



On the dispersion decay for crystals in the linearized Schrödinger–Poisson model

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ABSTRACT

The Schrödinger–Poisson–Newton equations for crystals with a cubic lattice and one ion per cell are considered. The ion charge density is assumed i) to satisfy the Wiener and Jellium conditions introduced in our previous paper [25], and ii) to be exponentially decaying at infinity. The corresponding examples are given. We study the linearized dynamics at the ground state. The dispersion relations are introduced via spectral resolution for the non-selfadjoint Hamilton generator using the positivity of the energy established in [25]. Our main result is the dispersion decay in the weighted Sobolev norms for solutions with initial states from the space of continuous spectrum of the Hamilton generator. We also prove the absence of singular spectrum and limiting absorption principle. The multiplicity of every eigenvalue is shown to be infinite. The proofs rely on novel exact bounds and compactness for the inversion of the Bloch generators and on uniform asymptotics for the dispersion relations. We derive the bounds by the energy positivity from [25]. We also use the theory of analytic sets.

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1. Introduction

First mathematical results on the stability of matter were obtained by Dyson and Lenard in [14,15], where the energy bound from below was established. The thermodynamic limit for the Coulomb systems was first studied by Lebowitz and Lieb [32,33], see the survey and further development in [36]. These results were extended by Catto, Le Bris, Lions, and others to the Thomas–Fermi and Hartree–Fock models [7–9]. Further results in this direction are due to Cancés, Lahbabi, Lewin, Sabin, Stoltz, and others [5,6,31,34,35]. All these results concern either the convergence of the ground state of finite particle systems in the

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thermodynamic limit or the existence of the ground state for infinite particle systems. Cancès and Le Bris proved the well-posedness for the Hartree–Fock molecular system [4].

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].

We consider the simplest Schrödinger–Poisson model for the crystal with one ion per cell. The electron cloud is described by the one-particle Schrödinger equation; the ions are looked upon as particles that correspond 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. Nevertheless, it provides a convenient framework to introduce suitable functional tools that might be instrumental for physically more realistic models (the Thomas–Fermi, Hartree–Fock, and second quantized models).

The Schrödinger–Poisson equations are extensively studied for molecular systems since P.-L. Lions paper [37], see [1,10,38] and the references therein. In present paper, we establish the dispersion decay for the linearized Schrödinger–Poisson equations at the ground state for infinite crystals. The decay is proved under the Jellium and Wiener conditions on the ion charge density introduced in [25]. The ground state for this model was constructed in [21].

We denote by $\sigma(x)$ the charge density of one ion, and define $Z > 0$ by the identity

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

where $e > 0$ is the elementary charge. We assume throughout the paper that

$$(\Delta - 1)\sigma \in L^1(\mathbb{R}^3) \quad (1.2)$$

which provides a suitable decay for the Fourier transform of σ . In particular, the series (1.15) are converging. Moreover, we assume the exponential decay of the ion charge density

$$|\sigma(x)| \leq Ce^{-\varepsilon|x|}, \quad x \in \mathbb{R}^3, \quad (1.3)$$

where $\varepsilon > 0$. The cubic lattice $\Gamma = \mathbb{Z}^3$ is chosen for the simplicity of notations. Let $\psi(x, t)$ be the wave function of the electron field, $q(n, t)$ denote the ions displacements, and $\Phi(x, t)$ be the electrostatic potential generated by the ions and electrons. We assume that $\hbar = c = m = 1$, where c is the speed of light and m is the electron mass. The coupled Schrödinger–Poisson–Newton equations read as

$$i\dot{\psi}(x, t) = -\frac{1}{2}\Delta\psi(x, t) - e\Phi(x, t)\psi(x, t), \quad x \in \mathbb{R}^3, \quad (1.4)$$

$$-\Delta\Phi(x, t) = \rho(x, t) := \sum_{n \in \mathbb{Z}^3} \sigma(x - n - q(n, t)) - e|\psi(x, t)|^2, \quad x \in \mathbb{R}^3, \quad (1.5)$$

$$M\ddot{q}(n, t) = -\langle \nabla\Phi(x, t), \sigma(x - n - q(n, t)) \rangle, \quad n \in \mathbb{Z}^3. \quad (1.6)$$

Here $t \in \mathbb{R}$, the brackets stand for the Hermitian scalar product on the real Hilbert space $L^2(\mathbb{R}^3)$ and for its various extensions, the series (1.5) converges in a suitable sense, and $M > 0$ is the mass of one ion. All the derivatives here and below are understood in the sense of distributions. The potential $\Phi(x, t)$ can be eliminated using the operator $G := (-\Delta)^{-1}$ defined by

$$G\rho(x) := \frac{1}{4\pi} \int \frac{\rho(y)dy}{|x-y|}, \quad x \in \mathbb{R}^3. \quad (1.7)$$

Then equations (1.4)–(1.6) can be formally written as a Hamilton system with the Hamilton functional (energy)

$$E(\psi, q, p) = \frac{1}{2} \int_{\mathbb{R}^3} [|\nabla \psi(x)|^2 + \rho(x)G\rho(x)]dx + \sum_n \frac{p^2(n)}{2M}, \quad (1.8)$$

where $q := (q(n) : n \in \mathbb{Z}^3)$, $p := (p(n) : n \in \mathbb{Z}^3)$, $\rho(x)$ is defined similarly to (1.5). Namely, system (1.4)–(1.6) can be formally written as

$$i\dot{\psi}(x, t) = \partial_{\bar{\psi}(x)} \mathcal{H}, \quad \dot{q}(n, t) = \partial_{p(n)} \mathcal{H}, \quad \dot{p}(n, t) = -\partial_{q(n)} \mathcal{H}, \quad (1.9)$$

where $\partial_{\bar{z}} := \frac{1}{2}(\partial_{z_1} + i\partial_{z_2})$ with $z_1 = \operatorname{Re} z$ and $z_2 = \operatorname{Im} z$.

A ground state of a crystal is a Γ -periodic solution

$$\psi^0(x)e^{-i\omega^0 t}, \quad \Phi^0(x), \quad q^0(n) = q^0 \text{ and } p^0(n) = 0 \quad \text{for } n \in \mathbb{Z}^3 \quad (1.10)$$

with a real ω^0 and minimal energy per cell. Such ground state was constructed in [21] for general lattice with several ions per cell. In our case the ion position $q^0 \in \mathbb{R}^3$ can be chosen arbitrarily, and we set $q^0 = 0$ everywhere below. In our framework $\psi^0(x)$ will be a real function up to a phase factor, see (1.10) below. This factor can be neglected due to $U(1)$ -symmetry of equations (1.4)–(1.6), and respectively, we will consider the real ground states $\psi^0(x)$.

In present paper, we prove the dispersion decay for the *formal linearization* of the nonlinear system (1.4)–(1.6) at the ground state (1.10). The linearization is obtained on substituting $\psi(x, t) = [\psi^0(x) + \Psi(x, t)]e^{-i\omega^0 t}$ into the nonlinear equations (1.4), (1.6) with $\Phi(x, t) = G\rho(x, t)$ and retaining the linear terms in $Y(t) = (\Psi(\cdot, t), q(\cdot, t), p(\cdot, t))$. For the real ground state the linearized equation reads as follows (see [25, (1.14)]):

$$\dot{Y}(t) = AY(t), \quad A = \begin{pmatrix} 0 & H^0 & 0 & 0 \\ -H^0 - 2e^2\psi^0 G\psi^0 & 0 & -S & 0 \\ 0 & 0 & 0 & M^{-1} \\ -2S^* & 0 & -T & 0 \end{pmatrix}. \quad (1.11)$$

Here, we denote $Y(t) = (\Psi_1(\cdot, t), \Psi_2(\cdot, t), q(\cdot, t), p(\cdot, t))$, where $\Psi_1(x, t) := \operatorname{Re} \Psi(x, t)$, $\Psi_2(x, t) := \operatorname{Im} \Psi(x, t)$, $H^0 := -\frac{1}{2}\Delta - e\Phi^0(x) - \omega^0$, the operators S and T are defined in Appendix, and ψ^0 denotes the operators of multiplication by the real function $\psi^0(x)$. From the Hamilton representation (1.9) we have

$$A = JB, \quad B = \begin{pmatrix} 2H^0 + 4e^2\psi^0 G\psi^0 & 0 & 2S & 0 \\ 0 & 2H^0 & 0 & 0 \\ 2S^* & 0 & T & 0 \\ 0 & 0 & 0 & M^{-1} \end{pmatrix}, \quad J = \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \quad (1.12)$$

The results [25] imply that the energy operator B is densely defined and is selfadjoint on the Hilbert space

$$\mathcal{X}^0(\mathbb{R}^3) := L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \oplus l^2(\mathbb{Z}^3) \oplus l^2(\mathbb{Z}^3). \quad (1.13)$$

Our main goal is to show the dispersion decay of solutions to (1.11) in the weighted norms

$$\|X\|_\alpha := \|\langle x \rangle^\alpha \Psi_1(x)\|_{L^2(\mathbb{R}^3)} + \|\langle x \rangle^\alpha \Psi_2(x)\|_{L^2(\mathbb{R}^3)} + \|\langle n \rangle^\alpha q(n)\|_{l^2(\mathbb{Z}^3)} + \|\langle n \rangle^\alpha p(n)\|_{l^2(\mathbb{Z}^3)} \quad (1.14)$$

with $\alpha < 0$ for $X = (\Psi_1, \Psi_2, q, p) \in \mathcal{X}^0(\mathbb{R}^3)$. We will prove the decay under two following conditions C1 and C2 on σ introduced in [25].

$$\text{C1. The Wiener Condition: } \Sigma(\theta) := \sum_m \left[\frac{\xi \otimes \xi}{|\xi|^2} |\hat{\sigma}(\xi)|^2 \right]_{\xi=2\pi m+\theta} > 0, \quad \text{for a.e. } \theta \in \Pi^* \setminus \Gamma^*. \quad (1.15)$$

Here $\hat{\sigma}(\xi)$ stands for the Fourier transform $\int e^{i\xi x} \sigma(x) dx$, $\Pi^* := [0, 2\pi]^3$ is the Brillouin zone, $\Gamma^* := 2\pi\mathbb{Z}^3$ and $\xi \otimes \xi$ denotes the matrix $\xi_i \xi_j$. The series of the matrices converges by (1.2), and the sum is a positive definite matrix.

This condition is an analog of the Fermi Golden Rule for crystals. It means a strong coupling of the ions to the electron field.

$$\text{C2. The Jellium Condition: } \hat{\sigma}(2\pi m) = 0, \quad m \in \mathbb{Z}^3 \setminus 0. \quad (1.16)$$

This condition cancels the negative energy which is provided by the electrostatic instability (‘Earnshaw’s Theorem’ [44], see [25, Remark 10.2]). It implies that the periodized ions charge density corresponding to the ground state is a positive constant everywhere in the space.

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 [19]. Moreover, this condition holds for a broad class of functions σ , see [26, Section B.2]. Here we study this model in the rigorous context of the Schrödinger–Poisson equations.

Under condition (1.16), the minimum of energy per cell corresponds to the opposite uniform negative electronic charge. So these ion and electronic densities cancel each other, and the potential $\Phi(x, t)$ vanishes by (1.5), see Lemma 2.1 in [25]:

$$\psi^0(x) \equiv e^{i\phi} \sqrt{Z}, \quad \phi \in [0, 2\pi]; \quad \Phi^0(x) \equiv 0, \quad \omega^0 = 0. \quad (1.17)$$

We give examples satisfying all our conditions (1.2), (1.3), (1.15), and (1.16), (see Example 3.2).

The key result of [25] is the positivity $B > 0$ of the energy operator (1.12) under the Wiener and Jellium conditions C1 and C2. Denote by \mathcal{W} the completion of the space $\mathcal{X}^1(\mathbb{R}^3) := H^1(\mathbb{R}^3) \oplus H^1(\mathbb{R}^3) \oplus l^2(\mathbb{Z}^3) \oplus l^2(\mathbb{Z}^3)$ with the norm

$$\|Y\|_{\mathcal{W}} := \|\Lambda Y\|_{\mathcal{X}^0(\mathbb{R}^3)}, \quad \Lambda := B^{1/2} > 0. \quad (1.18)$$

In [25] we have proved that for any $Y(0) \in \mathcal{W}$ there exists a unique *weak solution* $Y(t) \in C(\mathbb{R}, \mathcal{W})$ to (1.11). The main result of the present paper is the following theorem.

Theorem 1.1. *Let conditions (1.2), (1.3), (1.15), and (1.16) hold. Then every solution $Y(t) \in C(\mathbb{R}, \mathcal{W})$ to (1.11) splits as follows*

$$Y(t) = \sum_1^M Y_k e^{-i\omega_k^* t} + Y_c(t), \quad (1.19)$$

where $M \leq \infty$ and $Y_k \in \mathcal{W}$. Moreover,

$$|\omega_k^*| \rightarrow \infty, \quad k \rightarrow \infty, \quad (1.20)$$

if $M = \infty$. The remainder $Y_c(t)$ decays in the weighted norms: for any $\alpha < -3/2$,

$$\| \Lambda Y_c(t) \|_\alpha \rightarrow 0, \quad |t| \rightarrow \infty. \quad (1.21)$$

This theorem means the linear asymptotics stability of the ground state (1.17) when $M = 0$.

Let us comment on our approach. We develop our methods [25] relying on the Bloch transform. Namely, the generator A commutes with translations by vectors from Γ . Hence, the equation (1.11) can be reduced using the Fourier–Bloch–Gelfand–Zak transform $Y(t) \mapsto \tilde{Y}(\cdot, t) \in L^2(\Pi^*, \mathcal{X}^0(\mathbb{T}))$, where $\mathbb{T} := \mathbb{R}^3/\Gamma$ is the periodic cell, and

$$\mathcal{X}^s(\mathbb{T}) := H^s(\mathbb{T}) \oplus H^s(\mathbb{T}) \oplus \mathbb{C}^3 \oplus \mathbb{C}^3, \quad s \in \mathbb{R}. \quad (1.22)$$

In the Bloch transform equation (1.11) formally reads

$$\dot{\tilde{Y}}(\theta, t) = \tilde{A}(\theta) \tilde{Y}(\theta, t) \quad \text{for a.e. } \theta \in \Pi^*, \quad t \in \mathbb{R}, \quad (1.23)$$

where $\tilde{Y}(\cdot, t) \in \mathcal{X}^0(\mathbb{T})$ (see [25, (8.6)]). The Hamilton representation (1.12) implies that

$$\tilde{A}(\theta) = J \tilde{B}(\theta), \quad \theta \in \Pi^* \setminus \Gamma^*, \quad (1.24)$$

where the Bloch energy operators $\tilde{B}(\theta)$ are selfadjoint in $\mathcal{X}^0(\mathbb{T})$. The main crux here is that the generator $\tilde{A}(\theta)$ is not selfadjoint and even is not symmetric in the Hilbert space $\mathcal{X}^0(\mathbb{T})$. Hence we cannot diagonalize it using the von Neumann spectral theorem. Thus, even an introduction of the ‘dispersion relations’ $\omega_k(\theta)$, which are the eigenvalues of $\tilde{A}(\theta)$, is a nontrivial problem in our situation. Let us denote

$$\Pi_+^* := \{\theta \in \Pi^* \setminus \Gamma^* : \Sigma(\theta) > 0\}. \quad (1.25)$$

This is an open set of the complete Lebesgue measure, i.e., $\text{mes}(\Pi^* \setminus \Pi_+^*) = 0$, by (1.15). The key role in our approach is played by the positivity

$$\langle \tilde{Y}, \tilde{B}(\theta) \tilde{Y} \rangle \geq \varkappa(\theta) \|\tilde{Y}\|_{\mathcal{X}^1(\mathbb{T})}^2, \quad \tilde{Y} \in \mathcal{X}^1(\mathbb{T}), \quad \theta \in \Pi_+^*, \quad (1.26)$$

with $\varkappa(\theta) > 0$, the brackets denoting the scalar product in $\mathcal{X}^0(\mathbb{T})$. We have proved this bound in [25] under conditions (1.15)–(1.16) on the ion charge density σ .

In present paper we use this positivity to show that the eigenvectors of $\tilde{A}(\theta)$ span the Hilbert space $\mathcal{X}^0(\mathbb{T})$ by our spectral theory of the Hamilton operators with positive energy [23,24]. This is a special version of the Gohberg–Krein–Langer theory of selfadjoint operators in the Hilbert spaces with indefinite metric [20, Ch. VI] and [29,30]. Namely, setting $\tilde{\Lambda}(\theta) := \tilde{B}^{1/2}(\theta)$, we obtain that

$$\tilde{A}(\theta) = -i \tilde{\Lambda}^{-1}(\theta) \tilde{K}(\theta) \tilde{\Lambda}(\theta), \quad \theta \in \Pi_+^*, \quad (1.27)$$

where $\tilde{K}(\theta) = \tilde{\Lambda}(\theta) i J \tilde{\Lambda}(\theta)$ is a selfadjoint operator in $\mathcal{X}^0(\mathbb{T})$. Hence, all solutions to (1.23) admit the representation

$$\tilde{Y}(\theta, t) = \tilde{\Lambda}^{-1}(\theta) e^{-i \tilde{K}(\theta) t} \tilde{\Lambda}(\theta) \tilde{Y}(\theta, 0), \quad t \in \mathbb{R}, \quad \theta \in \Pi_+^*. \quad (1.28)$$

We prove that the spectrum of $\tilde{K}(\theta)$ is discrete and obtain the lower estimate for the eigenvalues $\omega_k(\theta)$ which are also the eigenvalues of $\tilde{A}(\theta)$ and are called the dispersion relations (or the Floquet eigenvalues).

Further, we represent the solution $Y(t)$ as the inversion of the Bloch transform (1.28). This inversion is the series of oscillatory integrals with the phase functions $\omega_k(\theta)$. Using the decay (1.3) we show that

- i) $\omega_k(\theta)$ are piecewise real-analytic in $\theta \in \Pi^* \setminus \Gamma^*$ for every k ;
- ii) If $\omega_k(\theta) \not\equiv \text{const}$, then the set

$$\{\theta \in \Pi^* \setminus \Gamma^* : \nabla \omega_k(\theta) = 0, \det \text{Hess} \omega_k(\theta) = 0\} \quad (1.29)$$

has the Lebesgue measure zero;

- iii) In the case $M = \infty$ the limit (1.20) holds for the constant dispersion relations $\omega_k(\theta) \equiv \omega_k^*$.

These properties of the phase functions provide the asymptotics (1.19) and (1.21). Finally, we establish the absence of singular spectrum and the limiting absorption principle for the selfadjoint operator $K := i\Lambda A \Lambda^{-1}$.

Note that all our methods and results extend obviously to equations (1.4)–(1.6) in the case of a general lattice

$$\Gamma = \{n_1 a_1 + n_2 a_2 + n_3 a_3 : (n_1, n_2, n_3) \in \mathbb{Z}^3\}, \quad (1.30)$$

where the generators $a_k \in \mathbb{R}^3$ are linearly independent. In this case the condition (1.16) becomes

$$\hat{\sigma}(\gamma^*) = 0, \quad \gamma^* \in \Gamma^* \setminus 0. \quad (1.31)$$

Here Γ^* denotes the dual lattice $\Gamma^* = \{m_1 b_1 + m_2 b_2 + m_3 b_3 : (m_1, m_2, m_3) \in \mathbb{Z}^3\}$, where $\langle a_k, b_j \rangle = 2\pi \delta_{kj}$. The condition (1.31) relates the properties of the ions with the crystal geometry.

Let us comment on previous results in these directions.

The Schrödinger–Poisson equations for crystal were introduced in [21,22], where the existence of the ground states was established for infinite crystals. Recently we have proved the linear stability of these ground states [25]. In [26,27] we have proved the orbital stability of the ground states for the Schrödinger–Poisson equations with one-particle and many-particle Schrödinger equation in the case of finite crystals with periodic boundary conditions.

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 [5], Cancès and Stoltz 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 [5, (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 [31] and in the introductions of [5,6].

In [6] E. Cancès, S. Lahbabi, and M. Lewin 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. They obtained suitable generalizations of the Hoffmann–Ostenhof and Lieb–Thirring inequalities for ergodic density matrices, and constructed a random potential satisfying the Poisson equation with the corresponding stationary stochastic charge density. The main result of [6] is the coincidence of this model with the thermodynamic limit in the case of the short-range Yukawa interaction.

In [34], Lewin and Sabin showed the well-posedness for the reduced von Neumann equation, describing the Fermi gas, with density matrices of infinite trace and pairwise interaction potentials $w \in L^1(\mathbb{R}^3)$. Moreover, they proved the asymptotic stability of translation-invariant stationary states for 2D Fermi gas [35].

The traditional *one-electron* Bethe–Bloch–Sommerfeld mathematical model of crystals is known to be the linear Schrödinger equation with a space-periodic static potential, which corresponds to the standing ions. The corresponding spectral theory is well developed, see [41] and the references therein. The scattering theory for short-range and long-range perturbations of such ‘periodic operators’ was constructed in [17,18].

The first results on the dispersion decay $\sim t^{-1}$ were obtained by Firsova [16] for 1D Schrödinger equation with space-periodic potential for finite band case. The proofs rely on Korotyaev's results [28] on stationary points of the dispersion relations.

The decay $\sim t^{-\varepsilon}$ with a small $\varepsilon > 0$ for the 1D Schrödinger equation with an infinite band potential was established by Cuccagna [12]. This decay was applied to the asymptotic stability of standing waves in presence of small nonlinear perturbations [11].

The absence of constant dispersion relations for the periodic Schrödinger equations was established by Thomas [45], see also Lemma 2 (c) of [41], p. 308.

Recently Prill [40] proved the decay $\sim t^{-p}$ with $p = 3/2$ and $p = 1/2$ (under distinct assumptions) for the 1D Klein–Gordon equation with a periodic Lamé potential and its short range perturbations.

The dispersion decay for the periodic Schrödinger and Klein–Gordon equations in higher dimensions $n \geq 2$ was not obtained previously.

Our paper is organized as follows. In Section 2 we recall some formulas from [25] for the Bloch representation. In Section 3 we introduce the dispersion relations and prove their properties. In Section 4 we prove the asymptotics (1.19), (1.21), and in Section 5 we justify the limiting absorption principle. In Appendix A we collect some formulas from [25] which we need in our calculations.

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2. The Bloch representation of the dynamics

In this section we recall some notations from [25] and establish novel exact bounds and compactness for the inversion of the Bloch generators.

2.1. The Bloch representation of the dynamics

We set $\mathcal{S}_+ := \cup_{\varepsilon>0} \mathcal{S}_\varepsilon$, where \mathcal{S}_ε is the space of functions $\Psi \in \mathcal{S}(\mathbb{R}^3)$ whose Fourier transforms $\hat{\Psi}(\xi)$ vanish in the ε -neighborhood of the lattice Γ^* , and let l_c be the space of compactly supported sequences $q(n) \in \mathbb{R}^3$.

Definition 2.1. Let $\mathcal{D} := \{Y = (\Psi_1, \Psi_2, q, p) : \Psi_1, \Psi_2 \in \mathcal{S}_+, \quad q, p \in l_c\}$.

Note that the space \mathcal{D} is dense in $\mathcal{X}^0(\mathbb{R}^3)$, and $A : \mathcal{D} \rightarrow \mathcal{X}^0(\mathbb{R}^3)$ by Theorem 4.2 of [25]. Denote by Π the primitive cell $\Pi := [0, 1]^3$ and $\mathcal{X}^0(\Pi) := L^2(\Pi) \oplus L^2(\Pi) \oplus \mathbb{R}^3 \oplus \mathbb{R}^3$. For $Y = (\Psi_1, \Psi_2, q, p) \in \mathcal{X}^0(\mathbb{R}^3)$ and $n \in \mathbb{Z}^3$ we set

$$Y(n) = (\Psi_1(n, \cdot), \Psi_2(n, \cdot), q(n), p(n)), \quad \text{where} \quad \Psi_j(n, y) = \Psi_j(n + y) \quad \text{for a.e. } y \in \Pi. \quad (2.1)$$

Obviously,

$$\|Y\|_{\mathcal{X}^0(\mathbb{R}^3)}^2 = \sum_{n \in \mathbb{Z}^3} \|Y(n)\|_{\mathcal{X}^0(\Pi)}^2. \quad (2.2)$$

Definition 2.2. We will call the sequence $Y(n)$ as the cell representation of $Y \in \mathcal{X}^0(\mathbb{R}^3)$.

The ground state (1.10) is invariant with respect to translations of the lattice Γ , and hence the generator A commutes with these translations. Therefore, the operator A can be reduced using the discrete Fourier transform

$$\hat{Y}(\theta) = F_{n \rightarrow \theta} Y(n) := \sum_{n \in \mathbb{Z}^3} e^{in\theta} Y(n) = (\hat{\Psi}_1(\theta, \cdot), \hat{\Psi}_2(\theta, \cdot), \hat{q}(\theta), \hat{p}(\theta)) \quad \text{for a.e. } \theta \in \Pi^*. \quad (2.3)$$

By the Parseval–Plancherel theorem the series converge in $L^2(\Pi^*, \mathcal{X}^0(\Pi))$ for $Y \in \mathcal{X}^0(\mathbb{R}^3)$.

Definition 2.3. (see [13,39,41], and [25]) The Bloch transform of $Y \in \mathcal{X}^0(\mathbb{R}^3)$ is defined as

$$\tilde{Y}(\theta) = [\mathcal{F}Y](\theta) := \mathcal{M}(\theta)\hat{Y}(\theta) := (\tilde{\Psi}_1(\theta, \cdot), \tilde{\Psi}_2(\theta, \cdot), \hat{q}(\theta), \hat{p}(\theta)) \quad \text{for a.e. } \theta \in \Pi^*, \quad (2.4)$$

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 $y \in \mathbb{R}^3$.

The transform $\mathcal{F} : \mathcal{X}^0(\mathbb{R}^3) \rightarrow L^2(\Pi^*, \mathcal{X}^0(\mathbb{T}))$ is an isomorphism by the Parseval–Plancherel identity. The inversion is given by

$$Y(n) = |\Pi^*|^{-1} \int_{\Pi^*} e^{-in\theta} \mathcal{M}(-\theta) \tilde{Y}(\theta) d\theta, \quad n \in \mathbb{Z}^3. \quad (2.5)$$

In the Bloch transform one has $\widetilde{AY}(\theta) = \tilde{A}(\theta)\tilde{Y}(\theta)$ for $Y \in \mathcal{D}$ and $\theta \in \Pi^* \setminus \Gamma^*$. Here $\tilde{A}(\theta)$ denotes the operator matrix

$$\tilde{A}(\theta) = \begin{pmatrix} 0 & \tilde{H}^0(\theta) & 0 & 0 \\ -\tilde{H}^0(\theta) - 2e^2\psi^0\tilde{G}(\theta)\psi^0 & 0 & \tilde{S}(\theta) & 0 \\ 0 & 0 & 0 & M^{-1} \\ -2\tilde{S}^*(\theta) & 0 & -\tilde{T}(\theta) & 0 \end{pmatrix}, \quad \theta \in \Pi^* \setminus \Gamma^*, \quad (2.6)$$

where the operator entries are given by (A.2)–(A.4). The operator $\tilde{A}(\theta)$ admits the representation

$$\tilde{A}(\theta) = J\tilde{B}(\theta), \quad \tilde{B}(\theta) = \begin{pmatrix} 2\tilde{H}^0(\theta) + 4e^2\psi^0\tilde{G}(\theta)\psi^0 & 0 & 2\tilde{S}(\theta) & 0 \\ 0 & 2\tilde{H}^0(\theta) & 0 & 0 \\ 2\tilde{S}^*(\theta) & 0 & \tilde{T}(\theta) & 0 \\ 0 & 0 & 0 & M^{-1} \end{pmatrix}, \quad \theta \in \Pi^* \setminus \Gamma^*. \quad (2.7)$$

Lemma 2.4. Let conditions (1.2) and (1.15), (1.16) hold. Then

i) For $\theta \in \Pi^* \setminus \Gamma^*$ the operator $\tilde{B}(\theta)$ is selfadjoint in $\mathcal{X}^0(\mathbb{T})$ with the domain $\mathcal{X}^2(\mathbb{T})$; the quadratic form $\langle \tilde{B}(\theta)\tilde{Y}, \tilde{Y} \rangle$ extends by continuity to $\tilde{Y} \in \mathcal{X}^1(\mathbb{T})$:

$$\langle \tilde{B}(\theta)\tilde{Y}, \tilde{Y} \rangle \leq C\|\tilde{Y}\|_{\mathcal{X}^1(\mathbb{T})}^2, \quad \tilde{Y} \in \mathcal{X}^1(\mathbb{T}). \quad (2.8)$$

ii) For $\theta \in \Pi_+^*$

$$\|\tilde{Y}\|_{\mathcal{X}^1(\mathbb{T})}^2 \leq \frac{1}{\varkappa(\theta)} \langle \tilde{B}(\theta)\tilde{Y}, \tilde{Y} \rangle, \quad \tilde{Y} \in \mathcal{X}^1(\mathbb{T}). \quad (2.9)$$

Proof. i) The representation $\tilde{A}(\theta) = J\tilde{B}(\theta)$ follows from (1.12). The operator $\tilde{B}(\theta)$ is symmetric on the domain $\mathcal{X}^2(\mathbb{T})$. Moreover, all operators in (2.7), except for $\tilde{H}^0(\theta)$, are bounded by (1.2). Finally, $\tilde{H}^0(\theta)$ is selfadjoint in $L^2(\mathbb{T})$ with the domain $H^2(\mathbb{T})$. Hence, $\tilde{B}(\theta)$ is selfadjoint on the domain $\mathcal{X}^2(\mathbb{T})$.

ii) The bound (2.9) holds by (1.26). \square

Corollary 2.5. Under conditions (1.2) and (1.15), (1.16)

- i) The operator $\tilde{\Lambda}(\theta) := \tilde{B}^{1/2}(\theta) : \mathcal{X}^1(\mathbb{T}) \rightarrow \mathcal{X}^0(\mathbb{T})$ is bounded.
- ii) For $\theta \in \Pi_+^*$ the operator $\tilde{\Lambda}(\theta)$ is invertible in $\mathcal{X}^0(\mathbb{T})$. Moreover,

$$\|\tilde{\Lambda}^{-1}(\theta)\tilde{Z}\|_{\mathcal{X}^1(\mathbb{T})}^2 \leq \frac{1}{\varkappa(\theta)} \|\tilde{Z}\|_{\mathcal{X}^0(\mathbb{T})}^2, \quad \tilde{Z} \in \mathcal{X}^0(\mathbb{T}) \quad (2.10)$$

Proof. i) $\tilde{\Lambda}(\theta)$ is bounded by (2.8), since

$$\langle \tilde{\Lambda}(\theta)\tilde{Y}, \tilde{\Lambda}(\theta)\tilde{Y} \rangle = \langle \tilde{B}(\theta)\tilde{Y}, \tilde{Y} \rangle, \quad \tilde{Y} \in \mathcal{X}^2(\mathbb{T}). \quad (2.11)$$

ii) $\tilde{\Lambda}(\theta)$ is invertible by the positivity (1.26), and (2.10) follows by (2.9) as applied to $\tilde{Y} = \tilde{\Lambda}^{-1}(\theta)\tilde{Z}$. \square

2.2. Reduction to selfadjoint generator

Definition 2.6. A function $Y(t) \in C(\mathbb{R}, \mathcal{X}^1(\mathbb{R}^3))$ is a weak solution to (1.11) if, for every $V \in \mathcal{D}$,

$$\langle Y(t) - Y(0), V \rangle = \int_0^t \langle Y(s), A^*V \rangle ds, \quad t \in \mathbb{R}. \quad (2.12)$$

In the Bloch transform the weak solution satisfies (1.23) in the sense of $\mathcal{X}^1(\mathbb{T})$ -valued distributions, see [25]. Applying $\tilde{\Lambda}(\theta)$ to both sides of (1.23), we obtain the equivalent equation $\dot{\tilde{Z}}(\theta, t) = -i\tilde{K}(\theta)\tilde{Z}(\theta, t)$ for $\theta \in \Pi_+^*$ in the sense of vector-valued distributions, where $\tilde{Z}(\theta, t) := \tilde{\Lambda}(\theta)\tilde{Y}(\theta, t)$ and $\tilde{K}(\theta) := \tilde{\Lambda}(\theta)iJ\tilde{\Lambda}(\theta)$ is formally symmetric operator in $\mathcal{X}^0(\mathbb{T})$. The main crux is that the domain of $\tilde{K}(\theta)$ is unknown, since the ion density $\sigma(x)$ is not smooth in general, and so the PDO machinery does not apply. The following lemma plays a key role in our approach.

Lemma 2.7. (cf. Lemma 8.2 of [25]) Let conditions (1.2) and (1.15), (1.16) hold. Then for $\theta \in \Pi_+^*$

- i) $\tilde{K}(\theta)$ is a selfadjoint operator in $\mathcal{X}^0(\mathbb{T})$ with dense domain $D(\tilde{K}(\theta)) \subset \mathcal{X}^1(\mathbb{T})$;
- ii) $\tilde{K}^{-1}(\theta)$ is a compact selfadjoint operator in $\mathcal{X}^0(\mathbb{T})$, and

$$\|\tilde{K}^{-1}(\theta)\tilde{Z}\|_{\mathcal{X}^1(\mathbb{T})}^2 \leq \frac{C}{\varkappa(\theta)} \|\tilde{Z}\|_{\mathcal{X}^0(\mathbb{T})}^2, \quad \tilde{Z} \in \mathcal{X}^0(\mathbb{T}). \quad (2.13)$$

Proof. i) The operator $\tilde{\Lambda}(\theta)$ is injective. Moreover, $\text{Ran } \tilde{\Lambda}(\theta) = \mathcal{X}^0(\mathbb{T})$. Hence, $\text{Ran } \tilde{K}(\theta) = \mathcal{X}^0(\mathbb{T})$. Consider the inverse operator

$$\tilde{R}(\theta) := \tilde{K}^{-1}(\theta) = i\tilde{\Lambda}^{-1}(\theta)J^{-1}\tilde{\Lambda}^{-1}(\theta). \quad (2.14)$$

This operator is selfadjoint, since it is bounded and symmetric. Hence, $D(\tilde{R}(\theta)) = \text{Ran } \tilde{K}(\theta) = \mathcal{X}^0(\mathbb{T})$. Therefore, $\tilde{K}(\theta) = \tilde{R}^{-1}(\theta)$ is a densely defined selfadjoint operator by Theorem 13.11 (b) of [42]:

$$\tilde{K}^*(\theta) = \tilde{K}(\theta), \quad D(\tilde{K}(\theta)) = \text{Ran } \tilde{R}(\theta) \subset \text{Ran } \tilde{\Lambda}^{-1}(\theta) \subset \mathcal{X}^1(\mathbb{T}),$$

where the last inclusion follows from (2.10).

ii) Estimate (2.13) follows from (2.10) and (2.14). Hence, $\tilde{K}^{-1}(\theta)$ is a compact operator in $\mathcal{X}^0(\mathbb{T})$ by the Sobolev embedding theorem. \square

As a consequence,

$$\tilde{Z}(\theta, t) = e^{-i\tilde{K}(\theta)t} \tilde{Z}(\theta, 0), \quad \tilde{Z}(\theta, 0) := \tilde{\Lambda}(\theta) \tilde{Y}(\theta, 0). \quad (2.15)$$

The definition (1.18) implies that the operator $\Lambda := \mathcal{F}^{-1} \tilde{\Lambda}(\theta)$ is the isomorphism $\mathcal{W} \rightarrow \mathcal{X}^0(\mathbb{R}^3)$.

Proposition 2.8. (Corollary 8.5 of [25]) *Let the positivity (1.26) hold. Then, for every initial state $Y(0) \in \mathcal{W}$, there exists a unique weak solution $Y(\cdot) \in C_b(\mathbb{R}, \mathcal{W})$ to equation (1.11). The solution is given by formula (1.28).*

3. Dispersion relations

Here we establish the properties of the eigenvalues of $\tilde{K}(\theta)$ which play the key role in the proof of the dispersion decay. Lemma 2.7 implies the spectral resolution

$$\tilde{K}(\theta) = \sum_{k=1}^{\infty} \omega_k(\theta) P_k(\theta), \quad \theta \in \Pi_+^*, \quad (3.1)$$

where $\omega_k(\theta)$ are the eigenvalues (dispersion relations) counted with their multiplicities,

$$|\omega_1(\theta)| \leq |\omega_2(\theta)| \leq \dots,$$

and $P_k(\theta)$ are the corresponding orthogonal projections.

Lemma 3.1. *Let conditions (1.2) and (1.15), (1.16) hold and Q be a compact subset of Π_+^* . Then*

$$|\omega_k(\theta)| \geq \varepsilon(Q) k^{2/3}, \quad k \geq 1, \quad \theta \in Q, \quad (3.2)$$

where $\varepsilon(Q) > 0$.

Proof. The key role in the proof of (3.2) is played by the estimate [25, (7.23)]:

$$b(Q) := \inf_{\theta \in Q} \kappa(\theta) > 0 \quad (3.3)$$

for any compact subset $Q \subset \Pi_+^*$. The expansion (3.1) implies that

$$|\tilde{K}^{-1}(\theta)| = \sum_{k=1}^{\infty} |\omega_k(\theta)|^{-1} P_k(\theta), \quad \theta \in \Pi_+^*. \quad (3.4)$$

Moreover, by duality we have from estimate (2.13)

$$\|\tilde{K}^{-1}(\theta) \tilde{Z}\|_{\mathcal{X}^0(\mathbb{T})}^2 \leq \frac{C}{b(Q)} \|\tilde{Z}\|_{\mathcal{X}^{-1}(\mathbb{T})}^2, \quad \tilde{Z} \in \mathcal{X}^0(\mathbb{T}), \quad \theta \in Q \quad (3.5)$$

due to (3.3), since the operator $\tilde{K}^{-1}(\theta)$ is selfadjoint. At last, the norm in the right-hand side of (3.5) can be written as $\|g\tilde{Z}\|_{\mathcal{X}^0(\mathbb{T})}$, where

$$g = \begin{pmatrix} (-\Delta + 1)^{-1/2} & 0 & 0 & 0 \\ 0 & (-\Delta + 1)^{-1/2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (3.6)$$

is the positive selfadjoint operator in $\mathcal{X}^0(\mathbb{T})$. Now (3.5) gives that

$$\|\tilde{K}^{-1}(\theta)\tilde{Z}\|_{\mathcal{X}^0(\mathbb{T})} \leq C(Q)\|g\tilde{Z}\|_{\mathcal{X}^0(\mathbb{T})}, \quad \tilde{Z} \in \mathcal{X}^0(\mathbb{T}), \quad \theta \in Q. \quad (3.7)$$

Hence, the Rayleigh–Courant–Fisher theorem ([2, Theorem 1, p. 110] and [41, Theorem XIII.1, p. 91]) implies that

$$|\omega_k(\theta)|^{-1} \leq C(Q)g_k, \quad k \geq 1, \quad \theta \in Q, \quad (3.8)$$

where $g_1 \geq g_2 \geq \dots$ are the eigenvalues of g counted with their multiplicities. Therefore, (3.2) holds, since $g_k \leq Ck^{-2/3}$. The last inequality is obvious, in as much as $k \leq \#\{n \in \mathbb{Z}^3 : n^2 + 1 \leq g_k^{-1}\} \leq C_1 g_k^{-3/2}$. \square

Further we use the exponential decay of the ion charge density (1.3). It is easy to construct examples of densities σ satisfying all conditions of Theorem 1.1: (1.2), (1.3) and the Wiener and Jellium conditions (1.15), (1.16).

Example 3.2. For example, all these conditions hold for $\sigma(x_1, x_2, x_3) := \sigma_1(x_1)\sigma_1(x_2)\sigma_1(x_3)$, where

$$\tilde{\sigma}_1(\xi) := \frac{\sin \frac{\xi}{2}}{\xi} e^{-\xi^2}, \quad \xi \in \mathbb{R}.$$

In particular, (1.3) holds by the Paley–Wiener theorem.

The condition (1.3) implies that the function $\tilde{\sigma}(\theta, y)$ is analytic with respect to θ in the complex tube

$$\Pi_\varepsilon^* := \{\theta \in [\Pi^* \setminus \Gamma^*] \oplus i\mathbb{R}^3 : |\operatorname{Im}\theta| < \varepsilon\}.$$

Hence, the finite rank operators $\tilde{S}(\theta)$ and $\tilde{T}(\theta)$ defined in (A.2)–(A.4) are also analytic in $\theta \in \Pi_\varepsilon^*$. Therefore, $\tilde{K}(\theta)$ is real-analytic on Π_+^* . Denote the set

$$\mathcal{R} := \{(\theta, \omega) : \theta \in \Pi_+^*, \omega \in \operatorname{Spec} \tilde{K}(\theta)\}. \quad (3.9)$$

The eigenvalues $\omega_k(\theta)$ and the projections $P_k(\theta)$ become single-valued functions on \mathcal{R} : for $R = (\theta, \omega_k(\theta))$

$$\theta(R) := \theta, \quad \omega(R) := \omega_k(\theta), \quad P(R) := P_k(\theta). \quad (3.10)$$

These functions are continuous on the manifold \mathcal{R} endowed with natural topology by the inclusion $\mathcal{R} \subset \Pi^* \times \mathbb{R}$. They are piecewise analytic on \mathcal{R} by the following lemma, which extends [43, Lemma 1.1] from the Schrödinger equation with periodic potential to the system (1.11).

Lemma 3.3. *Let all conditions of Theorem 1.1 hold. Then for every point $R^* = (\theta^*, \omega^*) \in \mathcal{R}$ there exists a neighborhood $U = U(R^*) \subset \mathcal{R}$ with its projection $V = V(R^*)$ onto Π_+^* , and a critical subset $\mathcal{C} = \mathcal{C}(R^*) \subset \Pi_\varepsilon^*$, which is a finite union of analytic submanifolds of positive complex codimension in Π_ε^* , with the following properties:*

- i) *For any point $R = (\theta, \omega) \in U$ we have $\omega(R) := \omega \in \operatorname{Spec} \tilde{K}(\theta)$.*
- ii) *For any point $\theta' \in V \setminus \mathcal{C}$ there exists a neighborhood $W = W(\theta') \subset V \setminus \mathcal{C}$ such that $R = (\theta, \omega) \in U$ with $\theta \in W$ if and only if $\omega = \omega_l(\theta)$ with some $l = 1, \dots, L = L(R^*)$.*
- iii) *The eigenvalues $\omega_l(\cdot)$ and the corresponding projections $P_l(\cdot)$ are real-analytic functions on W and admit an analytic continuation outside \mathcal{C} in a complex neighborhood of θ^* in Π_ε^* .*

iv) For each $l = 1, \dots, L(R^*)$, either

$$\nabla \omega_l(\theta) \neq 0, \quad \theta \in W, \quad (3.11)$$

or

$$\omega_l(\theta) \equiv \omega^*, \quad \theta \in W. \quad (3.12)$$

v) If (3.12) holds with some l for a point $R^* = (\theta^*, \omega^*)$, then the constant eigenvalue also exists for (θ, ω^*) with any $\theta \in \Pi_+^*$.

Proof. Let us set $r := \text{dist}(\omega^*, \text{Spec } \tilde{K}(\theta^*) \setminus \omega^*) > 0$. Then

$$P(\theta) = -\frac{1}{2\pi i} \int_{|\omega - \omega^*| = r/2} [\tilde{K}(\theta) - \omega]^{-1} d\omega \quad (3.13)$$

is a finite-rank Riesz projection, which is analytic in a complex neighborhood of θ^* . Its range $\text{Ran } P(\theta)$ is invariant under $\tilde{K}(\theta)$, and hence the bifurcated from ω^* eigenvalues of $\tilde{K}(\theta)$ coincide with the roots of the characteristic equation

$$\det[M(\theta) - \omega] = 0, \quad (3.14)$$

where $M(\theta) := \tilde{K}(\theta)|_{\text{Ran } P(\theta)}$. The coefficients of this polynomial are analytic functions of θ in a complex neighborhood of θ^* , and hence i)–iv) follow by the arguments from the proof of Lemma 1.1 of [43].

Finally, v) follows from the fact that the set of the corresponding $\theta \in \Pi_+^*$ is closed and open at the same time by the analyticity of each $\omega_l(\theta)$ in a connected open region of $\Pi_\varepsilon^* \setminus \mathcal{C}$. \square

Definition 3.4. Ω^* is the set of all ω^* which are constant eigenvalues (3.12) at least for one point $R^* \in \mathcal{R}$.

4. Dispersion decay

Here we prove our main Theorem 1.1. Recall that $\Lambda : \mathcal{W} \rightarrow \mathcal{X}^1(\mathbb{R}^3)$ is an isomorphism by the definition (1.18), and hence, it suffices to check the corresponding asymptotics for $Z(t) := \Lambda Y(t) \in C(\mathbb{R}, \mathcal{X}^0(\mathbb{R}^3))$:

$$Z(t) = \sum_1^M Z_k e^{-i\omega_k^* t} + Z^c(t); \quad \|Z^c(t)\|_\alpha \rightarrow 0, \quad |t| \rightarrow \infty, \quad (4.1)$$

where $Z_k \in \mathcal{X}^0(\mathbb{R}^3)$ and $\alpha < -3/2$. Substituting (2.15) for $\tilde{Z}(\theta, t)$ into the inversion formula (2.5) we obtain the corresponding cell representation

$$Z(n, t) = |\Pi^*|^{-1} \int_{\Pi^*} e^{-in\theta} \mathcal{M}(-\theta) e^{-i\tilde{K}(\theta)t} \tilde{Z}(\theta, 0) d\theta, \quad n \in \mathbb{Z}^3. \quad (4.2)$$

The weighted norms (1.14) are equivalent to the modified norms

$$\|Z\|_\alpha^2 := \sum_{n \in \mathbb{Z}^3} (1 + |n|)^{2\alpha} \|Z(n)\|_{\mathcal{X}^0(\Pi)}^2, \quad Z \in \mathcal{X}^0(\mathbb{R}^3), \quad (4.3)$$

where $Z(n)$ are defined by (2.1). Hence, the decay (4.1) for $Z^c(t)$ is equivalent to

$$\sum_{n \in \mathbb{Z}^3} (1 + |n|)^{2\alpha} \|Z^c(n, t)\|_{\mathcal{X}^0(\Pi)}^2 \rightarrow 0, \quad t \rightarrow \infty. \quad (4.4)$$

The spectral resolution (3.1) implies that

$$Z(n, t) = |\Pi^*|^{-1} \int_{\Pi^*} e^{-in\theta} \mathcal{M}(-\theta) \left[\sum_k e^{-i\omega_k(\theta)t} P_k(\theta) \right] \tilde{Z}(\theta, 0) d\theta, \quad n \in \mathbb{Z}^3. \quad (4.5)$$

Equivalently,

$$Z(n, t) = |\Pi^*|^{-1} \int_{\mathcal{R}} e^{-in\theta} \mathcal{M}(-\theta) e^{-i\omega t} P(\theta, \omega) \tilde{Z}(\theta, 0) d\theta, \quad n \in \mathbb{Z}^3, \quad (4.6)$$

where θ, ω and the projection $P(\theta, \omega)$ are the single-valued continuous functions (3.10) on \mathcal{R} . We denote by $d\theta$ is the corresponding differential form on \mathcal{R} . The integral is well defined by Lemma 3.3.

4.1. Discrete spectral component

We define the series of oscillating terms of (4.1) by its cell representation

$$\sum_k Z_k(n) e^{-i\omega_k^* t} = |\Pi^*|^{-1} \int_{\{(\theta, \omega) \in \mathcal{R} : \omega \in \Omega^*\}} e^{-in\theta} \mathcal{M}(-\theta) e^{-i\omega t} P(\theta, \omega) \tilde{Z}(\theta, 0) d\theta, \quad n \in \mathbb{Z}^3. \quad (4.7)$$

Now (1.20) follows from (3.2).

4.2. Continuous spectral component

It remains to prove the decay (4.1) for the remainder corresponding to the cell representation

$$Z^c(n, t) = |\Pi^*|^{-1} \int_{\mathcal{V}} e^{-in\theta} \mathcal{M}(-\theta) e^{-i\omega t} P(\theta, \omega) \tilde{Z}(\theta, 0) d\theta, \quad n \in \mathbb{Z}^3, \quad (4.8)$$

where the integration spreads over the set $\mathcal{V} := \{(\theta, \omega) \in \mathcal{R} : \omega \notin \Omega^*\}$. For every $\nu > 0$, we split $Z^c(t) = Z_-^\nu(t) + Z_+^\nu(t)$, where

$$Z_-^\nu(n, t) = |\Pi^*|^{-1} \int_{\mathcal{V}_-^\nu} e^{-in\theta} \mathcal{M}(-\theta) e^{-i\omega t} P(\theta, \omega) \tilde{Z}(\theta, 0) d\theta, \quad (4.9)$$

$$Z_+^\nu(n, t) = |\Pi^*|^{-1} \int_{\mathcal{V}_+^\nu} e^{-in\theta} \mathcal{M}(-\theta) e^{-i\omega t} P(\theta, \omega) \tilde{Z}(\theta, 0) d\theta. \quad (4.10)$$

Here $\mathcal{V}_-^\nu := \{(\theta, \omega) \in \mathcal{V} : |\omega| \leq \nu\}$ and $\mathcal{V}_+^\nu := \{(\theta, \omega) \in \mathcal{V} : |\omega| > \nu\}$.

High energy component. By (2.2) and the Parseval–Plancherel theorem

$$\|Z_+^\nu(t)\|_{\mathcal{X}^0(\mathbb{R}^3)}^2 = \sum_{n \in \mathbb{Z}^3} \|Z_+^\nu(n, t)\|_{\mathcal{X}^0(\Pi)}^2 = |\Pi^*|^{-1} \int_{\mathcal{V}_+^\nu} \|P(\theta, \omega) \tilde{Z}(\theta, 0)\|_{\mathcal{X}^0(\mathbb{T})}^2 d\theta. \quad (4.11)$$

According to definition (1.18) the condition $Y(0) \in \mathcal{W}$ means that $Z = \Lambda Y(0) \in \mathcal{X}^0(\mathbb{R}^3)$. Hence, the Parseval–Plancherel identity gives

$$\|Z(0)\|_{\mathcal{X}^0(\mathbb{R}^3)}^2 = |\Pi^*|^{-1} \int_{\Pi^*} \|\tilde{Z}(\theta, 0)\|_{\mathcal{X}^0(\mathbb{T})}^2 d\theta < \infty. \quad (4.12)$$

Therefore, (4.11) implies that

$$\|Z_+^\nu(t)\|_{\mathcal{X}^0(\mathbb{R}^3)} \rightarrow 0, \quad \nu \rightarrow \infty \quad (4.13)$$

uniformly in $t \in \mathbb{R}$ by the σ -additivity since $\cap_{\nu > 0} \mathcal{V}_+^\nu = \emptyset$.

Low energy component. It remains to prove the decay (4.1) for $Z_-^\nu(t)$ corresponding to the cell representation $Z_-^\nu(n, t)$. It suffices to check that every norm $\|Z_-^\nu(n, t)\|_{\mathcal{X}^0(\Pi)}$ decays to zero as $t \rightarrow \infty$, since $\alpha < -3/2$ and

$$\sum_{n \in \mathbb{Z}^3} \|Z_-^\nu(n, t)\|_{\mathcal{X}^0(\Pi)}^2 = \|Z_-^\nu(t)\|_{\mathcal{X}^0}^2 = \text{const}, \quad t \in \mathbb{R} \quad (4.14)$$

by (2.2) and formula of type (2.15) for $\tilde{Z}^\nu(\theta, t)$.

Reduction to a compact set and partition of unity. Consider an open precompact subset $Q \subset \Pi_+^*$ such that the Lebesgue measure of $\Pi_+^* \setminus Q$ is sufficiently small, and denote $\hat{Q}^\nu := \{R = (\theta, \omega) \in \mathcal{V}^\nu : \theta \in Q\}$. Then the $\mathcal{X}^0(\Pi)$ -norm of the integral of type (4.9) over $\mathcal{V}^\nu \setminus \hat{Q}^\nu$ is small uniformly in $t \in \mathbb{R}$ by (4.12). Hence, it remains to prove the decay for

$$Z_Q^\nu(n, t) := |\Pi^*|^{-1} \int_{\hat{Q}^\nu} e^{-in\theta} \mathcal{M}(-\theta) e^{-i\omega t} P(\theta, \omega) \tilde{Z}(\theta, 0) d\theta. \quad (4.15)$$

The asymptotics (3.2), which are uniform in $\theta \in Q$, imply that the set \hat{Q}^ν is open and precompact in \mathcal{R} . Neglecting an arbitrarily small term we can assume that Q does not intersect a small neighborhood of the critical submanifold $\mathcal{C}_j \subset V(\theta_j)$ for every j . Hence, we can cover \hat{Q}^ν by a finite number of neighborhoods $W(R_j)$ from Lemma 3.3 with $R_j = (\theta_j, \omega_j) \in \hat{Q}^\nu$. Then there exists a partition of unity $\chi_j \in C(\mathcal{R})$ with $\text{supp } \chi_j \subset W(R_j)$:

$$\sum_j \chi_j(R) = 1, \quad R = (\theta, \omega) \in \hat{Q}^\nu. \quad (4.16)$$

Hence, (4.15) becomes the finite sum

$$Z_{jl}^\nu(n, t) = \sum_{j,l} |\Pi^*|^{-1} \int_{W(R_j)} e^{-in\theta} \chi_j(\theta, \omega_{jl}(\theta)) \mathcal{M}(-\theta) e^{-i\omega_{jl}(\theta)t} P_{jl}(\theta) \tilde{Z}(\theta, 0) d\theta, \quad (4.17)$$

where the functions ω_{jl} and projections P_{jl} are constructed in Lemma 3.3. Note, that all constant dispersion relations (3.12) are excluded from the integration (4.17), and hence, the remaining nonconstant dispersion relations $\omega_{jl}(\theta)$ satisfy (3.11). Let us approximate

- i) $\chi_j(\theta, \omega_{jl}(\theta))$ by $\chi_{jl}(\cdot) \in C_0^\infty(W(R_j))$ and
- ii) $P_{jl}(\theta) \tilde{Z}(\theta, 0)$ by some functions $D_{jl}(\theta) \in C^\infty(W(R_j), \mathcal{X}^0(\mathbb{T}))$ in the norm of $L^2(Q, \mathcal{X}^0(\mathbb{T}))$.

Then the corresponding error in (4.17) is small in the norm $\mathcal{X}^0(\Pi)$ uniformly in $n \in \mathbb{Z}^3$ and $t \in \mathbb{R}$. Finally, (3.11) implies by a partial integration the decay of the integrals (4.17) with $\mu_{jl}(\theta)D_{jl}(\theta)$ instead of $\chi_j(\theta, \omega_{jl}(\theta))P_{jl}(\theta)\tilde{Z}(\theta, 0)$. ■

5. Spectral properties of the selfadjoint generator

Here we study spectral properties of the operator $K := \mathcal{F}^{-1}\tilde{K}\mathcal{F}$, where \tilde{K} denotes the operator of multiplication by $\tilde{K}(\theta)$ in the Hilbert space $L^2(\Pi^*, \mathcal{X}^0(\mathbb{T}))$.

Lemma 5.1. *K is a selfadjoint operator in $\mathcal{X}^0(\mathbb{R}^3)$ with a dense domain $D(K)$.*

Proof. Lemma 2.7 ii) implies that the operator \tilde{K}^{-1} of multiplication by $\tilde{K}^{-1}(\theta)$ is selfadjoint and injective in $L^2(\Pi^*, \mathcal{X}^0(\mathbb{T}))$. Hence, its inverse $\tilde{K}(\theta)$ is densely defined selfadjoint operator in $L^2(\Pi^*, \mathcal{X}^0(\mathbb{T}))$ by Theorem 13.11 (b) of [42]. □

Corollary 5.2. *The Hamilton generator A from (1.11) admits the representation*

$$AY = -i\Lambda^{-1}K\Lambda Y, \quad Y \in \Lambda^{-1}D(K), \quad (5.1)$$

where $\Lambda := \mathcal{F}^{-1}\tilde{\Lambda}(\theta) : \mathcal{W} \rightarrow \mathcal{X}^0(\mathbb{R}^3)$ is the isomorphism.

By (3.1),

$$KZ(n) = |\Pi^*|^{-1} \int_{\Pi_+^*} e^{-in\theta} \mathcal{M}(-\theta) \sum_k \omega_k(\theta) P_k(\theta) \tilde{Z}(\theta) d\theta, \quad n \in \mathbb{Z}^3 \quad (5.2)$$

for any $Z \in \mathcal{X}^0(\mathbb{R}^3)$. Similarly

$$Z(n) = |\Pi^*|^{-1} \int_{\Pi_+^*} e^{-in\theta} \mathcal{M}(-\theta) \sum_k P_k(\theta) \tilde{Z}(\theta) d\theta, \quad n \in \mathbb{Z}^3. \quad (5.3)$$

Therefore,

$$(K - \omega)Z(n) = |\Pi^*|^{-1} \int_{\Pi_+^*} e^{-in\theta} \mathcal{M}(-\theta) \sum_k (\omega_k(\theta) - \omega) P_k(\theta) \tilde{Z}(\theta) d\theta. \quad (5.4)$$

Hence, the discrete spectrum $\sigma_p(K)$ consists of constant dispersion relations.

Lemma 5.3. *Let all conditions of Theorem 1.1 hold. Then*

- i) $\sigma_p(K) = \Omega^*$.
- ii) *The multiplicity of every eigenvalue is infinite.*

Proof. Let $\omega^* \in \Omega^*$ is a constant eigenvalue (3.12) corresponding to a point $R^* = (\theta^*, \omega^*) \in \mathcal{R}$. Let us take any $Z \in \mathcal{X}^0(\mathbb{R}^3)$ with the Bloch transform $\tilde{Z}(\theta) \in \text{Ran } P(\omega^*)$ for $\theta \in V(\theta^*)$ and $\tilde{Z}(\theta) \equiv 0$ for $\theta \notin V(\theta^*)$. Then (3.12) and (5.4) imply that $(K - \omega^*)Z = 0$. Obviously, the space of such Z is infinite dimensional.

Conversely, let $(K - \omega^*)Z = 0$ for some $Z \in \mathcal{X}^0(\mathbb{R}^3)$, and $\tilde{Z}(\theta^*) \neq 0$. Then (5.4) implies (3.12) with some $l = 1, \dots, L(\theta^*, \omega^*)$. □

Let us show that the continuous spectrum of K is absolutely continuous. First, (5.4) implies that the resolvent $R_K(\omega) := (K - \omega)^{-1}$ for $\text{Im } \omega \neq 0$ is given by

$$R_K(\omega)Z(n) = |\Pi^*|^{-1} \int_{\Pi_+^*} e^{-in\theta} \mathcal{M}(-\theta) \sum_k (\omega_k(\theta) - \omega)^{-1} P_k(\theta) \tilde{Z}(\theta) d\theta, \quad Z \in \mathcal{X}^0(\mathbb{R}^3). \quad (5.5)$$

Denote by \mathcal{X}_d the space of discrete spectrum of K .

Lemma 5.4. *Let all conditions of Theorem 1.1 hold. Then the singular spectrum of K is empty.*

Proof. This follows by Theorem XIII.20 of [41]. Namely, it suffices to check the corresponding criterion

$$\sup_{0 < \varepsilon < 1} \int_a^b |\text{Im} \langle Z, R_K(\omega + i\varepsilon)Z \rangle|^p d\omega < \infty \quad (5.6)$$

with any $a, b \in \mathbb{R}$ and some $p > 1$ for a dense set of $Z \in \mathcal{X}_d^\perp$. For example, for the linear span of vectors $Z \in \mathcal{X}^0(\mathbb{R}^3)$ with the Bloch transform

$$\tilde{Z}(\theta) = P_l(\theta)D(\theta), \quad D \in C_0^\infty(W, \mathcal{X}^0(\mathbb{T})), \quad (5.7)$$

as constructed in Lemma 3.3 for each $R^* = (\theta^*, \omega^*) \in \mathcal{R}$, where $P_l(\theta)$ is the projection corresponding to an eigenvalue $\omega_l(\theta)$ satisfying (3.11). It suffices to check (5.6) only for the vectors of type (5.7). Applying Sokhotski–Plemelj’s formula, we obtain for these vectors

$$\begin{aligned} \text{Im} \langle Z, R_K(\omega + i\varepsilon)Z \rangle &= \int_W \text{Im} \langle P_l(\theta)D(\theta), (\omega - \omega_l(\theta) - i\varepsilon)^{-1} P_l(\theta)D(\theta) \rangle_{\mathcal{X}(\mathbb{T})} d\theta \\ &\rightarrow -\pi \int_{\omega_l(\theta)=\omega} \frac{\langle P_l(\theta)D(\theta), P_l(\theta)D(\theta) \rangle_{\mathcal{X}(\mathbb{T})}}{|\nabla \omega_l(\theta)|} d\theta, \quad \varepsilon \rightarrow 0+, \end{aligned} \quad (5.8)$$

which implies (5.6) with any $p \geq 1$. \square

In conclusion, let us prove the Limiting Absorption Principle. Let us denote by \mathcal{X}_α the Hilbert space of functions with the finite norm (4.3).

Lemma 5.5. *Let all conditions of Theorem 1.1 hold, and let $Z \in \mathcal{X}_d^\perp$ be a finite linear combination of the vectors with the Bloch transform of type (5.7). Then for any $\omega \in \mathbb{R}$ and $\alpha < -7/2$*

$$R_K(\omega \pm i\varepsilon)Z \xrightarrow{\mathcal{X}_\alpha} R_K(\omega \pm i0)Z, \quad \varepsilon \rightarrow +0. \quad (5.9)$$

Proof. It suffices to prove (5.9) for every vector of type (5.7). By (4.5) the corresponding solution $Z(t)$ with $Z(0) = Z$ reads

$$Z(n, t) = |\Pi^*|^{-1} \int_W e^{-in\theta} \mathcal{M}(-\theta) e^{-i\omega_l(\theta)t} P_l(\theta) \tilde{Z}(\theta) d\theta, \quad n \in \mathbb{Z}^3$$

The partial integration shows the time-decay

$$\|Z(n, t)\|_{\mathcal{X}^0(\Pi)} \leq C(1 + |n|)^2(1 + |t|)^{-2}.$$

Hence,

$$\|Z(t)\|_{\mathcal{X}_\alpha} \leq C(1 + |t|)^{-2}.$$

Now the convergence (5.9) follows from the integral representation

$$R_K(\omega \pm i\varepsilon)Z = \int_0^{\pm\infty} e^{(i\omega \mp \varepsilon)t} Z(t) dt. \quad \square$$

Appendix A. Matrix entries of the Bloch generators

Let us recall some notations from [25]. For $f \in C_0^\infty(\mathbb{R}^3)$ the Fourier transform is defined by

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

For the real ground state (1.10) the generator A of the linearized dynamics is given by (1.11), where S denotes the operator with the ‘matrix’

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

by formula (3.3) of [25] and T is the real matrix with entries

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

by formula (3.4) of [25]. The operators $G\psi^0 : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$ and $S : l^2 := l^2(\mathbb{Z}^3) \otimes \mathbb{C}^3 \rightarrow L^2(\mathbb{R}^3)$ are not bounded due to the ‘infrared divergence’ at $\xi = 0$. On the other hand, the operator T is bounded in $l^2(\mathbb{Z}^3) \otimes \mathbb{C}^3$ by Lemma 3.1 of [25]. In the Bloch representation all these operators are given by

$$\tilde{S}(\theta) = e\psi^0 \tilde{G}(\theta)(\nabla - i\theta)\tilde{\sigma}(\theta, \cdot), \quad \tilde{G}(\theta) = (i\nabla + \theta)^{-2}, \quad (\text{A.2})$$

$$\tilde{H}^0(\theta) = \frac{1}{2}(i\nabla + \theta)^2 - e\Phi^0 - \omega^0, \quad \tilde{T}(\theta) = \tilde{T}_1(\theta) + \tilde{T}_2 + \mathcal{O}(e^4) \text{ as } e \rightarrow 0, \quad (\text{A.3})$$

$$\tilde{T}_1(\theta) = \sum_m \left[\frac{\xi \otimes \xi}{|\xi|^2} |\tilde{\sigma}(\xi)|^2 \right]_{\xi=2\pi m - \theta}, \quad \tilde{T}_2 = - \sum_{m \neq 0} \left[\frac{\xi \otimes \xi}{|\xi|^2} |\tilde{\sigma}(\xi)|^2 \right]_{\xi=2\pi m}, \quad (\text{A.4})$$

in accordance with the formulas (6.22)–(6.24), and (10.4), (10.12) of [25].

Remarks A.1.

- i) $\tilde{T}_2 = 0$ under the Jellium condition (1.16).
- ii) The operators $\tilde{G}(\theta) : L^2(\mathbb{T}) \rightarrow H^2(\mathbb{T})$ are bounded for $\theta \in \Pi^* \setminus \Gamma^*$; however $\|\tilde{G}(\theta)\| \sim d^{-2}(\theta)$, where $d(\theta) := \text{dist}(\theta, \Gamma^*)$.

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