \mathscr{X}$ is compact by the Sobolev theorem, and hence, (B.13) holds by (B.10) for $t \in D$, where D is a countable dense set. Finally, let us use the interpolation inequality and (B.10), (B.12): for any $\varepsilon > 0$

$$d_{\mathscr{X}}(X_m(t), X_m(s)) \le \varepsilon d_{\mathscr{V}}(X_m(t), X_m(s)) + C(\varepsilon) d_{\mathscr{V}^{-1}}(X_m(t), X_m(s)) \le 2\varepsilon R + C(\varepsilon, R)|t-s|. \tag{B.14}$$

This inequality implies the equicontinuity of the Galerkin approximations with values in $\mathscr{X}$. Hence, convergence (B.13) holds for all $t \in \mathbb{R}$ since it holds for the dense set of $t \in D$. The same equicontinuity also implies the continuity of the limit function $X \in C(\mathbb{R}, \mathscr{X})$.

ii) Integrating equation (B.6), we obtain

$$\int_0^t \langle \dot{X}_m(t), Y\rangle \, ds = \int_0^t \langle X_m(s), HY\rangle \, ds + \int_0^t \langle N(X_m(s)), Y\rangle \, ds, \qquad Y \in \mathscr{W}_m, \tag{B.15}$$

Below we will write m instead of m'. To prove (2.12) it suffices to check that in the limit $m \to \infty$, we get

$$\int_0^t \langle \dot{X}(t), Y\rangle \, ds = \int_0^t (X(s), HY) \, ds + \int_0^t \langle N(X(s)), Y\rangle \, ds, \qquad Y \in \mathscr{W}_n, \qquad n \in \mathbb{N}. \tag{B.16}$$

The convergence of the left hand side and of the first term on the right hand side of (B.15) follow from (B.13) and (B.8) since $HY \in \mathscr{W}_m$.

It remains to consider the last integral in (B.15). The integrand is uniformly bounded by (B.10) and Proposition A.3. Hence, it suffices to check the pointwise convergence

$$\langle N(X_m(s), Y\rangle \longrightarrow \langle N(X(s), Y\rangle, \qquad Y \in \mathscr{W}_n \tag{B.17}$$

for any $s \in \mathbb{R}$. Here $N(X_m(s)) = (ie\Phi_m^{\otimes}(s)\psi_m(s), p_m(s), f_m(s))$ according to the notation (2.13), and $Y = (\varphi, \varkappa, v) \in \mathscr{W}_n$. Hence, (B.17) reads

$$ie[\Phi_m^{\otimes}(s)\psi_m(s), \varphi] + p_m(s)\varkappa + f_m(s)v \to ie(\Phi^{\otimes}(s)\,\psi(s), \varphi) + p(s)\varkappa + f(s)v, \tag{B.18}$$

where $[\cdot,\cdot]$ is the scalar product in $L^2(\overline{\mathbb{T}})$. The convergence of $p_m(s)\varkappa$ follows from (B.13) (with $m' = m$) . To prove the convergence of the two remaining terms we first show that

$$\Phi_m(s) := G\rho_m \xrightarrow{C(\mathbb{T})} \Phi(s) := G\rho. \tag{B.19}$$

Indeed, (B.13) implies that

$$\psi_m(s) \xrightarrow{L^2(\overline{\mathbb{T}})} \psi(s), \qquad q_m(s) \to q(s) \tag{B.20}$$

Further, the sequence $\psi_m(s)$ is bounded in $H^1(\overline{\mathbb{T}})$ by (B.10). Hence, the sequence $\rho_m(s)$ is bounded in the Sobolev space $W^{1,3/2}(\mathbb{T})$ by (A.2). Therefore, the sequence $\rho_m(s)$ is precompact in $L^2(\mathbb{T})$ by the Sobolev compactness theorem. Hence,

$$\rho_m \xrightarrow{L^2(\mathbb{T})} \rho \tag{B.21}$$

by (B.20). Therefore, (B.19) holds since the operator $G : L^2(\mathbb{T}) \to C(\mathbb{T})$ is continuous. Finally, (B.19) and (B.20) imply that

$$\Phi_m^{\otimes}(s)\psi_m(s) \xrightarrow{L^2(\overline{\mathbb{T}})} \Phi^{\otimes}(s)\psi(s), \qquad f_m(s) \to f(s), \tag{B.22}$$

which proves (B.18). Now (B.16) is proved for $Y \in \mathscr{V}_n$ with any $n \in \mathbb{N}$. Hence, $X(t)$ is a solution to (2.3). Finally, $N(X(t))$ is bounded in $\mathscr{W}$ by (B.10) and Proposition A.3. Hence, (2.12) implies that

$X(\cdot) \in C(\mathbb{R}, \mathscr{V})$.

iii) The conservation laws (B.7) and the convergences (B.8), (B.13) imply that

$$E(X(t)) \le E(X(0)), \quad Q(X(t)) \le Q(X(0)), \qquad t \in \mathbb{R}. \tag{B.23}$$

The last inequality holds by the first convergence of (B.20). The first inequality follows from the representation

$$E(X_m(t)) = \frac{1}{2}\|\nabla\psi_m(t)\|^2_{L^2(\mathbb{T})} + \frac{1}{2}\|\sqrt{G}\rho_m(t)\|^2_{L^2(\mathbb{T})} + \sum_{n\in\Gamma_n} \frac{p_m^2(n,t)}{2M}. \tag{B.24}$$

Namely, the last two terms on the right hand side converge by (B.21) and (B.13). Moreover, the first term is bounded by (B.10). Hence, the first convergence of (B.20) implies the weak convergence

$$\nabla\psi_m(t) \xrightarrow{L^2_w(\overline{\mathbb{T}})} \nabla\psi(t) \tag{B.25}$$

by the Banach theorem. Now the first inequality of (B.23) follows by the property of the weak convergence in the Hilbert space. Finally, the opposite inequalities to (B.23) are also true by the uniqueness of solutions $X(\cdot) \in C(\mathbb{R}, \mathscr{V})$, which is proved in Proposition A.2. □

References

[1] R.A. Adams, Sobolev Spaces, Academic Press, NY, 1975.

[2] V. Arnold, Mathematical Methods of Classical Mechanics, Springer, New York, 1978.

[3] F. Bonetto, J. L. Lebowitz, L. Rey-Bellet, Fourier's law: a challenge to theorists, p. 128-150 in: Fokas, A. (ed.) et al., Mathematical physics 2000. International congress, London, GB, 2000, Imperial College Press, London, 2000.

[4] M. Born, K. Huang, Dynamical Theory of Crystal Lattices, The Clarendon Press, Oxford University Press, New York, 1998.

[5] E. Cancès, S. Lahbabi, M. Lewin, Mean-field models for disordered crystals, *J. Math. Pures Appl. (9)* **100** (2013), no. 2, 241-274.

[6] E. Cancès, G. Stoltz, A mathematical formulation of the random phase approximation for crystals, *Ann. I. H. Poincaré - AN* **29** (2012), 887-925.

[7] L. Catto, C. Le Bris, P.-L. Lions, The Mathematical Theory of Thermodynamic Limits: Thomas-Fermi Type Models, Clarendon Press, Oxford, 1998.

[8] L. Catto, C. Le Bris, P.-L. Lions, On the thermodynamic limit for Hartree-Fock type models, *Ann. Inst. Henri Poincaré, Anal. Non Linéaire* **18** (2001), no. 6, 687-760.

[9] L. Catto, C. Le Bris, P.-L. Lions, On some periodic Hartree-type models for crystals, *Ann. Inst. Henri Poincaré, Anal. Non Linéaire* **19** (2002), no. 2, 143-190.

[10] Yu. A. Dubinsky, Weak convergence in non-linear elliptic and parabolic equations, *Mat. USSR Sb.* **67** (4) (1965), 609-642 (in Russian).

[11] F.J. Dyson, Ground-state energy of a finite system of charged particles, J. Math. Phys. 8, 1538-1545 (1967).

[12] F.J. Dyson, A. Lenard, Stability of matter I, *J. Math. Phys.* **8** (1967), 423-434; II, ibid. **9** (1968), 698-711.

[13] G. Giuliani, G. Vignale, Quantum Theory of the Electron Liquid, Cambridge University Press, Cambridge, 2005.

[14] M. Grillakis, J. Shatah, W. Strauss, Stability theory of solitary waves in the presence of symmetry. I, *J. Funct. Anal.* **74** (1987), 160-197.

[15] L. Hörmander, The Analysis of Linear Partial Differential Operators. I. Distribution Theory and Fourier Analysis, Springer, Berlin, 2003.

[16] C. Kittel, Introduction to Solid State Physics, Wiley & Sons, Hoboken, NJ, 2005.

[17] A. I. Komech, Quantum Mechanics: Genesis and Achievements, Springer, Dordrecht, 2013.

[18] A. I. Komech, On crystal ground state in the Schrödinger–Poisson model, *SIAM J. Math. Anal.* **47** (2015), no. 2, 1001-1021. arXiv:1310.3084

[19] A. I. Komech, On crystal ground state in the Schrödinger–Poisson model with point ions, submitted to *J. Math. Anal. Appl.*, 2015. arXiv:1409.1847

[20] A. Komech, E. Kopylova, On the linear stability of crystals for the Schrödinger-Poisson model, *J. Stat. Phys.* **165** (2016), no. 2, 246-273.

arXiv:1505.07074

[21] C. Le Bris, P.-L. Lions, From atoms to crystals: a mathematical journey, *Bull. Am. Math. Soc., New Ser.* **42** (2005), no. 3, 291-363.

[22] J.L. Lebowitz, E.H. Lieb, Existence of thermodynamics for real matter with Coulomb forces, *Phys. Rev. Lett.* **22** (13) (1969), 631-634.

[23] J.L. Lebowitz, E.H. Lieb, Lectures on the thermodynamic limit for Coulomb systems, in: Springer Lecture Notes in Physics, Vol. 20, Springer, 1973, pp. 136-161.

[24] M. Lewin, J. Sabin, The Hartree equation for infinitely many particles. I. Well-posedness theory, arXiv:1310.0603.

[25] M. Lewin, J. Sabin, The Hartree equation for infinitely many particles. II. Dispersion and scattering in 2D, arXiv:1310.0604.

[26] E.H. Lieb, R. Seiringer, The Stability of Matter in Quantum Mechanics, Cambridge University Press, Cambridge, 2009.

[27] J.-L. Lions, Quelques méthodes de résolution des problèmes aux limites non linéaires, Dunod; Gauthier-Villars, Paris, 1969.

[28] M. Reed, B. Simon, Methods of Modern Mathematical Physics, II: Fourier Analysis, Self-Adjointness, Academic Press, NY, 1975.

[29] J.A. Stratton, Electromagnetic Theory, John Wiley & Sons, Inc., Hoboken, New Jersey, 2007.

[30] M. Ziman, The Calculation of Bloch Functions, Academic Press, NY, 1971.