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On linear stability of crystals in the Schrödinger–Poisson model

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Abstract

We consider the Schrödinger–Poisson–Newton equations for crystals with a cubic lattice and one ion per cell. We linearize this dynamics at the ground state and introduce a novel class of the ion charge densities which provide the stability of the linearized dynamics. This is the first result on linear stability for crystals.

Our key result is the *energy positivity* for the Bloch generators of the linearized dynamics under a Wiener-type condition on the ion charge density. We also assume an additional condition which cancels the negative contribution caused by electrostatic instability.

The proof of the energy positivity relies on a novel factorization of the corresponding Hamilton functional. We show that the energy positivity can fail if the additional condition breaks down while the Wiener condition holds.

The Bloch generators are nonselfadjoint (and even nonsymmetric) Hamilton operators. We diagonalize these generators using our theory of spectral resolution of the Hamilton operators *with positive definite energy* [15, 16]. Using this spectral resolution, we establish the stability of the linearized crystal dynamics.

Key words and phrases: crystal; lattice; field; Schrödinger–Poisson equations; Hamilton equation; ground state; linearization; stability; positivity; Bloch transform; Hamilton operator; self-adjoint operator; spectral resolution.

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1 Introduction

First mathematical results on stability of matter were obtained by Dyson and Lenard in [8, 9] where the energy bound from below has been established. The thermodynamic limit for the Coulomb systems was studied first by Lebowitz and Lieb [18, 19], see the survey and further development in [20]. These results were extended by Catto, L. Lions, Le Bris and others to Thomas-Fermie and Hartree-Fock models [4, 5, 6]. 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. The dynamical stability of infinite particle ground states was never considered previously.

We establish for the first time the dynamical stability of crystal ground state in linear approximation for the simplest Schrödinger-Poisson model. The ground state for this model was constructed in [14].

We consider crystals with the cubic lattice $\Gamma = \mathbb{Z}^3$ and with one ion per cell. The electron cloud is described by one-particle Schrödinger equation. The ions are described as classical particles that corresponds to the Born and Oppenheimer approximation. The ions interact with the electron cloud via the scalar potential, which is a solution to the corresponding Poisson equation.

This model does not respect the Pauli exclusion principle for electrons. However, it provides a convenient framework to introduce suitable functional tools, which might be useful for physically more realistic models (Thomas–Fermie, Hartree–Fock, and second quantized models). In particular, we find a novel Wiener-type stability criterion (1.23), (1.24).

This investigation is motivated by the lack of a suitable mathematical model 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 [1].

We denote by $\sigma(x)$ the charge density of one ion:

$$\int_{\mathbb{R}^3} \sigma(x)dx = eZ > 0, \tag{1.1}$$

where $e > 0$ is the elementary charge. Let $\psi(x,t)$ be the wave function of the electron field, and $\Phi(x)$ 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. Then the coupled equations read

$$i\dot{\psi}(x,t) = -\frac{1}{2}\Delta\psi(x,t) - e\Phi(x,t)\psi(x,t), \qquad x \in \mathbb{R}^3, \tag{1.2}$$

$$-\Delta\Phi(x,t) = \rho(x,t) := \sum_n \sigma(x - n - q(n,t)) - e|\psi(x,t)|^2, \qquad x \in \mathbb{R}^3, \tag{1.3}$$

$$M\ddot{q}(n,t) = -\langle \nabla\Phi(x,t), \sigma(x - n - q(n,t))\rangle, \qquad n \in \mathbb{Z}^3. \tag{1.4}$$

Here the brackets stand for the Hermitian scalar product in the Hilbert space $L^2(\mathbb{R}^3)$ and for its different extensions, and the series (1.3) converges in a suitable sense. All derivatives here and below are understood in the sense of distributions. These equations can be written as the Hamilton system with a formal Hamilton functional

$$\mathscr{H}(\psi, q, p) = \frac{1}{2}\int_{\mathbb{R}^3} [|\nabla\psi(x)|^2 + \rho(x)G\rho(x)]dx + \sum_n \frac{p^2(n)}{2M}, \tag{1.5}$$

where $G := -\Delta^{-1}$ and $q := (q(n) :\ n \in \mathbb{Z}^3)$, $p := (p(n) :\ n \in \mathbb{Z}^3)$, and $\rho(x)$ is defined similarly to (1.3). Namely, the system (1.2)-(1.4) can be formally written as

$$i\dot{\psi}(x,t) = \partial_{\overline{\psi}(x)}\mathscr{H}, \quad \dot{q}(n,t) = \partial_{p(n)}\mathscr{H}, \quad \dot{p}(n,t) = -\partial_{q(n)}\mathscr{H}, \tag{1.6}$$

where $\partial_{\overline{z}} := \frac{1}{2}(\partial_{z_1} + i\partial_{z_2})$ with $z_1 = \mathrm{Re}\, z$ and $z_2 = \mathrm{Im}\, z$. A ground state of a crystal is a Γ-periodic stationary solution

$$\psi^0(x)e^{-i\omega^0 t}\ , \quad \Phi^0(x)\ , \quad q^0(n) = q^0 \ \text{ for } \ n \in \mathbb{Z}^3 \tag{1.7}$$

with a real ω^0 (and $q^0 \in \mathbb{R}^3$ can be chosen arbitrary). A ground state was constructed in [14]. Substituting (1.7) into (1.2)-(1.4), we obtain the system

$$\omega^0\psi^0(x) \ = \ -\frac{1}{2}\Delta\psi^0(x) - e\Phi^0(x)\psi^0(x), \qquad x \in T^3 := \mathbb{R}^3/\Gamma, \tag{1.8}$$

$$-\Delta\Phi^0(x) \ = \ \rho^0(x) := \sigma^0(x) - e|\psi^0(x)|^2, \qquad x \in T^3, \tag{1.9}$$

$$0 \ = \ -\langle\nabla\Phi^0(x), \sigma(x-n-q^0)\rangle, \qquad n \in \mathbb{Z}^3, \tag{1.10}$$

where we denote

$$\sigma^0(x) := \sum_n \sigma(x-n-q^0). \tag{1.11}$$

In present paper we prove the stability for the *formal linearization* of the nonlinear system (1.2)-(1.4) at the ground state (1.7). Namely, substituting

$$\psi(x,t) = [\psi^0(x) + \Psi(x,t)]e^{-i\omega^0 t}, \quad q(n,t) = q^0 + Q(n,t) \tag{1.12}$$

into the nonlinear equations (1.2), (1.4) with $\Phi(x,t) = G\rho(x,t)$, we *formally* obtain the linearized equations (see Appendix A)

$$\left.\begin{aligned} &[i\partial_t + \omega^0]\Psi(x,t) = -\tfrac{1}{2}\Delta\Psi(x,t) - e\Phi^0(x)\Psi(x,t) - e\psi^0(x)G\rho_1(x,t) \\ &\dot{Q}(n,t) = P(n,t)/M \\ &\dot{P}(n,t) = -\langle\nabla G\rho_1(t), \sigma(x-n-q^0)\rangle + \langle\nabla\Phi^0, \nabla\sigma(x-n-q^0)Q(n,t)\rangle \end{aligned}\right| \begin{array}{l} x \in \mathbb{R}^3 \\ n \in \mathbb{Z}^3 \end{array} \tag{1.13}$$

Here $\rho_1(x,t)$ is the linearized charge density

$$\rho_1(x,t) = -\sum_n \nabla\sigma(x-n-q^0)Q(n,t) - 2e\mathrm{Re}\,[\psi^0(x)\overline{\Psi(x,t)}], \tag{1.14}$$

The system (1.13) is linear over $\mathbb{R}$ but it is not complex linear. This is due to the last term in (1.14), which appears from the linearization of the term $|\psi|^2 = \psi\overline{\psi}$ in (1.3). However, we need the complex linearity for the application of the spectral theory. This why we will consider below the complexification of the system (1.13) writing it in the variables $\Psi_1(x,t) := \mathrm{Re}\,\Psi(x,t), \Psi_2(x,t) := \mathrm{Im}\,\Psi(x,t)$. We will consider the case when the ground state $\psi^0(x)$ can be taken to be a real function. In this case

$$\mathrm{Re}\,[\psi^0(x)\overline{\Psi(x,t)}] = \psi^0(x)\Psi_1(x,t). \tag{1.15}$$

Further we denote

$$Y(t) = (\Psi_1(\cdot,t), \Psi_2(\cdot,t), Q(\cdot,t), P(\cdot,t)). \tag{1.16}$$

Then (1.13) can be written as

$$\dot{Y}(t) = AY(t), \qquad A = \begin{pmatrix} 0 & H^0 & 0 & 0 \\ -H^0 - 2e^2\psi^0 G\psi^0 & 0 & -S & 0 \\ 0 & 0 & 0 & M^{-1} \\ -2S^* & 0 & -T & 0 \end{pmatrix}, \tag{1.17}$$

where $H^0 := -\frac{1}{2}\Delta - e\Phi^0(x) - \omega^0$, the operators S and T correspond to matrices (4.4) and (4.5) respectively, and ψ^0 denotes the operators of multiplication by the real function $\psi^0(x)$. The Hamilton representation (1.6) implies that

$$A = JB, \qquad B = D^2\mathscr{H}(\psi^0, q^0, 0) = \begin{pmatrix} 2H^0 + 4e^2\psi^0 G\psi^0 & 0 & 2S & 0 \\ 0 & 2H^0 & 0 & 0 \\ 2S^* & 0 & T & 0 \\ 0 & 0 & 0 & M^{-1} \end{pmatrix}, \tag{1.18}$$

where J is the skew-symmetric matrix (5.2). Our basic result is the stability for the linearized system (1.17): for any finite energy initial state there exists a unique global solution, and it is bounded in the energy norm.

We show that the generator A is densely defined in the Hilbert space $\mathscr{X} := L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \oplus \mathbb{R}^3 \oplus \mathbb{R}^3$ and commutes with translations by vectors from Γ. Hence, the equation (1.17) can be reduced by the Fourier–Bloch–Gelfand–Zak transform to equations with the corresponding Bloch generators $\tilde{A}(\theta) = J\tilde{B}(\theta)$, which depend on the parameter θ from the Brillouin zone $\Pi^* := [0, 2\pi]^3$. The Bloch energy operator $\tilde{B}(\theta)$ is given by

$$\tilde{B}(\theta) = \begin{pmatrix} 2\tilde{H}^0(\theta) + 4e^2\psi^0\tilde{G}(\theta)\psi^0 & 0 & 2\tilde{S}(\theta) & 0 \\ 0 & 2\tilde{H}^0(\theta) & 0 & 0 \\ 2\tilde{S}^*(\theta) & 0 & \hat{T}(\theta) & 0 \\ 0 & 0 & 0 & M^{-1} \end{pmatrix}, \qquad \theta \in \Pi^* \setminus \Gamma^*, \tag{1.19}$$

where $\Gamma^* := 2\pi\mathbb{Z}^3$, and $\tilde{H}^0(\theta) := -\frac{1}{2}(\nabla + i\theta)^2 - e\Phi^0(x) - \omega^0$. Further, $\tilde{G}(\theta)$ is the inverse to the operator $(i\nabla - \theta)^2 : H^2(T^3) \to L^2(T^3)$. Finally, $\tilde{S}(\theta)$ and $\hat{T}(\theta) = \hat{T}_2(\theta) + \hat{T}_1(\theta)$ are defined respectively by (7.22) and (4.10), (4.13).

However, the operator A is not selfadjoint and even not symmetric, which is a typical situation for the linearization of $U(1)$-invariant nonlinear equations [15, Appendix B]. Respectively, the Bloch generators $\tilde{A}(\theta)$ are not selfadjoint in the Hilbert space

$$\mathscr{X}(T^3) := L^2(T^3) \oplus L^2(T^3) \oplus \mathbb{C}^3 \oplus \mathbb{C}^3, \qquad T^3 := \mathbb{R}^3/\Gamma. \tag{1.20}$$

The main crux here is that we cannot apply the von Neumann spectral theorem to the nonselfadjoint generators A and $\tilde{A}(\theta)$. We solve this problem by applying our spectral theory of the Hamilton operators with positive energy [15, 16], which is an infinite-dimensional version of some Gohberg and Krein ideas from the theory of parametric resonance [12, Chap. VI]. This is why we need the positivity of the energy operator $\tilde{B}(\theta)$:

$$\mathscr{E}(\theta, Y) := \langle Y, \tilde{B}(\theta)Y\rangle_{T^3} \geq \varkappa(\theta)\|Y\|^2_{\mathscr{V}(T^3)}, \qquad \text{a.e. } \theta \in \Pi^* \setminus \Gamma^*, \tag{1.21}$$

where $\varkappa(\theta) > 0$, the brackets stand for the scalar product in $\mathscr{X}(T^3)$, and we denote

$$\mathscr{V}(T^3) := H^1(T^3) \oplus H^1(T^3) \oplus \mathbb{C}^3 \oplus \mathbb{C}^3. \tag{1.22}$$

This positivity allows us to construct the spectral resolution of $\tilde{A}(\theta)$ which implies the stability for the linearized dynamics (1.17).

The key result of the present paper is the proof of the positivity (1.21) for the ions's charge densities σ satisfying the following conditions on the corresponding Fourier transform $\tilde{\sigma}(\xi)$. The first one is the Wiener-type condition

Wiener Condition:
$$\Sigma(\theta) := \sum_m \Big[\frac{\xi \otimes \xi}{|\xi|^2}|\tilde{\sigma}(\xi)|^2\Big]_{\xi = 2\pi m - \theta} > 0\,, \qquad \text{a.e. } \theta \in \Pi^* \setminus \Gamma^*. \tag{1.23}$$

This condition is an analog of Fermi Golden Rule for crystals. The second condition reads

$$\tilde{\sigma}(2\pi m) = 0, \quad m \in \mathbb{Z}^3 \setminus 0. \tag{1.24}$$

The proof of the positivity (1.21) relies on a novel factorization of the Hamilton functional. This positivity necessarily breaks down at $\theta \in \Gamma^*$. Examples 8.1 and 8.2 demonstrate that the positivity can break down at some other points and submanifolds of Π^*.

Our main novelties are the following:

I. The factorization of energy (6.4), (6.6) and (8.8), (8.10).

II. The energy bound from below (6.1) for general densities $\sigma(x)$.

III. The energy positivity (1.21) under conditions (1.23) and (1.24) on $\sigma(x)$: we show that the Wiener condition (1.23) is necessary and sufficient for the positivity (1.21) under assumption (1.24) (Theorem 8.3).

IV. An asymptotics of the ground state as $e \to 0$.

V. An example of negative energy when the condition (1.24) breaks down while the Wiener condition (1.23) holds (Lemma 10.1).

VI. Spectral resolution of nonselfadjoint Hamilton generators and stability of the linearized dynamics.

Remark 1.1. *The condition (1.24) cancels a negative contribution to the energy, which is due to the electrostatic instability (”Earnshaw Theorem” [27], see Remark 10.2).*

Let us comment on previous results in these directions.

The crystal ground state for the Hartree-Fock equations was constructed by Catto, Le Bris, and Lions [5, 6]. For the Thomas-Fermie model similar results were obtained in [4].

The corresponding ground state in the Schrödinger-Poisson model was constructed in [14]. The stability for the linearized dynamics was not established previously in any model.

In [3], Cancés and Stoltz have established the well-posedness for local perturbations of the ground state density matrix in an infinite crystal for the reduced Hartree-Fock model of crystal in the *random phase approximation* with the Coulomb potential $w(x-y) = 1/|x-y|$. However, the space-periodic nuclear potential in the equation [3, (3)] does not depend on time that corresponds to the fixed ions’s positions. Thus the back reaction of the electrons onto the nuclei is neglected.

The nonlinear Hartree-Fock dynamics for compact perturbations of the ground state without the random phase approximation is not studied yet, see the discussion in [17] and in the introductions of [2, 3].

The paper [2] deals with 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 obtain suitable generalizations of the Hoffmann-Ostenhof and Lieb-Thirring inequalities for ergodic density matrices, and construt 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 [21], Lewin and Sabin established the well-posedness for the reduced von Neumann equation with density matrices of infinite trace for pair-wise interaction potentials $w \in L^1(\mathbb{R}^3)$. The authors also proved the asymptotic stability of the ground state for 2D crystals [22]. Nevertheless, the case of the Coulomb potential in 3D remains open.

The spectral theory of the Schrödinger operators with space-periodic potentials is well developed, see [24] and the references therein. The scattering theory for short-range and long-range perturbations of such operators was constructed in [10, 11].

The plan of our paper is the following. In Section 2 we recall our result [14] on the existence of a ground state, and in Section 3 we establish small charge asymptotics of the ground state. In Sections 4–6 we study the Hamilton structure of the linearized dynamics and establish the energy bound from below. In Section 7 we calculate the generator of the linearized dynamics in the Fourier–Bloch representation. In Section 8 we prove the positivity of energy. In Section 9 we apply this positivity to the stability of the linearized dynamics. Finally, in Section 10 we construct examples of negative energy. Appendices concern some technical calculations.

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2 Space-periodic ground state

Let us recall the results of [14] on the existence of the ground state (1.7). The Poisson equation (1.9) for the Γ-periodic potential Φ^0 implies the neutrality of the periodic cell $T^3 = \mathbb{R}^3/\Gamma$:

$$\int_{T^3} \rho^0(x)dx = 0, \tag{2.1}$$

which is equivalent to the normalization condition

$$\int_{T^3} |\psi^0(x)|^2 dx = Z \tag{2.2}$$

by (1.1). We assume that $Z > 0$, since otherwise the theory is trivial. The existence of the ground state (1.7) is proved in [14] under the condition

$$\sigma_{\rm per}(x) := \sum_n \sigma(x-n) \in L^2(T^3). \tag{2.3}$$

The ion position $q^0 \in T^3$ can be chosen arbitrary, and we will set $q^0 = 0$.

2.1 Minimization of energy per cell

The wave function ψ^0 is constructed as a minimal point of the energy per cell

$$U(\psi) = \frac{1}{2}\int_{T^3} [|\nabla\psi(x)|^2 + \rho(x)G_{\rm per}\rho(x)]dx, \tag{2.4}$$

where

$$\rho(x) := \sigma_{\rm per}(x) - e|\psi(x)|^2, \tag{2.5}$$

while the operator $G_{\rm per} := -\Delta_{\rm per}^{-1}$ is defined by

$$G_{\rm per}\varphi(x) = \sum_{m\in\mathbb{Z}^3\setminus 0} e^{-i2\pi mx}\frac{\check{\varphi}(m)}{|2\pi m|^2}, \qquad \check{\varphi}(m) = \int_{T^3} e^{i2\pi mx}\varphi(x)dx. \tag{2.6}$$

More precisely,

$$U(\psi^0) = \min_{\psi\in\mathscr{M}} U(\psi), \tag{2.7}$$

where $\mathscr{M}$ denotes the manifold

$$\mathscr{M} := \{\psi \in H^1(T^3) : \int_{T^3} |\psi(x)|^2 dx = Z\}. \tag{2.8}$$

2.2 Smoothness of the ground state

The results [14] imply that there exists a ground state with $\psi^0, \Phi^0 \in H^2(T^3)$. Hence $\psi^0\Phi^0 \in H^2(T^3)$, and the equation (1.8) implies that

$$\psi^0 \in H^4(T^3) \subset C^2(T^3). \tag{2.9}$$

In other words,

$$\psi^0(x) = \sum_{m\in\mathbb{Z}^3} \check{\psi}^0(m)e^{i2\pi mx}, \qquad \sum_{m\in\mathbb{Z}^3} \langle m\rangle^8 |\check{\psi}^0(m)|^2 < \infty, \qquad \langle m\rangle := (1+|m|^2)^{1/2}. \tag{2.10}$$

3 Small-charge asymptotics of the ground state

We will need below the asymptotics as $e \to 0$ of the ground state (1.7) corresponding to a one-parametric family of ion densities

$$\sigma(x) = e\mu(x) \tag{3.1}$$

with some fixed function $\mu \in L^2(\mathbb{R}^3)$. We assume that

$$\mu_{\rm per}(x) := \sum_{n\in\mathbb{Z}^3} \mu(x-n) \in L^2(T^3) \tag{3.2}$$

in accordance with (2.3). Now the energy (2.4) reads

$$U(\psi) = \frac{1}{2}\int_{T^3} [|\nabla\psi(x)|^2 + e^2\nu(x)G_{\rm per}\nu(x)]dx, \qquad \nu(x) := \mu_{\rm per}(x) - |\psi(x)|^2. \tag{3.3}$$

Denote by ψ_e^0, ω_e^0 the family of ground states with the parameter $e \in (0,1]$. The energy (3.3) is obviously bounded uniformly in $e \in (0,1]$ for any fixed $\psi \in \mathscr{M}$. Hence, the energy of the minimizers is also bounded uniformly in $e \in (0,1]$. In particular, the family ψ_e^0 is bounded in $H^1(T^3)$,

$$\|\psi_e^0\|_{H^1(T^3)} \le C, \qquad e \in (0,1]. \tag{3.4}$$

On the other hand,

$$\int \nu_e^0(x)G_{\rm per}\nu_e^0(x)dx \le C, \qquad \nu_e^0(x) := \mu_{\rm per}(x) - |\psi_e^0(x)|^2. \tag{3.5}$$

This estimate is due to the uniform bound

$$\|\nu_e^0\|_{L^2(T^3)} \le C, \qquad e \in (0,1] \tag{3.6}$$

which holds by (3.2) and (3.4). Further, the equation (1.9) reads

$$-\Delta\Phi_e^0(x) = e\nu_e^0(x). \tag{3.7}$$

We will choose the solution $\Phi_e^0 = eG_{\rm per}\nu_e^0$, where the operator $G_{\rm per}$ is defined by (2.6). The definition (2.6) implies the bound

$$\|\Phi_e^0\|_{H^2(T^3)} \le e\|\nu_e^0\|_{L^2(T^3)} \le Ce, \qquad e \in (0,1] \tag{3.8}$$

by (3.6).

Lemma 3.1. *Let condition (3.2) hold. Then for sufficiently small $e > 0$,*

$$H_e^0 := -\frac{1}{2}\Delta - e\Phi_e^0(x) - \omega_e^0 \ge 0, \tag{3.9}$$

and the ground state admits the following asymptotics as $e \to 0$:

$$\omega_e^0 = \mathscr{O}(e^2), \tag{3.10}$$

$$\psi_e^0(x) = \gamma_e + \chi_e(x), \qquad |\gamma_e|^2 = Z + \mathscr{O}(e^4), \qquad \|\chi_e\|_{H^2(T^3)} = \mathscr{O}(e^2). \tag{3.11}$$

Proof i) Equation (1.8) reads

$$\omega_e^0\psi_e^0(x) = -\frac{1}{2}\Delta\psi_e^0(x) - e\Phi_e^0(x)\psi_e^0(x). \tag{3.12}$$

Hence,

$$\omega_e^0\langle\psi_e^0,\psi_e^0\rangle_{T^3} = \omega_e^0 Z = \frac{1}{2}\langle\nabla\psi_e^0,\nabla\psi_e^0\rangle_{T^3} - e\langle\Phi_e^0\psi_e^0,\psi_e^0\rangle_{T^3}, \tag{3.13}$$

which implies the uniform bound

$$|\omega_e^0| \le C < \infty, \qquad e\in(0,1] \tag{3.14}$$

by (2.2), (3.4) and (3.8). Moreover, (3.12) and (3.8) suggest that ω_e^0 is close to an eigenvalue of $-\frac{1}{2}\Delta$:

$$\omega_e^0 \approx |2\pi k|^2 \tag{3.15}$$

with some $k\in\mathbb{Z}^3$. Indeed, (3.12) can be rewritten as

$$(\frac{1}{2}|2\pi m|^2 - \omega_e^0)\check{\psi}_e^0(m) = \check{r}_e(m), \qquad r_e := e\Phi_e^0\psi_e^0 \tag{3.16}$$

and hence,

$$\sum_{m\in\mathbb{Z}^3}(\frac{1}{2}|2\pi m|^2 - \omega_e^0)^2|\check{\psi}_e^0(m)|^2 = \mathscr{O}(e^4), \tag{3.17}$$

since $\|r_e\|_{L^2(T^3)} = \mathscr{O}(e^2)$ by (3.8). Denote by λ_e the value of $|2\pi m|^2$ corresponding to the minimal magnitude of $|\frac{1}{2}|2\pi m|^2 - \omega_e^0|$. Then (3.17) implies that

$$\sum_{|2\pi m|^2\ne\lambda_e}|\check{\psi}_e^0(m)|^2 = \mathscr{O}(e^4), \tag{3.18}$$

since the set of possible values of $\frac{1}{2}|2\pi m|^2 - \omega_e^0$ is discrete and possible values of ω_e^0 are bounded by (3.14). Moreover, (3.17) can be rewritten as

$$(\frac{1}{2}\lambda_e - \omega_e^0)^2 Z + \sum_{|2\pi m|^2\ne\lambda_e}\Big[(\frac{1}{2}|2\pi m|^2 - \omega_e^0)^2 - (\frac{1}{2}\lambda_e - \omega_e^0)^2\Big]|\check{\psi}_e^0(m)|^2 = \mathscr{O}(e^4) \tag{3.19}$$

since

$$\sum_{m\in\mathbb{Z}^3}|\check{\psi}_e^0(m)|^2 = Z \tag{3.20}$$

due to the normalization (2.2). Hence,

$$|\frac{1}{2}\lambda_e - \omega_e^0| = \mathscr{O}(e^2), \tag{3.21}$$

since the sum in (3.19) is nonnegative. Let us show that (3.19) also implies that

$$\sum_{|2\pi m|^2\ne\lambda_e}(|2\pi m|^2 - \lambda_e)^2|\check{\psi}_e^0(m)|^2 = \mathscr{O}(e^4). \tag{3.22}$$

First, (3.19) gives that

$$\sum_{|2\pi m|^2\ne\lambda_e}(|2\pi m|^2 - \lambda_e)(\frac{1}{2}|2\pi m|^2 + \frac{1}{2}\lambda_e - 2\omega_e^0)|\check{\psi}_e^0(m)|^2 = \mathscr{O}(e^4)$$

However, $2\omega_e^0 = \lambda_e + \mathscr{O}(e^2)$ by (3.21). Hence,

$$\sum_{|2\pi m|^2\ne\lambda_e}(|2\pi m|^2 - \lambda_e)(|2\pi m|^2 - \lambda_e + \mathscr{O}(e^2))|\check{\psi}_e^0(m)|^2 = \mathscr{O}(e^4).$$

Now (3.22) follows from (3.18) since λ_e is bounded for small $e>0$ by (3.21) and (3.14).

ii) Now let us prove that $\lambda_e = 0$ for small $e>0$. Indeed, the energy of the ground state reads

$$U(\psi_e^0) = \frac{1}{2}\sum_{m\in\mathbb{Z}^3} |2\pi m|^2 |\check{\psi}_e^0(m)|^2 + \mathscr{O}(e^2) \tag{3.23}$$

by (3.3) and (3.5). On the other hand, (3.22) implies

$$\sum_m |2\pi m|^2 |\check{\psi}_e^0(m)|^2 = \lambda_e Z + \sum_{|2\pi m|^2\neq\lambda_e} (|2\pi m|^2 - \lambda_e)|\check{\psi}_e^0(m)|^2 = \lambda_e Z + \mathscr{O}(e^4). \tag{3.24}$$

Substituting (3.24) into (3.23), we obtain

$$U(\psi_e^0) = \frac{1}{2}\lambda_e Z + \mathscr{O}(e^2), \quad \lambda_e \geq 0. \tag{3.25}$$

On the other hand, taking $\psi(x)\equiv\sqrt{Z}$, we ensure that the energy minimum (2.7) does not exceed $\mathscr{O}(e^2)$. Hence, (3.25) implies that $\lambda_e = 0$ for small $e>0$, since the set of all possible values of $\lambda_e Z$ is discrete. Therefore, (3.10) holds by (3.21).

iii) Now we can prove the asymptotics (3.11). Namely, the first identity holds if we set

$$\gamma_e = \check{\psi}_e^0(0), \qquad \chi_e(x) = \sum_{m\neq 0} e^{-i2\pi mx}\check{\psi}_e^0(m). \tag{3.26}$$

Then the second asymptotics of (3.11) holds by (3.20) and (3.18) with $\lambda_e = 0$. The last asymptotics of (3.11) holds since

$$\sum_{m\neq 0} |2\pi m|^4 |\check{\psi}_e^0(m)|^2 = \mathscr{O}(e^4) \tag{3.27}$$

due to (3.22) with $\lambda_e = 0$. Finally, (3.8) and (3.10) with small $e>0$ imply that the lowest eigenvalue of the Schrödinger operator H_e^0 in $L^2(T^3)$ is close to zero. Hence, its zero eigenvalue is exactly the lowest eigenvalue, since the spectrum of this operator is discrete. Therefore, the nonnegativity (3.9) is proved for small $e>0$. ■

4 Linearized dynamics

Let us consider the linearized system (1.13). We recall that $G := -\Delta^{-1}$. The meaning of the terms with G will be adjusted below, see Lemma 5.3. We assume further that (2.3) holds, and additionally,

$$\langle x\rangle^2\sigma \in L^2(\mathbb{R}^3), \qquad (\Delta-1)\sigma \in L^1(\mathbb{R}^3). \tag{4.1}$$

For $f(x)\in C_0^\infty(\mathbb{R}^3)$ the Fourier transform is defined by

$$f(x) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} e^{-i\xi x}\tilde{f}(\xi)d\xi, \qquad x\in\mathbb{R}^3; \qquad \tilde{f}(\xi) = \int_{\mathbb{R}^3} e^{i\xi x} f(x)dx, \qquad \xi\in\mathbb{R}^3. \tag{4.2}$$

The conditions (4.1) imply that

$$(\Delta-1)\tilde{\sigma} \in L^2(\mathbb{R}^3), \qquad \langle\xi\rangle^2\tilde{\sigma}(\xi) \leq \mathrm{const}. \tag{4.3}$$

We consider the case when the ground state $\psi^0(x)$ can be taken to be a real function. Then (1.13)–(1.15) imply that the operator-matrix A is given by (1.17) where S denotes the operator with the "matrix"

$$S(x,n) := e\psi^0(x)G\nabla\sigma(x-n): \quad n\in\mathbb{Z}^3,\ x\in\mathbb{R}^3. \tag{4.4}$$

Finally, T is the real matrix with entries

$$T(n,n') := -\langle G\nabla\otimes\nabla\sigma(x-n'),\sigma(x-n)\rangle + \langle\Phi^0,\nabla\otimes\nabla\sigma\rangle\delta_{nn'} = T_1(n-n') + T_2(n-n'). \tag{4.5}$$

The operators $G\psi^0 : L^2(\mathbb{R}^3)\to L^2(\mathbb{R}^3)$ and $S : l^2_3 := l^2_3(\mathbb{Z}^3)\otimes\mathbb{C}^3 \to L^2(\mathbb{R}^3)$ are not bounded due to the "infrared divergence", see Remark 5.4. In the next section, we will construct a dense domain for all these operators.

On the other hand, the corresponding operators T_1 and T_2 are bounded by the following lemma. Denote by Π the primitive cell

$$\Pi := \{(x_1,x_2,x_3) : 0 \le x_k \le 1,\ k = 1,2,3\}. \tag{4.6}$$

Let us define the Fourier transform on l^2_3 as

$$\hat{Q}(\theta) = \sum_{n\in\mathbb{Z}^3} e^{in\theta}Q(n), \qquad \text{a.e. } \theta\in\Pi^*; \qquad Q(n) = \frac{1}{|\Pi^*|}\int_{\Pi^*} e^{-in\theta}\hat{Q}(\theta)d\theta,\ \ n\in\mathbb{Z}^3, \tag{4.7}$$

where $\Pi^* = 2\pi\Pi$ denotes the primitive cell of the lattice Γ^* and the series converges in $L^2(\Pi^*)$.

Lemma 4.1. *The operators T_1 and T_2 are bounded in l^2_3 under condition (4.1).*

Proof The first operator T_1 reads as the convolution: $T_1Q(n) = \sum T_1(n-n')Q(n')$, where

$$T_1(n) = -\langle\nabla\otimes G\nabla\sigma(x),\sigma(x-n)\rangle. \tag{4.8}$$

In the Fourier transform (4.7), the convolution operator T_1 becomes the multiplication,

$$\widehat{T_1Q}(\theta) = \hat{T}_1(\theta)\hat{Q}(\theta), \qquad \text{a.e. } \theta\in\Pi^*\setminus\Gamma^*. \tag{4.9}$$

By the Parseval identity, it suffices to check that the "symbol" $\hat{T}_1(\theta)$ is a bounded function. This follows by direct calculation from (4.5). First, we apply the Parseval identity:

$$\begin{aligned}\hat{T}_1(\theta) &= -\sum_n e^{in\theta}\langle\nabla\otimes G\nabla\sigma(x),\sigma(x-n)\rangle = \frac{1}{(2\pi)^3}\sum_n e^{in\theta}\langle\frac{\xi\otimes\xi}{|\xi|^2}\tilde{\sigma}(\xi),\tilde{\sigma}(\xi)e^{in\xi}\rangle\\ &= \frac{1}{(2\pi)^3}\langle\frac{\xi\otimes\xi}{|\xi|^2}\tilde{\sigma}(\xi),\tilde{\sigma}(\xi)\sum_n e^{in(\theta+\xi)}\rangle = \sum_m\Big[\frac{\xi\otimes\xi}{|\xi|^2}|\tilde{\sigma}(\xi)|^2\Big]_{\xi=2\pi m-\theta}, \quad \theta\in\Pi^*\setminus\Gamma^*\end{aligned} \tag{4.10}$$

since the sum over n equals $|\Pi^*|\sum\limits_m\delta(\theta+\xi-2\pi m)$ by the Poisson summation formula [13]. Finally, $|\tilde{\sigma}(\xi)| \le C\langle\xi\rangle^{-2}$ by (4.3). Hence,

$$|\hat{T}_1(\theta)| \le C_1\sum_m|\tilde{\sigma}(2\pi m-\theta)\tilde{\sigma}(2\pi m-\theta)| \le C_2\sum_m\langle m\rangle^{-4} < \infty. \tag{4.11}$$

ii) Finally,

$$\widehat{T_2Q}(\theta) = \hat{T}_2\hat{Q}(\theta), \qquad \theta\in\Pi^*, \tag{4.12}$$

where

$$\hat{T}_2 = \langle\Phi^0(x),\nabla\otimes\nabla\sigma(x)\rangle \tag{4.13}$$

by (1.9). The expression is finite by (4.1), since $\Phi^0\in H^2(T^3)$ is a bounded periodic function. ■

5 The Hamilton structure and the domain

To construct solutions of the system (1.17), we need to diagonalize its generator A. The main problem is that this generator is neither selfadjoint and even not symmetric, so we cannot apply the von Neumann spectral theorem. We will solve this problem by applying our spectral theory of Hamilton operators with positive energy [15, 16] to the Bloch representation of A.

In this section we study the domain of the generator A. Denote

$$\mathscr{V} := H^1(\mathbb{R}^3) \oplus H^1(\mathbb{R}^3) \oplus l_3^2 \oplus l_3^2, \qquad l_3^2 := l^2(\mathbb{Z}^3) \otimes \mathbb{C}^3. \tag{5.1}$$

It is easy to check that the Hamilton representation (1.18) formally holds with the symplectic matrix

$$J = \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \tag{5.2}$$

Definition 5.1. *i) $\mathscr{S}_+ := \cup_{\varepsilon>0}\mathscr{S}_\varepsilon$, where $\mathscr{S}_\varepsilon$ is the space of functions $\varphi \in \mathscr{S}(\mathbb{R}^3)$, whose Fourier transforms $\hat\varphi(\xi)$ vanish in the ε-neighborhood of the lattice Γ^*,*

ii) $l_c = \cup_{R\in\mathbb{N}} l_c(R)$, where $l_c(R) := \{Q \in l_3^2 : Q(n) = 0 \ \text{ for } \ |n| > R\}$.

iii) $\mathscr{D} := \{Y = (\Psi_1, \Psi_2, Q, P) \in \mathscr{X} : \Psi_1, \Psi_2 \in \mathscr{S}_+, \quad Q \in l_c, \quad P \in l_c\}$.

Obviously, $\mathscr{D}$ is dense in $\mathscr{X}$.

Theorem 5.2. *Let conditions (4.1) hold. Then B is a symmetric operator on the domain $\mathscr{D} \subset \mathscr{X}$.*

Proof Formally the matrix (1.18) is symmetric. The following lemma implies that B is defined on $\mathscr{D}$.

Lemma 5.3. *i) $\psi^0 G \psi^0 \varphi \in L^2(\mathbb{R}^3)$ and $S^*\varphi \in l_3^2$ for $\varphi \in \mathscr{S}_+$.*

ii) $SQ \in L^2(\mathbb{R}^3)$ for $Q \in l^c$.

Proof i) First, note that

$$G\psi^0\varphi = F^{-1}\frac{[\tilde\psi^0 * \tilde\varphi](\xi)}{|\xi|^2}. \tag{5.3}$$

Further, $\tilde\psi^0(\xi) = (2\pi)^3 \sum_{m\in\mathbb{Z}^3} \check\psi^0(m)\delta(\xi - 2\pi m)$. Respectively,

$$[\tilde\psi^0 * \tilde\varphi](\xi) = (2\pi)^3 \sum_{m\in\mathbb{Z}^3} \check\psi^0(m)\hat\varphi(\xi - 2\pi m) = 0, \qquad |\xi| < \varepsilon \tag{5.4}$$

if $\varphi \in \mathscr{S}_\varepsilon$ with some $\varepsilon > 0$. Moreover, $\tilde\psi^0 * \tilde\varphi \in L^2(\mathbb{R}^3)$, since $\psi^0\varphi \in L^2(\mathbb{R}^3)$. Hence, φ belongs to the domain of $G\psi^0$ and of $\psi^0 G\psi^0$.

Now consider $S^*\varphi$. Applying (4.4), the Parseval identity and (5.4) we get for $\varphi \in \mathscr{S}_\varepsilon$

$$\begin{aligned} [S^*\varphi](n) &= e\int \psi^0(x)\varphi(x)G\nabla\sigma(x-n)dx = e\langle\psi^0(x)\varphi(x), G\nabla\sigma(x-n)\rangle \\ &= \frac{ie}{(2\pi)^3}\int_{|\xi|>\varepsilon} [\tilde\psi^0 * \tilde\varphi](\xi)\frac{\xi\overline{\tilde\sigma}(\xi)e^{-in\xi}}{|\xi|^2}d\xi. \end{aligned} \tag{5.5}$$

Here $\partial^\alpha[\tilde\psi^0 * \tilde\varphi](\xi)\langle\xi\rangle^4 \in L^2(\mathbb{R}^3)$ for all α by (2.10), since $\tilde\varphi \in \mathscr{S}(\mathbb{R}^3)$. Moreover, $\partial^\alpha\tilde\sigma \in L^2(\mathbb{R}^3)$ for $|\alpha| \le 2$ by (4.3). Hence, integrating by parts twice, and taking into account (5.4), we obtain

$$|[S^*\varphi](n)| \le C\langle n\rangle^{-2}, \tag{5.6}$$

which implies that $S^*\varphi \in l^2_3$.

ii) Let us check that $SQ \in L^2(\mathbb{R}^3)$ for $Q \in l_c$. The Fourier transform of SQ reads as

$$\begin{aligned}\widetilde{SQ}(\xi) &= eF_{x\to\xi}\sum_n \psi^0(x)G\nabla\sigma(x-n)Q(n) = e\sum_n \tilde{\psi}^0 * F_{x\to\xi}[G\nabla\sigma(x-n)]Q(n)\\ &= e(2\pi)^3\int\sum_m \check{\psi}^0(m)\delta(\eta-2\pi m)\widetilde{G\nabla\sigma}(\xi-\eta)\sum_n e^{in(\xi-\eta)}Q(n)d\eta\\ &= e(2\pi)^3\sum_m \check{\psi}^0(m)\widetilde{G\nabla\sigma}(\xi-2\pi m)\tilde{Q}(\xi-2\pi m). \end{aligned} \tag{5.7}$$

Hence, the Parseval identity gives that

$$\|SQ\|_{L^2(\mathbb{R}^3)} = C\|\widetilde{SQ}\|_{L^2(\mathbb{R}^3)} \le C_1\sum_m |\check{\psi}^0(m)|\|\widetilde{G\nabla\sigma}(\xi)\tilde{Q}(\xi)\|_{L^2(\mathbb{R}^3)} \tag{5.8}$$

It remains to note that the sum over m is finite by (2.10) because

$$\|\widetilde{G\nabla\sigma}\tilde{Q}\|^2_{L^2(\mathbb{R}^3)} = \int\frac{1}{|\xi|^2}|\tilde{\sigma}(\xi)\tilde{Q}(\xi)|^2d\xi \le C(Q)\int\frac{|\tilde{\sigma}(\xi)|^2}{|\xi|^2}d\xi \tag{5.9}$$

since the function $\tilde{Q}(\xi)$ is bounded for $Q \in l_c$. Finally, the last integral is finite by (4.3). ■

This lemma implies that $BY \in \mathscr{X}$ for $Y \in \mathscr{D}$. The symmetry of B on $\mathscr{D}$ is evident from (1.18). Theorem 5.2 is proved. ■

Remark 5.4. *The infrared singularity at $\xi = 0$ of the integrands (5.3), (5.5) and (5.9) demonstrates that all operators $G\psi^0 : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, $S : l^2_3 \to L^2(\mathbb{R}^3)$ and $S^* : L^2(\mathbb{R}^3) \to l^2_3$ are unbounded.*

Corollary 5.5. *The proof of Theorem 5.2 shows that the operator A is defined on $\mathscr{D}$, as well as the "formal adjoint" A^*, which is defined by the identity*

$$\langle AY_1, Y_2\rangle = \langle Y_1, A^*Y_2\rangle, \qquad Y_1, Y_2 \in \mathscr{D}. \tag{5.10}$$

6 Factorization of energy and bound from below

The equation (1.17) is formally a Hamiltonian system with Hamilton functional $\frac{1}{2}\langle Y, BY\rangle$. Next theorem means the stability property of the linearized crystal.

Theorem 6.1. *Let conditions (4.1) hold. Then the operator B on the domain $\mathscr{D}$ is bounded from below:*

$$\langle Y, BY\rangle \ge -C\|Y\|^2_{\mathscr{X}}, \qquad Y \in \mathscr{D}. \tag{6.1}$$

Proof For $Y = (\Psi_1, \Psi_2, Q, P) \in \mathscr{D}$ the quadratic form reads (with the notations (4.4)–(4.5))

$$\begin{aligned}\langle Y, BY\rangle \;=\; & 2\sum_j\langle\Psi_j, H^0\Psi_j\rangle + 4e^2\langle\psi^0\Psi_1, G\psi^0\Psi_1\rangle + 2[\langle\Psi_1, SQ\rangle + \langle Q, S^*\Psi_1\rangle] + \langle Q, T_1Q\rangle\\ & + \langle Q, T_2Q\rangle + \langle P, M^{-1}P\rangle. \end{aligned} \tag{6.2}$$

Here the first sum is bounded from below, the operator T_2 is bounded in l^2_3 by Lemma 4.1, while the operator M^{-1} is positive. Our basic observation is that

$$\beta(\Psi_1, Q) := 4e^2\langle\psi^0\Psi_1, G\psi^0\Psi_1\rangle + 2[\langle\Psi_1, SQ\rangle + \langle Q, S^*\Psi_1\rangle] + \langle Q, T_1Q\rangle \ge 0. \tag{6.3}$$

Indeed, the operators factorize as follows:

$$e^2\psi^0 G\psi^0 = f^* f, \qquad S = f^* g, \qquad T_1 = g^* g, \tag{6.4}$$

where

$$f := e\sqrt{G}\psi^0, \qquad g(x,n) = \nabla\sqrt{G}\sigma(x-n). \tag{6.5}$$

Then the quadratic form (6.3) becomes the "perfect square"

$$\beta(\Psi, Q) = \langle 2f\Psi_1 + gQ, 2f\Psi_1 + gQ\rangle \geq 0. \qquad \blacksquare \tag{6.6}$$

Corollary 6.2. *The operator B admits selfadjoint extensions by the Friedrichs Theorem [23].*

7 Generator in the Fourier–Bloch transform

We reduce the operators $A = JB$ and K by the Fourier–Bloch–Gelfand–Zak transform [7, 26].

7.1 The discrete Fourier transform

Let us consider a vector $Y = (\Psi_1, \Psi_2, Q, P) \in \mathscr{X}$, and denote

$$Y(n) = (\Psi_1(n,\cdot), \Psi_2(n,\cdot), Q(n), P(n)), \qquad n \in \mathbb{Z}^3, \tag{7.1}$$

where

$$\Psi_j(n,y) = \begin{cases} \Psi_j(n+y), & \text{a.e. } y \in \Pi, \\ 0, & y \notin \Pi. \end{cases} \tag{7.2}$$

Obviously, $Y(n)$ with different $n \in \mathbb{Z}^3$ are orthogonal vectors in $\mathscr{X}$, and

$$Y = \sum_n Y(n), \tag{7.3}$$

where the sum converges in $\mathscr{X}$. The norms in $\mathscr{X}$ and $\mathscr{V}$ can be represented as

$$\|Y\|^2_{\mathscr{X}} = \sum_{n\in\mathbb{Z}^3} \|Y(n)\|^2_{\mathscr{X}(\Pi)}, \qquad \|Y\|^2_{\mathscr{V}} = \sum_{n\in\mathbb{Z}^3} \|Y(n)\|^2_{\mathscr{V}(\Pi)}, \tag{7.4}$$

where

$$\mathscr{X}(\Pi) := L^2(\Pi) \oplus L^2(\Pi) \oplus \mathbb{C}^3 \oplus \mathbb{C}^3, \qquad \mathscr{V}(\Pi) := H^1(\Pi) \oplus H^1(\Pi) \oplus \mathbb{C}^3 \oplus \mathbb{C}^3. \tag{7.5}$$

Further, the ground state (1.7) is invariant with respect to translations of the lattice Γ, and hence the operator A commutes with these translations. Namely, (4.4) implies that

$$S(x,n) = S(x-n, 0), \tag{7.6}$$

since $\psi^0(x)$ is a Γ-periodic function. Similarly, (4.5) implies that T commutes with translations of Γ. Hence, A can be reduced by the discrete Fourier transform. Namely, applying the Fourier transform $F_{n\to\theta}$ to the function $Y(\cdot)$ from (7.1), we obtain

$$\hat{Y}(\theta) = F_{n\to\theta} Y(n) := \sum_{n\in\mathbb{Z}^3} e^{in\theta} Y(n) = (\hat{\Psi}_1(\theta,\cdot), \hat{\Psi}_2(\theta,\cdot), \hat{Q}(\theta), \hat{P}(\theta)), \qquad \text{a.e. } \theta \in \mathbb{R}^3, \tag{7.7}$$

where

$$\hat{\Psi}_j(\theta,y) = \sum_{n\in\mathbb{Z}^3} e^{in\theta} \Psi_j(n+y), \qquad \text{a.e. } \theta \in \mathbb{R}^3, \qquad \text{a.e. } y \in \mathbb{R}^3. \tag{7.8}$$

The function $\hat{Y}(\theta)$ is Γ^*-periodic in θ. The series (7.7) converges in $L^2(\Pi^*, \mathscr{X}(\Pi))$, since the series (7.3) converges in $\mathscr{X}$. The inversion formula is given by

$$Y(n) = |\Pi^*|^{-1} \int_{\Pi^*} e^{-in\theta} \hat{Y}(\theta) d\theta \tag{7.9}$$

(cf. (4.7)). The Parseval–Plancherel identity gives

$$\|Y\|^2_{\mathscr{V}} = |\Pi^*|^{-1} \|\hat{Y}\|^2_{L^2(\Pi^*, \mathscr{V}(\Pi))}, \qquad \|Y\|^2_{\mathscr{X}} = |\Pi^*|^{-1} \|\hat{Y}\|^2_{L^2(\Pi^*, \mathscr{X}(\Pi))}. \tag{7.10}$$

The functions $\hat{\Psi}_j(\theta, y)$ are Γ-quasiperiodic in y; i.e.,

$$\hat{\Psi}_j(\theta, y+m) = e^{-im\theta} \hat{\Psi}_j(\theta, y), \qquad m \in \mathbb{Z}^3. \tag{7.11}$$

7.2 Generator in the discrete Fourier transform

Let us consider $Y \in \mathscr{D}$ and calculate the Fourier transform (7.7) for AY. Using (4.5), (5.5), (7.6), and taking into account the Γ-periodicity of $\Phi^0(x)$ and $\psi^0(x)$, we obtain that

$$\widehat{AY}(\theta) = \hat{A}(\theta)\hat{Y}(\theta), \qquad \text{a.e. } \theta \in \mathbb{R}^3 \setminus \Gamma^*, \tag{7.12}$$

where $\hat{A}(\theta)$ is a Γ^*-periodic operator function,

$$\hat{A}(\theta) = \begin{pmatrix} 0 & H^0 & 0 & 0 \\ -H^0 - 2e^2\psi^0 \hat{G}(\theta)\psi^0 & 0 & \hat{S}(\theta) & 0 \\ 0 & 0 & 0 & M^{-1} \\ -2\hat{S}^*(\theta) & 0 & -\hat{T}(\theta) & 0 \end{pmatrix}. \tag{7.13}$$

by (1.17) and (1.18). Here

$$\hat{G}(\theta)\hat{\varphi}(\theta, y) = \sum_m \frac{\check{\varphi}(\theta, m)}{(2\pi m - \theta)^2} e^{i(2\pi m - \theta)y}, \qquad \text{a.e. } \theta \in \mathbb{R}^3 \setminus \Gamma^*. \tag{7.14}$$

This expression is well-defined for $\varphi(x) = \psi^0(x)\Psi_1(x)$ with $\Psi_1 \in \mathscr{S}_\varepsilon$ since

$$\check{\varphi}(\theta, m) = \tilde{\varphi}(2\pi m - \theta) = 0 \quad \text{for} \quad |2\pi m - \theta| < \varepsilon \tag{7.15}$$

according to (5.4).

Lemma 7.1. *The operator $\hat{S}(\theta)$ acts as follows:*

$$\hat{S}(\theta)\hat{Q}(\theta) = \hat{S}(\theta)\hat{Q}(\theta), \quad \text{where} \quad \hat{S}(\theta) = e\psi^0 \hat{G}(\theta) \nabla \hat{\sigma}(\theta, y). \tag{7.16}$$

Proof. For $x = y + n$ equations (1.11) and (4.4) imply

$$\begin{aligned} SQ(y+n) &= e\psi^0(y+n) \sum_m G\nabla\sigma^0(m, y+n) Q(m) \\ &= e\psi^0(y) \sum_m G\nabla\sigma(y+n-m) Q(m) \end{aligned}$$

due to the Γ-periodicity of ψ^0. Applying the Fourier transform (7.7), we obtain (7.16). □

Furthermore, $\hat{S}^*(\theta)$ in (7.13) is the corresponding adjoint operator, and $\hat{T}(\theta)$ is the operator matrix expressed by (4.10). Note that $\hat{S}(\theta)$, $\hat{S}^*(\theta)$ and $\hat{T}(\theta)$ are finite dimensional operators.

7.3 Generator in the Bloch transform

Definition 7.2. *The Bloch transform of Y is defined as*

$$\tilde{Y}(\theta)=[\mathscr{F}Y](\theta):=\mathscr{M}(\theta)\hat{Y}(\theta):=(\tilde{\Psi}_1(\theta,y),\tilde{\Psi}_2(\theta,y),\hat{Q}(\theta),\hat{P}(\theta)),\qquad \text{a.e. } \theta\in\mathbb{R}^3, \tag{7.17}$$

where $\tilde{\Psi}_j(\theta,y)=M(\theta)\hat{\Psi}_j:=e^{i\theta y}\hat{\Psi}_j(\theta,y)$ *are* Γ*-periodic functions in* $y\in\mathbb{R}^3$.

Now the Parseval-Plancherel identities (7.10) read

$$\|Y\|^2_{\mathscr{V}}=|\Pi^*|^{-1}\|\tilde{Y}\|^2_{L^2(\Pi^*,\mathscr{V}(T^3))},\qquad \|Y\|^2_{\mathscr{X}}=|\Pi^*|^{-1}\|\tilde{Y}\|^2_{L^2(\Pi^*,\mathscr{X}(T^3))}. \tag{7.18}$$

Hence, $\mathscr{F}:\mathscr{X}\to L^2(\Pi^*,\mathscr{X}(T^3))$ is the isomorphism. The inversion is given by

$$Y(n)=|\Pi^*|^{-1}\int_{\Pi^*}e^{-in\theta}\mathscr{M}(-\theta)\tilde{Y}(\theta)d\theta,\qquad n\in\mathbb{Z}^3. \tag{7.19}$$

Finally, the above calculations can be summarised as follows: (7.12) implies that for $Y\in\mathscr{D}$

$$\widetilde{AY}(\theta)=\tilde{A}(\theta)\tilde{Y}(\theta),\qquad \text{a.e. } \theta\in\Pi^*\setminus\Gamma^*. \tag{7.20}$$

Here

$$\tilde{A}(\theta)=\mathscr{M}(\theta)\hat{A}(\theta)\mathscr{M}(-\theta)=\begin{pmatrix}0 & \tilde{H}^0(\theta) & 0 & 0\\ -\tilde{H}^0(\theta)-2e^2\psi^0\tilde{G}(\theta)\psi^0 & 0 & \tilde{S}(\theta) & 0\\ 0 & 0 & 0 & M^{-1}\\ -2\tilde{S}^*(\theta) & 0 & -\hat{T}(\theta) & 0\end{pmatrix}, \tag{7.21}$$

where

$$\tilde{S}(\theta)\quad:=\quad M(\theta)\hat{S}(\theta)=e\psi^0\tilde{G}(\theta)\nabla\tilde{\sigma}^0(\theta), \tag{7.22}$$

$$\tilde{H}^0(\theta)\quad:=\quad M(\theta)H^0M(-\theta)=-\frac{1}{2}(\nabla+i\theta)^2-e\Phi^0(x)-\omega^0, \tag{7.23}$$

$$\tilde{G}(\theta)\quad:=\quad M(\theta)\hat{G}(\theta)M(-\theta)=(i\nabla-\theta)^{-2}. \tag{7.24}$$

Remark 7.3. *The operators* $\tilde{G}(\theta):L^2(T^3)\to H^2(T^3)$ *are bounded for* $\theta\in\Pi^*\setminus\Gamma^*$.

Lemma 7.4. *Let the condition (1.21) hold. Then the operator* $\tilde{A}(\theta)$ *admits the representation*

$$\tilde{A}(\theta)=J\tilde{B}(\theta),\qquad \theta\in\Pi^*\setminus\Gamma^*, \tag{7.25}$$

where $\tilde{B}(\theta)$ *is the selfadjoint operator (1.19) in* $\mathscr{X}(T^3)$ *with the domain*

$$\tilde{D}:=H^2(T^3)\oplus H^2(T^3)\oplus\mathbb{C}^3\oplus\mathbb{C}^3. \tag{7.26}$$

Proof The representation (7.25) follows from (1.18) and (1.18). The operator $\tilde{B}(\theta)$ is symmetric on the domain $\tilde{D}$. Moreover, operators in (1.19) are all bounded, except for $\tilde{H}^0(\theta)$, which is selfadjoint in $L^2(T^3)$ with the domain $H^2(T^3)$. Hence, $\tilde{B}(\theta)$ is also selfadjoint on the domain $\tilde{D}$. ∎

8 The positivity of energy

Here we prove the positivity (1.21) for the linearized dynamics (1.17) under conditions (1.23) and (1.24). It is easy to construct the corresponding examples of densities $\sigma(x)$.

Example 8.1. *(1.23) holds for $\sigma(x) \in L^1(\mathbb{R}^3)$ if*

$$\tilde{\sigma}(\xi) \neq 0, \qquad \text{a.e. } \xi \in \mathbb{R}^3. \tag{8.1}$$

Example 8.2. *Let us define the function $f(x)$ by its Fourier transform $\tilde{f}(\xi) := \dfrac{2\sin\dfrac{\xi}{2}}{\xi} e^{-\xi^2}$, and set*

$$\sigma(x) := eZ f(x_1) f(x_2) f(x_3), \qquad x \in \mathbb{R}^3. \tag{8.2}$$

Then $\sigma(x)$ is the smooth function satisfying the Wiener condition (1.23), as well as (1.24) and (1.1), and

$$|\sigma(x)| \leq C(a) e^{-a|x|}, \quad x \in \mathbb{R}^3, \tag{8.3}$$

for any $a > 0$ by the Paley–Wiener theorem.

The matrix (1.23) is a continuous function of $\theta \in \Pi^* \setminus \Gamma^*$. Let us denote

$$\Pi^*_+ := \{\theta \in \Pi^* \setminus \Gamma^* : \Sigma(\theta) > 0\}. \tag{8.4}$$

Then the Wiener condition (1.23) means that $|\Pi^*_+| = |\Pi^*|$. In the rest of this paper we assume condition (1.24) and consider the linearized dynamics (1.17) corresponding to a real minimizer of energy per cell. In Appendix B we show that the real minimizer exists and is unique.

Theorem 8.3. *Let conditions (4.1), and (1.24) hold. Then the Wiener condition (1.23) is necessary and sufficient for the positivity (1.21) of the generator corresponding to the real minimizer of energy per cell.*

Proof i) First, let us check that the Wiener condition (1.23) is necessary. Namely, let us consider the inequality (1.21) for $Y_0 = (0,0,Q,P) \in \mathscr{V}(T^3)$: (1.19) and (1.21) imply that

$$\mathscr{E}(\theta, Y_0) = Q\hat{T}(\theta)Q + PM^{-1}P \geq \varkappa(\theta)[|Q|^2 + |P|^2], \qquad \text{a.e. } \theta \in \Pi^* \setminus \Gamma^*. \tag{8.5}$$

Formula (4.13) implies that $\hat{T}_2 = 0$ by (B.5). Hence,

$$\hat{T}(\theta) = \hat{T}_1(\theta) = \Sigma(\theta), \qquad \theta \in \Pi^* \setminus \Gamma^* \tag{8.6}$$

by (4.10). Therefore, (8.5) becomes

$$\mathscr{E}(\theta, Y_0) = Q\Sigma(\theta)Q + PM^{-1}P \geq \varkappa(\theta)[|Q|^2 + |P|^2]. \tag{8.7}$$

Hence, the condition (1.23) is necessary for the positivity (1.21).

ii) It remains to show that the Wiener condition (1.23) together with (1.24) is sufficient for the positivity (1.21). Let us translate the calculations (6.2)–(6.5) into the Fourier–Bloch transform. The operators (6.5) commute with the Γ-translations, and therefore

$$e^2\psi^0\tilde{G}(\theta)\psi^0 = \tilde{f}^*(\theta)\tilde{f}(\theta), \quad \tilde{S}(\theta) = \tilde{f}^*(\theta)\tilde{g}(\theta), \quad \hat{T}_1(\theta) = \tilde{g}^*(\theta)\tilde{g}(\theta), \tag{8.8}$$

where $\tilde{f}(\theta) := e\sqrt{\tilde{G}(\theta)}\psi^0$ and $\tilde{g}(\theta) = \sqrt{\tilde{G}(\theta)}\nabla\tilde{\sigma}(\cdot,\theta)$. Hence, (1.19) implies that

$$\mathscr{E}(\theta, Y) := \langle Y, \tilde{B}(\theta)Y\rangle_{T^3} = b(\theta, \Psi_1, Q) + 2\langle \Psi_2, \tilde{H}^0(\theta)\Psi_2\rangle_{T^3} + PM^{-1}P, \quad Y = (\Psi_1, \Psi_2, Q, P) \in \mathscr{V}(T^3), \tag{8.9}$$

where

$$b(\theta,\Psi_1,Q):=2\langle\Psi_1,\tilde H^0(\theta)\Psi_1\rangle_{T^3}+\langle 2\tilde f(\theta)\Psi_1+\tilde g(\theta)Q,\ 2\tilde f(\theta)\Psi_1+\tilde g(\theta)Q\rangle_{T^3}. \tag{8.10}$$

Let us note that $\tilde H^0(\theta)=-\frac{1}{2}(\nabla+i\theta)^2$ by (B.5). Hence, the eigenvalues of $\tilde H^0(\theta)$ equal to $\frac{1}{2}|2\pi m-\theta|^2$ where $m\in\mathbb{Z}^3$. Therefore, $\tilde H^0(\theta)$ is positive definite:

$$\langle\Psi_1,\tilde H^0(\theta)\Psi_1\rangle\geq\frac{1}{2}d^2(\theta)\|\Psi_1\|^2_{H^1(T^3)}\,,\qquad \theta\in\Pi^*\setminus\Gamma^*, \tag{8.11}$$

where $d(\theta):=\operatorname{dist}(\theta,\Gamma^*)$. Hence, it remains to prove the following proposition.

Proposition 8.4. *Under conditions of Theorem 8.3*

$$b(\theta,\Psi_1,Q)\geq\varepsilon(\theta)[\|\Psi_1\|^2_{H^1(T^3)}+|Q|^2],\qquad \theta\in\Pi^*_+, \tag{8.12}$$

where $\varepsilon(\theta)>0$.

Proof Let us denote $\alpha:=\langle\Psi_1,\tilde H^0(\theta)\Psi_1\rangle_{T^3}$, and

$$\beta_{11}:=\langle 2\tilde f(\theta)\Psi_1,2\tilde f(\theta)\Psi_1\rangle_{T^3},\quad \beta_{12}:=\langle 2\tilde f(\theta)\Psi_1,\tilde g(\theta)Q\rangle_{T^3},\quad \beta_{22}:=\langle\tilde g(\theta)Q,\tilde g(\theta)Q\rangle_{T^3}. \tag{8.13}$$

Then we can write the quadratic form (8.10) as

$$b=2\alpha+\beta,\qquad \beta:=\beta_{11}+2\mathrm{Re}\,\beta_{12}+\beta_{22}. \tag{8.14}$$

The positivity (8.11) implies that

$$\alpha\geq\delta(\theta)\beta_{11},\qquad \theta\in\Pi^*\setminus\Gamma^*, \tag{8.15}$$

where $\delta(\theta)>0$. Hence,

$$b\geq\alpha+(1+\delta(\theta))\beta_{11}+2\mathrm{Re}\,\beta_{12}+\beta_{22},\qquad \theta\in\Pi^*\setminus\Gamma^*. \tag{8.16}$$

On the other hand, the Cauchy-Schwarz inequality implies that

$$|\beta_{12}|\leq\beta_{11}^{1/2}\beta_{22}^{1/2}\leq\frac{1}{2}[\gamma\beta_{11}+\frac{1}{\gamma}\beta_{22}] \tag{8.17}$$

for any $\gamma>0$. Hence,

$$b\geq\alpha+(1+\delta(\theta)-\gamma)\beta_{11}+(1-\frac{1}{\gamma})\beta_{22},\qquad \theta\in\Pi^*\setminus\Gamma^*. \tag{8.18}$$

Therefore, choosing $1<\gamma\leq 1+\delta(\theta)$, we obtain (8.12) from (8.11) since

$$\beta_{22}=Q\hat T_1(\theta)Q=\Sigma(\theta)|Q|^2 \tag{8.19}$$

by (8.8) and (8.6). ■

9 Weak solutions and linear stability

Weak solutions are introduced and the linear stability is proved.

9.1 Weak solutions

We will consider solutions to (1.17) in the sense of distributions. Let us recall that $A^*V \in \mathscr{X}$ for $V \in \mathscr{D}$ by Corollary 5.5.

Definition 9.1. *$Y(t) \in C(\mathbb{R}, \mathscr{X})$ is a weak solution to (1.17) if*

$$-\int \langle Y(t), \dot{\varphi}(t)V\rangle dt = \int \langle Y(t), \varphi(t)A^*V\rangle dt, \qquad \varphi \in C_0^\infty(\mathbb{R}),\ V \in \mathscr{D}. \tag{9.1}$$

Let us translate this definition into the Fourier–Bloch transform: by the Parseval–Plancherel identity

$$-\int \Big[\int_{\Pi^*} \langle \tilde{Y}(\theta,t), \dot{\varphi}(t)\tilde{V}(\theta)\rangle_{T^3} d\theta\Big] dt = \int \Big[\int_{\Pi^*} \langle \tilde{Y}(\theta,t), \varphi(t)\tilde{A}^*(\theta)\tilde{V}(\theta)\rangle_{T^3} d\theta\Big] dt \tag{9.2}$$

Respectively, (9.1) is equivalent to the identity

$$-\int \langle \tilde{Y}(\theta,t), \dot{\varphi}(t)\tilde{V}\rangle_{T^3} dt = \int \langle \tilde{Y}(\theta,t), \varphi(t)\tilde{A}^*(\theta)\tilde{V}\rangle_{T^3} dt,\ \ \varphi \in C_0^\infty(\mathbb{R}),\ \ \tilde{V} \in \mathscr{D}(T^3),\ \ \text{a.e. } \theta \in \Pi^* \setminus \Gamma^*, \tag{9.3}$$

where $\mathscr{D}(T^3) := C^\infty(T^3) \oplus C^\infty(T^3) \oplus \mathbb{C}^3 \oplus \mathbb{C}^3$. In other words,

$$\dot{\tilde{Y}}(\theta,t) = \tilde{A}(\theta)\tilde{Y}(\theta,t), \qquad \text{a.e. } \theta \in \Pi^* \setminus \Gamma^* \tag{9.4}$$

in the sense of vector-valued distributions.

9.2 Linear stability

The equation (9.4) is equivalent to

$$\dot{\tilde{Y}}(\theta,t) = J\tilde{B}(\theta)\tilde{Y}(\theta,t)\ , \quad t \in \mathbb{R}, \qquad \text{a.e. } \theta \in \Pi^* \setminus \Gamma^*. \tag{9.5}$$

We reduce it, using (1.21), to an equation with a selfadjoint generator by our methods [15, 16] which is an infinite-dimensional version of some Gohberg and Krein ideas from the theory of parametric resonance [12, Chap. VI]. We reproduce some details of [15] for the convenience of the reader. Namely, let us denote

$$\tilde{\Lambda}(\theta) = \tilde{B}^{1/2}(\theta) > 0, \qquad \theta \in \Pi_+^*. \tag{9.6}$$

This is a selfadjoint operator with the domain $\mathscr{V}(T^3)$, that follows by the interpolation arguments, and the range $\operatorname{Ran} \tilde{\Lambda}(\theta) = \mathscr{X}(T^3)$. Its inverse is bounded in $\mathscr{X}(T^3)$ by (1.21), and

$$\|\tilde{\Lambda}^{-1}(\theta)Z\|_{\mathscr{V}(T^3)} \le \frac{1}{\sqrt{\varkappa(\theta)}}\|Z\|_{\mathscr{X}(T^3)}, \quad Z \in \mathscr{X}(T^3), \qquad \theta \in \Pi_+^*. \tag{9.7}$$

Let us set $\tilde{Z}(\theta,t) := \tilde{\Lambda}(\theta)\tilde{Y}(\theta,t)$, and now equation (9.5) implies that

$$\dot{\tilde{Z}}(\theta,t) = -i\tilde{K}(\theta)\tilde{Z}(\theta,t), \quad t \in \mathbb{R}, \qquad \text{a.e. } \theta \in \Pi_+^* \tag{9.8}$$

in the sense of vector-valued distributions, where $\tilde{K}(\theta) = i\tilde{\Lambda}(\theta)J\tilde{\Lambda}(\theta)$.

Lemma 9.2. (Lemma 2.1 of [15]) *$K(\theta)$ is a selfadjoint operator in $\mathscr{X}(T^3)$ with a dense domain $D(K(\theta)) \subset \mathscr{V}(T^3)$ for every $\theta \in \Pi_+^*$.*

Proof The operator $\tilde{K}(\theta)$ is injective. On the other hand, $\mathrm{Ran}\,\tilde{\Lambda}(\theta)=\mathscr{X}(T^3)$, and $J:\mathscr{X}(T^3)\to\mathscr{X}(T^3)$ is a bounded invertible operator. Hence, $\mathrm{Ran}\,\tilde{K}(\theta)=\mathscr{X}(T^3)$. Consider the inverse operator

$$\tilde{R}(\theta):=\tilde{K}^{-1}(\theta)=i\tilde{\Lambda}^{-1}(\theta)J\tilde{\Lambda}^{-1}(\theta). \tag{9.9}$$

It is selfadjoint since $D(\tilde{R}(\theta))=\mathrm{Ran}\,K(\theta)=\mathscr{X}(T^3)$ and $\tilde{R}(\theta)$ is bounded and symmetric. Finally, $\tilde{R}(\theta)$ is injective, and hence, $\tilde{K}(\theta)=\tilde{R}^{-1}(\theta)$ is a densely defined selfadjoint operator by Theorem 13.11 (b) of [25]:

$$\tilde{K}^*(\theta)=\tilde{K}(\theta)\;,\quad D(\tilde{K}(\theta))=\mathrm{Ran}\,\tilde{R}(\theta)\subset\;\mathrm{Ran}\,\tilde{\Lambda}^{-1}(\theta)\subset\mathscr{V}(T^3)$$

by (9.7). ■

This lemma implies that each weak solution to (9.8) is given by

$$\tilde{Z}(\theta,t)=e^{-i\tilde{K}(\theta)t}\tilde{Z}(\theta,0)\in C_b(\mathbb{R},\mathscr{X}(T^3)),\qquad \text{a.e. }\;\theta\in\Pi^*_+ \tag{9.10}$$

for $\tilde{Z}(\theta,0)\in\mathscr{X}(T^3)$. Hence, we obtain the well posedness of the Cauchy problem for equation (9.5).

Theorem 9.3. *Let all conditions of Theorem 8.3 hold and $\theta\in\Pi^*_+$. Then for every initial state $\tilde{Y}(\theta,0)\in\mathscr{V}(T^3)$ there exists a unique weak solution $\tilde{Y}(\theta,t)\in C_b(\mathbb{R},\mathscr{V}(T^3))$ to equation (9.5), and*

$$\langle\tilde{\Lambda}(\theta)\tilde{Y}(\theta,t),\tilde{\Lambda}(\theta)\tilde{Y}(\theta,t)\rangle_{T^3}=\mathrm{const},\qquad t\in\mathbb{R}. \tag{9.11}$$

Proof $\tilde{Z}(\theta,0):=\tilde{\Lambda}(\theta)\tilde{Y}(\theta,0)\in\mathscr{X}(T^3)$ since $Y(\theta,0)\in\mathscr{V}(T^3)$. Hence, (9.10) and (9.7) imply that

$$\tilde{Y}(\theta,t)=\tilde{\Lambda}^{-1}(\theta)e^{-iK(\theta)t}\tilde{Z}(\theta,0)\in C_b(\mathbb{R},\mathscr{V}(T^3)). \tag{9.12}$$

Finally, (9.11) holds since $e^{-iK(\theta)t}$ is the unitary group in $\mathscr{X}(T^3)$, and hence

$$\langle\tilde{\Lambda}(\theta)\tilde{Y}(\theta,t),\tilde{\Lambda}(\theta)\tilde{Y}(\theta,t)\rangle_{T^3}=\langle\tilde{Z}(\theta,t),\tilde{Z}(\theta,t)\rangle_{T^3}=\mathrm{const},\qquad t\in\mathbb{R}.\quad ■$$

Now we apply this theory to equation (1.17). Let us note that $\tilde{\Lambda}(\theta)\tilde{Y}(\theta)\in L^2(\Pi^*_+,\mathscr{X}(T^3))$ for $Y\in\mathscr{D}$, see Definition 5.1.

Definition 9.4. *The Hilbert space $\mathscr{W}$ is the completion of $\mathscr{D}$ in the norm*

$$\|Y\|_{\mathscr{W}}:=\|\tilde{\Lambda}(\theta)\tilde{Y}(\theta)\|_{L^2(\Pi^*_+,\mathscr{X}(T^3))} \tag{9.13}$$

Formally, $\|Y\|_{\mathscr{W}}=\langle Y,BY\rangle^{1/2}$. The Fourier-Bloch transform (7.17) extends to the isomorphism

$$\mathscr{F}:\mathscr{W}\to\tilde{\mathscr{W}}:=\{\tilde{Y}(\cdot)\in L^2_{\mathrm{loc}}(\Pi^*_+,\mathscr{X}(T^3)):\|\tilde{\Lambda}(\theta)\tilde{Y}(\theta)\|_{L^2(\Pi^*_+,\mathscr{X}(T^3))}<\infty\}. \tag{9.14}$$

Finally, let us extend definition of weak solutions to $Y(t)\in C_b(\mathbb{R},\mathscr{W})$ by the identity (9.5) in the sense of vector-valued distributions (9.3). Then Theorem 9.3 implies the following corollary.

Corollary 9.5. *Let all conditions of Theorem 8.3 hold. Then for every initial state $Y(0)\in\mathscr{W}$ there exists a unique weak solution $Y(t)\in C_b(\mathbb{R},\mathscr{W})$ to equation (1.17), and the energy norm is conserved*:

$$\|Y(t)\|_{\mathscr{W}}=\mathrm{const},\qquad t\in\mathbb{R}. \tag{9.15}$$

The solution is given by the formula (9.12):

$$Y(t)=\mathscr{F}^{-1}\tilde{\Lambda}^{-1}(\theta)e^{-iK(\theta)t}\tilde{Z}(\theta,0)\in C_b(\mathbb{R},\mathscr{W}(T^3)). \tag{9.16}$$

This means that the linearized dynamics (1.17) is stable: global solutions exist for all initial states of finite energy, and the norm is constant in time.

10 Examples of negative energy

We show that the positivity (1.21) can fail if the condition (1.24) breaks down even when the Wiener condition (1.23) holds. Namely, for $Y_0 = (0,0,Q,0) \in \mathscr{V}(T^3)$ we have

$$\mathscr{E}(\theta, Y_0) = Q\hat{T}(\theta)Q \tag{10.1}$$

by (8.5).

Lemma 10.1. *There exist functions $\mu(x)$ such that the positivity (1.21) fails for $\sigma(x)$ from (3.1) with small $e > 0$ while (4.1) and the Wiener condition (1.23) hold.*

Proof It suffices to construct an example of $\sigma(x)$ which provides

$$Q\hat{T}(\theta_0)Q < 0 \tag{10.2}$$

for some $\theta_0 \in \Pi^* \setminus \Gamma^*$ and $Q \in \mathbb{C}^3$. The representation (4.10) can be written as

$$\hat{T}_1(\theta) = e^2 \sum_m \Big[\frac{\xi \otimes \xi}{|\xi|^2} |\tilde{\mu}(\xi)|^2\Big]_{\xi = 2\pi m - \theta}, \quad \theta \in \Pi^* \setminus \Gamma^* \tag{10.3}$$

Similarly, (4.13) can be written in the Fourier representation as

$$\hat{T}_2 = -e^2 \frac{1}{(2\pi)^3} \langle \tilde{v}_e^0(\xi) \frac{\xi \otimes \xi}{|\xi|^2}, \tilde{\mu}(\xi) \rangle \tag{10.4}$$

with $v_e^0 := \mu_{\rm per}(x) - |\psi_e^0(x)|^2$ according to (3.5). The asymptotics (3.11) of the ground state $\psi_e^0(x)$ implies

$$\tilde{v}_e^0(\xi) = \tilde{\mu}_{\rm per}(\xi) - |\gamma_e|^2 (2\pi)^3 \delta(\xi) - \tilde{s}(\xi) = \tilde{\mu}_{\rm per}(\xi) - Z(2\pi)^3 \delta(\xi) - \tilde{s}(\xi), \tag{10.5}$$

since $|\gamma_e|^2 = Z$ by (3.11). Here $s(x) = \gamma_e \overline{\chi}_e(x) + \overline{\gamma}_e \chi_e(x) + |\chi_e(x)|^2$, and

$$\|s\|_{L^2(T^3)} \le C_1 e^2 \tag{10.6}$$

by (3.11). Further, (3.2) gives

$$\tilde{\mu}_{\rm per}(\xi) = \sum_n \tilde{\mu}(\xi) e^{in\xi} = \tilde{\mu}(\xi)(2\pi)^3 \sum_m \delta(\xi - 2\pi m) \tag{10.7}$$

by the Poisson summation formula [13]. Substituting (10.7) into (10.5) we get

$$\tilde{v}_e^0(\xi) = \tilde{\mu}(\xi)(2\pi)^3 \sum_{m \ne 0} \delta(\xi - 2\pi m) - \tilde{s}(\xi) \tag{10.8}$$

by (1.1) and (3.1). Substituting this expression into (4.13) we obtain

$$\hat{T}_2 = -e^2 \langle \tilde{\mu}(\xi) \sum_{m \ne 0} \delta(\xi - 2\pi m) \frac{\xi \otimes \xi}{|\xi|^2}, \tilde{\mu}(\xi) \rangle + \frac{e^2}{(2\pi)^3} \langle \tilde{s}(\xi) \frac{\xi \otimes \xi}{|\xi|^2}, \tilde{\mu}(\xi) \rangle. \tag{10.9}$$

At last, $s(x)$ is a Γ-periodic function and

$$\int_{T^3} s(x)dx = \int_{T^3} v_e^0(x)dx = 0$$

by (3.7). Hence,

$$\tilde{s}(\xi) = \sum_{m \ne 0} \check{s}(m) \delta(\xi - 2\pi m), \qquad \sum_m |\check{s}(m)|^2 = \mathscr{O}(e^4), \qquad e \to 0 \tag{10.10}$$

by (10.6). Therefore,

$$\hat{T}_2 = -e^2 \sum_{m\neq 0} \Big[\frac{\xi\otimes\xi}{|\xi|^2} |\tilde{\mu}(\xi)|^2 \Big]_{\xi=2\pi m} + \mathscr{O}(e^4), \qquad e\to 0. \tag{10.11}$$

Hence, there exists a $Q\in\mathbb{C}^3$ such that

$$Q\hat{T}_2 Q < 0 \tag{10.12}$$

for small $e>0$ if the condition (B.2) breaks down. For example, we can take $Q=2\pi m$ with $m\in\mathbb{Z}^3\setminus 0$ if $\tilde{\mu}(2\pi m)\neq 0$. Finally, for any $\theta_0\notin\Gamma^*$ we can reduce $|\hat{\mu}(\theta)|$ in all points $\theta\in\theta_0+\Gamma^*$ keeping it in the points of Γ^* to have

$$Q\hat{T}(\theta_0)Q = Q\hat{T}_1(\theta_0)Q + Q\hat{T}_2 Q < 0. \tag{10.13}$$

At the same time, we can keep (4.1) and the Wiener condition (1.23) to hold. ■

Remark 10.2. *The operator T_2 corresponds to the last term in the last line of (1.13). This term describes the "virtual repulsion" of the ion located at $n+q^0$ from the same ion deflected to the point $n+q^0+Q(n,t)$. This means that the negative energy contribution is provided by the electrostatic instability ("Earnshaw Theorem"* [27]*).*

A Formal linearization at the ground state

Let us substitute

$$\psi(x,t) = [\psi^0(x)+\Psi(x,t)]e^{-i\omega^0 t}, \quad q(n,t) = q^0+Q(n,t)$$

into the nonlinear equations (1.2), (1.4) with $\Phi(x,t)=G\rho(x,t)$. First, (1.3) implies that

$$\rho(x,t) = \sum_n \sigma(x-n-q^0-Q(n,t)) - e|\psi^0(x)+\Psi(x,t)|^2$$

and the Taylor expansion *formally* gives

$$\begin{aligned}\rho(x,t) \;=\; &\sum_n \Big[\sigma(x-n-q^0) - \nabla\sigma(x-n-q^0)Q(n,t) + \frac{1}{2}\nabla\nabla\sigma(x-n-q^0)Q(n,t)\otimes Q(n,t) + \ldots\Big] \\ &- \; e\Big[|\psi^0(x)|^2 + 2\mathrm{Re}\,(\psi^0(x)\overline{\Psi}(x,t)) + |\Psi(x,t)|^2\Big] = \rho^0(x)+\rho_1(x,t)+\rho_2(x,t)+\ldots\end{aligned} \tag{A.1}$$

Here $\rho^0(x):=\sigma^0(x)-e|\psi^0(x)|^2$ and ρ_k are polynomials in $\Psi(x,t)$ and $Q(t)$ of degree k. In particular, $\rho_1(x,t)$ is given by (1.14). As a result, we obtain the system (1.13) in the linear approximation.

B Ground states with minimal energy per cell

Let us consider any ion density $\sigma(x)\in L^2(\mathbb{R}^3)$ satisfying (1.24):

$$\tilde{\sigma}(2\pi m) = 0, \quad m\in\mathbb{Z}^3\setminus 0. \tag{B.2}$$

Let us note that

$$\tilde{\sigma}(0) = \int \sigma(x)dx = eZ > 0 \tag{B.3}$$

by (1.1). Then $\sigma_{\rm per}(x) := \sum_n \sigma(x-n) \equiv eZ$ since

$$\check{\sigma}_{\rm per}(m) = \int_{T^3} e^{i2\pi mx}\sigma_{\rm per}(x)dx = \int_{R^3} e^{i2\pi mx}\sigma(x)dx = 0, \qquad m\in\mathbb{Z}^3\setminus 0 \tag{B.4}$$

by (B.2). Therefore, the functions

$$\psi^0(x) \equiv \sqrt{Z}, \qquad \Phi^0(x) \equiv 0, \qquad \omega^0 = 0 \tag{B.5}$$

give a solution to (1.8)–(1.10) with zero energy per cell (2.4). On the other hand, the energy (2.4) is nonnegative. Hence, the set of all minimizers of energy per cell consists of $\psi^0(x) \equiv e^{i\phi}\sqrt{Z}$, with $\phi \in [0, 2\pi]$.

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