On stability of crystals in the Schrödinger - Poisson model

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Abstract

We consider 1D, 2D and 3D crystals in $\mathbb{R}^3$ with N ions per cell. The electron field is coupled to the ions via the Schrödinger - Poisson - Newton equations. Our main results are

i) the existence of ground state (GS) for 1D, 2D and 3D cases and

ii) linear and nonlinear stability of the ground state for 3D case.

The stability of the GS for 1D case ("carbon nanotube") and 2D case ("graphene") is an open problem.

[1] A.I. Komech, On the crystal ground state in the Schrödinger - Poisson model, *SIAM J. Math. Anal* **47** (2015), no.2, 1001-2021. arXiv:1310.3084

[2] A. Komech, E. Kopylova, On linear stability and dispersion for crystals in the Schrödinger - Poisson model, arXiv:1505.07074

Plan:

I. The existence of ground state (GS)

II. Linearization of Schrödinger-Poisson-Newton Eqns at the GS

III. Positivity of "linearized" energy

IV. Linear stability

V. Dispersion decay

VI. Positivity of renormalized energy

VII. Nonlinear stability: low energy weak solutions

d-dimesional lattice in R^3:$d = 1, 2, 3$ and $\mathbf{a}_k \in \mathbb{R}^3$

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

Elementary cell $T_d := \mathbb{R}^3/\Gamma_d$:
$d = 3$: T_d is 3D torus
$d = 2$: T_d is the direct product of 2D torus by $\mathbb{R}$
$d = 1$: T_d is the direct product of 1D torus (circle) by $\mathbb{R}^2$

The Schrödinger-Poisson-Newton equations for crystal:

$$(SPN) \begin{cases} i\hbar\dot{\psi}(x,t) = -\frac{\hbar^2}{2\mathrm{m}}\Delta\psi(x,t) - e\Phi(x,t)\psi(x,t), \qquad x \in \mathbb{R}^3 \\ -\Delta\Phi(x,t) = \sum_{j=1}^{N} \sum_{n\in\mathbb{Z}^d} \sigma_j(x - \gamma(n) - x_j(n,t)) - e|\psi(x,t)|^2 \\ M_j\ddot{x}_j(n,t) = -\langle\nabla\Phi(x,t), \sigma_j(x - \gamma(n) - x_j(n,t))\rangle, n \in \mathbb{Z}^d, \forall j \end{cases}$$

$e > 0$ is the elementary charge, m is the electron mass,

Physical motivation

Dynamical theory of crystals is indispensable for theoretical decription of heat and electric conductivity, thermoelectronic emission, photoelectric effect, Compton effect. etc.
In particular, a rigorous theory of the Fourier law and Ohm law for metals are missing up to now.

Ground state: Γ_d-periodic stationary solution $\psi^0(x)e^{-i\omega^0 t}$, $\Phi^0(x)$, $x_j^0(n) = x_j^0$, $n \in \mathbb{Z}^n$, $j = 1, ..., N$

$$\begin{cases} \hbar\omega^0\psi(x) = -\frac{\hbar^2}{2\mathrm{m}}\Delta\psi^0(x) - e\Phi^0(x)\psi^0(x), \qquad x \in T_d := \mathbb{R}^3/\Gamma_d \\ -\Delta\Phi^0(x) = \rho^0(x) := \sum_{j=1}^N \sum_{n\in\mathbb{Z}^d} \sigma_j(x - \gamma(n) - x_j^0) - e|\psi^0(x)|^2 \\ 0 = -\langle\nabla\Phi^0(x), \sigma_j(x - \gamma(n) - x_j^0)\rangle, n \in \mathbb{Z}^d, \forall j \end{cases}$$

Neutrality condition: $\displaystyle\int_{T_d} \rho^0(x)dx = 0.$ Equivalently,

$$\psi^0 \in \mathcal{M} := \{\psi^0 \in L^2(T_d) : \|\psi^0(x)\|^2_{L^2(T_d)} = Z\}, \quad Z := \sum_1^N Z_j > 0,$$

where $Z_j := \displaystyle\int_{\mathbb{R}^3} \sigma_j(x)dx/e.$

Condition (σ): $\sigma_j^{\rm per}(x):=\sum_n \sigma_j(x-\gamma(n))\in L^1(T_d)\cap L^2(T_d), \forall j$

Theorem 1. Let $d=3$ and (σ) hold. Then there exists a ground state with $\psi^0, \Phi^0 \in H^2(T_3)$ and $\omega^0 \in \mathbb{R}$.

For $d=2$ the lattice Γ_2 lies in the plan $x_3=0$

Theorem 2. Let $d=2$, $N=1$ and (σ) hold $+$ .... Then there exists a ground state with $\psi^0 \in H^1(T_2)\cap H^2_{\rm loc}(T_2)$, $\Phi^0 \in H^2_{\rm loc}(T_2)$ and $\omega^0 \in \mathbb{R}$. The bound holds $|\Phi^0(x)| \le C(1+|x_3|)^{1/2}$.

For $d=1$ the lattice Γ_1 lies on the line $x_2=x_3=0$

Theorem 3. Let $d=1$, $N=1$ and (σ) hold $+$ .... Then there exists a ground state with $\psi^0 \in H^1(T_1)\cap H^2_{\rm loc}(T_1)$, $\Phi^0 \in H^2_{\rm loc}(T_1)$ and $\omega^0 \in \mathbb{R}$. The bound holds $|\Phi^0(x)| \le C(1+|x_2|+|x_3|)^{1/2}$.

Proofs: minimization of *energy per cell* $E(\psi, \overline{x})$ over $(\psi, \overline{x}) \in \mathcal{M} \times T_d^N$, $\overline{x} := (x_1, ..., x_N)$:

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

$$E(\psi,\overline{x}) := \int_{T_d} \Big[\frac{\hbar^2}{2\mathrm{m}}|\nabla\psi(x)|^2 + \frac{1}{2}|\Lambda\rho(x)|^2\Big] d\mathbf{x}, \qquad \Lambda\rho := (-\Delta)^{-1/2}\rho$$

$$\int_{T_d} \rho(x) dx = 0$$

Linearization of Eqns (SPN) at the ground state

Substitute into the nonlinear equations (SPN)

$$\psi(x,t)=[\psi^0(x)+\Psi(x,t)]e^{-i\omega^0 t},\;\; x_j(n,t)=\gamma(n)+x_j^0+X_j(n,t)$$

The linearized equation reads

$$(L)\quad \dot{Y}(t)=AY(t),\qquad A=JB,\qquad J^*=-J,\qquad B^*=B$$

where $Y(t)=(\Psi_1(x,t),\Psi_2(x,t),X(t),P(t))$

$$\Psi_1(x,t):=\mathrm{Re}\,\Psi(x,t),\quad \Psi_2(x,t):=\mathrm{Im}\,\Psi(x,t)$$

$$X(t):=(X_j(n,t):j\!=\!1,...,N,\;\; n\in\mathbb{Z}^3)$$

$$P(t):=(P_j(n,t):j\!=\!1,...,N,\;\; n\in\mathbb{Z}^3)$$

$A^*\neq A$!!

Wiener condition and energy positivity

Energy positivity (EPL) $\langle Y, BY\rangle \geq \varkappa \|Y\|^2_{\mathcal{V}}, \quad Y \in \mathcal{V}, \qquad \varkappa > 0$

$\mathcal{V} := H^1(\mathbb{R}^3) \oplus H^1(\mathbb{R}^3) \oplus l^2_{3N} \oplus l^2_{3N}, \qquad l^2_{3N} := l^2(\mathbb{Z}^3) \otimes \mathbb{R}^{3N}$

Consider $\sigma_j(x) = e\mu_j(x), \qquad j = 1, ..., N$, and denote

$$\Sigma_j := \sum_{m\neq 0}[\sum_{j'} e^{ix^0_j \xi}\tilde{\mu}_j(\xi)\frac{\xi\otimes\xi}{|\xi|^2}\overline{\tilde{\mu}_{j'}(\xi)e^{ix^0_{j'}\xi}}]|_{\xi=\gamma^*(m)}$$

Wiener condition (W) : $\quad \Sigma_j > 0, \qquad j = 1, ..., N$

Remarks i) $\Sigma_1 \geq 0$ for $N = 1$.
ii) (W) holds for $N = 1$ if $\tilde{\mu}_1(\xi) \neq 0$ for $\xi \in \mathbb{R}^3$:
in particular, for Gaussian $\mu_1(x) = Ce^{-\alpha|x|^2}$

Energy positivity for small elementary charge

$(\mu) \quad (-\Delta + \langle x\rangle^2)\mu_j \in L^2(\mathbb{R}^3); \quad \partial^\alpha \mu_j \in L^1(\mathbb{R}^3), \quad |\alpha| \le 5$

Theorem 4*. Let (W), (σ) and (μ) hold. Then the positivity (EP) holds for $\sigma_j(x) = e\mu_j(x)$ with sufficiently small $e > 0$.

Corollary 1. The generator $A = JB$ admits a spectral resolution for sufficiently small $e > 0$.

Proof (M.G.Krein) Denote $\Lambda := B^{1/2} > 0$. Then $A = JB = J\Lambda^2$, and hence $A = -i\Lambda^{-1}K\Lambda$ where $K := \Lambda iJB\Lambda$ is selfadjoint.

Corollary 2. i) Solutions to the linearized equation (L) with small $e > 0$ read

$$(Y) \qquad Y(t) = \Lambda^{-1}e^{-iKt}\Lambda Y(0)$$

ii) The energy is conserved:

$$\|Y(t)\|_{\mathcal{W}} := \langle Y(t), BY(t)\rangle = \text{const}$$

Proof of (*EPL*): small charge asymptotics of GS

Theorem 5. Let (σ) hold and $\sigma_j(x) = e\mu_j(x)$.

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

$$\omega_e^0 = \mathcal{O}(e^2)$$

$$\psi_e^0(x) = C_e + \chi_e(x), \quad |C_e|^2 = \frac{Z}{|T_3|} + \mathcal{O}(e^2), \quad \|\chi_e\|_{H^2(T^3)} = \mathcal{O}(e^2)$$

Dispersion decay

Weighted Sobolev norms: $Y = (\Psi_1(x), \Psi_2(x), X(n), P(n)) \in \mathcal{V}_s$

$$\|Y\|_s := \quad \|\langle x\rangle^s \Psi_1(x)\|_{H^1(\mathbb{R}^3)} + \|\langle x\rangle^s \Psi_2(x)\|_{H^1(\mathbb{R}^3)}$$

$$+\|\langle n\rangle^s X(n)\|_{l^2_{3N}} + \|\langle n\rangle^s P(n)\|_{l^2_{3N}} < \infty$$

Theorem 6. Let $Y(0) \in \mathcal{V}_0$. Then for $\sigma_j(x) = e\mu_j(x)$ with sufficiently small $e > 0$

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

$$\|Y_c(t)\|_{\mathcal{V}_{-\alpha}} \to 0, \qquad |t| \to \infty, \quad \alpha > 3/2.$$

Proof Oscillatory integral representation of formula (Y) in the Bloch transform.

Definition: renormalized energy

$$\mathcal{H}_r(Y) := \mathcal{H}(\psi^0 + \Psi, \overline{x}^0 + X, P) - \mathcal{H}(\psi^0, \overline{x}^0), \qquad Y = (\Psi, X, P)$$

Theorem 7. Let conditions (W), (σ) and (μ) hold. Then for the charge densities $\sigma_j(x) = e\mu_j(x)$ with small $e > 0$

$$(EPNL) \qquad \mathcal{H}_r(Y) \geq \nu(e)\|Y\|^2_{\mathcal{W}}, \qquad \|Y\|_{\mathcal{W}} \leq \varepsilon(e),$$

where $\nu(e) > 0$ and $\varepsilon(e) > 0$.

Theorem 8*. Let conditions (W), (σ) and (μ) hold. Then the system (SPN) admits a global weak solution

$Y(t) \in C_b(\mathbb{R}, \mathcal{W})$ for initial state with $\|Y(0)\|_{\mathcal{W}} \leq \varepsilon(e)$.

Remark: The uniqueness is not proved yet!

THANK YOU!