Derivation of the Transport Equation for the Harmonic Crystal coupled to a Klein–Gordon Field

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International Conference

Mathematical Physics, Dynamical Systems and Infinite-Dimensional Analysis

dedicated to the 100th anniversary of V.S. Vladimirov, the 100th anniversary of L.D. Kudryavtsev and the 85th anniversary of O.G. Smolyanov

July 5–13, 2023, online, Dolgoprudny, Moscow Region, Russia

Problem I: Convergence to equilibrium distribution

Consider a dynamical system:

$$\dot{Y}(t) = \mathcal{A}(Y(t)), \quad t \in \mathbb{R}; \quad Y(0) = Y_0.$$

Initial data $Y_0 \in \mathcal{E}$ (phase space)

$$W(t) : Y_0 \to Y(t), \quad t \in \mathbb{R}.$$

Let μ_0 be a Borel probability measure on $\mathcal{E}$.

Def. μ_t, $t \in \mathbb{R}$, is the distribution of $Y(t)$, $\mu_t(B) = \mu_0(W^{-1}(t)B)$, $B \in \mathcal{B}(\mathcal{E})$.

The objective is to prove *the weak convergence of measures μ_t* in the space $\mathcal{E}$ to a limiting measure μ_∞ as $t \to \infty$.

By definition, this means that $\displaystyle\int_{\mathcal{E}} f(Y)\,\mu_t(dY) \to \int_{\mathcal{E}} f(Y)\,\mu_\infty(dY)$ as $t \to \infty$

for any continuous bounded functional f in $\mathcal{E}$.

The model

Hamiltonian: $H(\varphi, \pi, u, v) = H_F(\varphi, \pi) + H_L(u, v) + H_I(\varphi, u)$, where

$$H_F(\varphi, \pi) := \frac{1}{2} \int\limits_{\mathbb{R}^d} \left(|\nabla \varphi(x)|^2 + |\pi(x)|^2 + m_0^2 |\varphi(x)|^2 \right) \, dx,$$

$$H_L(u, v) = \sum_{k \in \mathbb{Z}^d} \Big(\sum_{k' \in \mathbb{Z}^d} u(k) \cdot V(k - k') u(k') + |v(k)|^2 \Big),$$

$$H_I(\varphi, u) := \sum_{k \in \mathbb{Z}^d} \int\limits_{\mathbb{R}^d} R(x - k) \cdot u(k) \varphi(x) \, dx.$$

Here $m_0 > 0$, $\varphi(\cdot) \in \mathbb{R}$, $u(\cdot), v(\cdot) \in \mathbb{R}^n$, $R(\cdot) \in \mathbb{R}^n$, $V(k) \in \mathbb{R}^n \times \mathbb{R}^n$, $d, n \geq 1$.

The given system can be considered as the description of the motion of electrons (so-called *Bloch electrons*) in the periodic medium which is generated by the ionic cores, i.e., $\varphi(x, t)$ describes the motion of electron field, $u(k, t)$ is the (small) displacements of the ionic cores from their equilibrium positions.
Understanding of this motion is one of the central problem of solid state physics.

Cauchy problem

$$\left\{\begin{array}{rcl}\dot\varphi(x,t) &=& \pi(x,t), \qquad x\in\mathbb{R}^d, \qquad t\in\mathbb{R},\\ \dot\pi(x,t) &=& (\Delta-m_0^2)\varphi(x,t)-\sum\limits_{k'\in\mathbb{Z}^d} u(k',t)\cdot R(x-k'),\\ \dot u(k,t) &=& v(k,t), \qquad k\in\mathbb{Z}^d,\\ \dot v(k,t) &=& -\sum\limits_{k'\in\mathbb{Z}^d} V(k-k')u(k',t)-\int_{\mathbb{R}^d} R(x'-k)\varphi(x',t)\,dx'.\end{array}\right. \tag{1}$$

Initial Data: $$\left\{\begin{array}{rclrcll}\varphi(x,0) &=& \varphi_0(x), & \pi(x,0) &=& \pi_0(x), & x\in\mathbb{R}^d,\\ u(k,0) &=& u_0(k), & v(k,0) &=& v_0(k), & k\in\mathbb{Z}^d.\end{array}\right. \tag{2}$$

Def. $\widetilde V(\theta):=F_{k\to\theta}[V(k)]=\sum\limits_{k\in\mathbb{Z}^d} e^{ik\cdot\theta}V(k), \quad \theta\in\mathbb{T}^d\equiv\mathbb{R}^d/(2\pi\mathbb{Z})^d$ (d-torus)

Conditions on the interaction matrix $V\in\mathbb{R}^n\times\mathbb{R}^n$:

V1 $\exists C,\gamma>0:\ \|V(k)\|\le Ce^{-\gamma|k|}$
V2 $V^T(-k)=V(k), \quad k\in\mathbb{Z}^d$
$\Longrightarrow$ $\widetilde V(\theta)=\widetilde V^*(\theta)$ is real-analytic matrix-valued function $\theta\in\mathbb{T}^d$

V3 $\widetilde V(\theta)>0 \quad \forall\,\theta\in\mathbb{T}^d$, i.e., $\exists\,\nu_0>0:\ \overline{u}\cdot\widetilde V(\theta)u\ge\nu_0^2|u|^2, \quad u\in\mathbb{C}^n$.

Notation: $Y_0 = (\varphi_0, u_0, \pi_0, v_0)$, $Y(t) = (Y^0(t), Y^1(t))$, where

$$Y^0(t) \equiv Y^0(\cdot, t) := (\varphi(x,t), u(k,t)), \quad Y^1(t) = \dot{Y}^0(t) = (\pi(x,t), v(k,t)).$$

In other words, $Y(\cdot, t)$, $Y^j(\cdot, t)$ are functions defined on the disjoint union $\mathbb{P}^d := \mathbb{R}^d \bigsqcup \mathbb{Z}^d$, for example, $Y^0(t) \equiv Y^0(p,t) = \begin{cases} \varphi(x,t), & p = x \in \mathbb{R}^d, \\ u(k,t), & p = k \in \mathbb{Z}^d. \end{cases}$

Then, the Cauchy problem (1)–(2) has a form

$$\dot{Y}(t) = \mathcal{A}(Y(t)), \quad t \in \mathbb{R}; \quad Y(0) = Y_0. \tag{3}$$

$$\mathcal{A} = \begin{pmatrix} 0 & \mathrm{I} \\ -\mathcal{H} & 0 \end{pmatrix}, \ \mathcal{H} = \begin{pmatrix} -\Delta + m_0^2 & S \\ S^* & \mathcal{V} \end{pmatrix}, \ \mathcal{V}u := \sum_{k' \in \mathbb{Z}^d} V(k-k')u(k'),$$

$$(Su)(x) = \sum_{k \in \mathbb{Z}^d} R(x-k)u(k), \quad (S^*\varphi)(k) = \int_{\mathbb{R}^d} R(x-k)\varphi(x)dx,$$

$$\langle \varphi, Su \rangle_{L^2(\mathbb{R}^d)} = \langle S^*\varphi, u \rangle_{[\ell^2(\mathbb{Z}^d)]^n}, \quad \varphi \in L^2(\mathbb{R}^d), \ u \in [\ell^2(\mathbb{Z}^d)]^n.$$

Note that **the dynamics of problem (3) is invariant w.r.t. shifts in $\mathbb{Z}^d$**.

Bloch–Floquet–Zak transform (= Zak transform): $\varphi(x)$ $(x \in \mathbb{R}^d) \to \widetilde{\varphi}_e(\theta, y)$ $(\theta \in [-\pi, \pi]^d,\ \ y \in \mathbb{T}_1^d)$

Split $x \in \mathbb{R}^d$ as $x = k + y$, $k = [x] \in \mathbb{Z}^d$, $y \in [0,1]^d$, and apply *the discrete Fourier transform* $k \to \theta$: $\widetilde{\varphi}(\theta, y) = \sum\limits_{k \in \mathbb{Z}^d} e^{ik\cdot\theta}\varphi(k+y)$

Def. *The Zak transform of a function* $\varphi(x)$ *is* $\mathcal{Z}(\varphi) \equiv \widetilde{\varphi}_e(\theta, y) := e^{iy\cdot\theta}\widetilde{\varphi}(\theta, y)$. ($\widetilde{\varphi}_e(\theta, y)$ *is periodic in* $y \in \mathbb{T}_1^d \equiv \mathbb{R}^d/\mathbb{Z}^d$ *and quasi-periodic in* θ*).*

Apply the Zak transform to solutions $Y(t)$:

$$\mathcal{Z} : Y(\cdot, t) \to \widetilde{Y}_e(\theta, t) \equiv \widetilde{Y}_e(\theta, y, t) = (\widetilde{\varphi}_e(\theta, y, t), \widetilde{u}(\theta, t), \widetilde{\pi}_e(\theta, y, t), \widetilde{v}(\theta, t)).$$

Then, the Cauchy problem (3) is reduced to the *Bloch problem on the torus* ($y \in \mathbb{T}_1^d$) with the parameter θ (so-called *Bloch momentum*), $\theta \in [-\pi, \pi]^d$:

$$\left\{ \begin{array}{l} \dot{\widetilde{Y}}_e(\theta, t) = \widetilde{\mathcal{A}}(\theta)(\widetilde{Y}_e(\theta, t)), \ \ t \in \mathbb{R}, \\ \widetilde{Y}_e(\theta, 0) = \widetilde{Y}_{0,e}(\theta), \end{array} \right. \qquad \widetilde{\mathcal{A}}(\theta) = \begin{pmatrix} 0 & 1 \\ -\widetilde{\mathcal{H}}(\theta) & 0 \end{pmatrix},$$

where $\widetilde{\mathcal{H}}(\theta)$ is a self-adjoint operator in $L^2(\mathbb{T}_1^d) \otimes \mathbb{C}^n$ with the discrete positive spectrum, since we assume that $\widetilde{\mathcal{H}}(\theta) > 0$ for $\theta \in [-\pi, \pi]^d$.

$$\widetilde{\mathcal{H}}(\theta) = \mathcal{Z}\mathcal{H}\mathcal{Z}^{-1} = \begin{pmatrix} (i\nabla_y + \theta)^2 + m_0^2 & \widetilde{S}(\theta) \\ \widetilde{S}^*(\theta) & \widetilde{V}(\theta) \end{pmatrix}, \text{ where } \mathcal{Z} \text{ is the Zak transform,}$$

$$(\widetilde{S}(\theta)\widetilde{u}) = \widetilde{R}_e(\theta, y) \cdot \widetilde{u}(\theta), \quad (\widetilde{S}^*(\theta)\widetilde{\psi}_e(\theta, \cdot)) = \int_{\mathbb{T}_1^d} \overline{\widetilde{R}_e(\theta, y)}\, \widetilde{\psi}_e(\theta, y)\, dy.$$

Conditions on the coupling function $R(\cdot) \in \mathbb{R}^n$:

(R1) $R \in C^\infty(\mathbb{R}^d)$, $\quad |R(x)| \le \bar{R}\exp(-\gamma|x|)$ with some $\gamma > 0$ and $\bar{R} < \infty$.

(R2) (*hyperbolicity of the problem*) The operator $\widetilde{\mathcal{H}}(\theta) > 0$ for $\theta \in [-\pi, \pi]^d$.

This is equivalent to the uniform bound

$$\left(\widetilde{Y}_e^0, \widetilde{\mathcal{H}}(\theta)\widetilde{Y}_e^0\right) \ge \kappa^2 \left\|\widetilde{Y}_e^0\right\|^2_{H^1(\mathbb{T}_1^d)\oplus\mathbb{C}^n} \quad \text{for} \quad \widetilde{Y}_e^0 \equiv (\widetilde{\varphi}_e(y), \widetilde{u}) \in H^1(\mathbb{T}_1^d) \oplus \mathbb{C}^n,$$

where a constant $\kappa > 0$, $\quad (\cdot, \cdot)$ stands for the scalar product in $H^0(\mathbb{T}_1^d) \oplus \mathbb{C}^n$.

Condition (R2) holds for functions R satisfying condition (R1) with $\bar{R}\gamma^{-d} \ll 1$.

Phase space

- The weighted Sobolev spaces $H^s_\alpha(\mathbb{R}^d)$: $\|\varphi\|_{s,\alpha} \equiv \|\langle x\rangle^\alpha \Lambda^s \varphi\|_{L^2(\mathbb{R}^d)} < \infty$, $\langle x\rangle := \sqrt{|x|^2+1}$, $s,\alpha\in\mathbb{R}$.

  Here $\Lambda^s\varphi := F^{-1}_{\xi\to x}(\langle\xi\rangle^s\widehat{\varphi}(\xi))$, $\quad \widehat{\varphi}(\xi) := \int_{\mathbb{R}^d} e^{i\,x\cdot\xi}\varphi(x)\,dx$

- $\ell^2_\alpha = \left\{ u(k)\in\mathbb{R}^n:\ \|u\|^2_\alpha \equiv \sum\limits_{k\in\mathbb{Z}^d}\langle k\rangle^{2\alpha}|u(k)|^2 < \infty \right\}$, $\alpha\in\mathbb{R}$.

- $Y = (\varphi, u, \pi, v) \in \mathcal{E}^s_\alpha \equiv H^{1+s}_\alpha(\mathbb{R}^d)\oplus\ell^2_\alpha\oplus H^s_\alpha(\mathbb{R}^d)\oplus\ell^2_\alpha$ with finite norm $\|Y\|^2_{s,\alpha} = \|\varphi\|^2_{1+s,\alpha} + \|u\|^2_\alpha + \|\pi\|^2_{s,\alpha} + \|v\|^2_\alpha < \infty$.

Def. $Y_0 = (\varphi_0, u_0, \pi_0, v_0)\in\mathcal{E}\equiv\mathcal{E}^0_\alpha$ with $\alpha < -d/2$.

Lemma. *For any $Y_0\in\mathcal{E}$ there exists a unique solution $Y(t) = W(t)Y_0 \in C(\mathbb{R},\mathcal{E})$ to the Cauchy problem (3). Moreover,* $\sup\limits_{|t|\le T}\|W(t)Y_0\|_{0,\alpha} \le C(T)\|Y_0\|_{0,\alpha}$.

Assume that the initial data $Y_0 = (Y_0^0, Y_0^1)$, $Y_0^0 \equiv (\varphi_0, u_0)$, $Y_0^1 \equiv (\pi_0, v_0)$ is a random measurable function with values in $\mathcal{E}$, μ_0 denotes the distribution of Y_0.

Conditions on the initial measure μ_0:

1. $\mathbb{E}(Y_0(p)) \equiv \int_{\mathcal{E}} Y_0(p)\,\mu_0(dY_0) = 0, \quad p \in \mathbb{P}^d := \mathbb{R}^d \cup \mathbb{Z}^d.$
2. μ_0 has a finite mean energy density, $\mathbb{E}(|\nabla\varphi_0(x)|^2 + |\varphi_0(x)|^2 + |\pi_0(x)|^2 + |u_0(k)|^2 + |v_0(k)|^2) \le C < \infty.$
3. $Q_0(p,p') := \mathbb{E}(Y_0(p) \otimes Y_0(p'))$, $p, p' \in \mathbb{P}^d$, is translation invariant w.r.t. shifts in $\mathbb{Z}^d$, i.e., $Q_0(p+k, p'+k) = Q_0(p,p') \quad \forall\, k \in \mathbb{Z}^d$.

   Write
   $Q_0(k+r, k'+r') =: q_0(k-k', r, r'), \quad k, k' \in \mathbb{Z}^d, \quad r, r' \in [0,1]^d \cup \{0\}.$
4. $|Q_0(p,p')| \le C(1+|p-p'|)^{-\gamma}$, $\gamma > d$.
5. μ_0 satisfies a *mixing condition*. This means roughly that $Y_0(p)$ and $Y_0(p')$ are asymptotically independent as $|p-p'| \to \infty$.

Rosenblatt mixing condition

Let $\sigma(\mathcal{A}) := \sigma\{Y_0 \in \mathcal{E} : \ \mathrm{supp}\, Y_0 \subset \mathcal{A}\}, \ \ \mathcal{A} \subset \mathbb{P}^d$.

The Rosenblatt mixing coefficient of a probability measure μ_0 on $\mathcal{E}$ is

$$\alpha(r) \equiv \sup_{\mathcal{A},\mathcal{B}\subset\mathbb{P}^d:\rho(\mathcal{A},\mathcal{B})\geq r} \ \sup_{A\in\sigma(\mathcal{A}),B\in\sigma(\mathcal{B})} |\mu_0(A\cap B) - \mu_0(A)\mu_0(B)|.$$

Def. *A measure μ_0 satisfies the strong Rosenblatt mixing condition* [a] *if the mixing coefficient $\alpha(r) \to 0$ as $r \to \infty$.*

[a] Ibragimov I.A., Linnik Yu.V., *Independent and Stationary Sequences of Random Variables*.
Rosenblatt, M.A., *A central limit theorem and a strong mixing condition* (1956).
Bulinskii A.V., *Limit theorems under weak dependence conditions*. MSU Press (1989) [in Russian]
Bradley R.C., *Basic properties of strong mixing conditions*, Probability Surveys (2005)

Assume that μ_0 satisfies the strong Rosenblatt mixing condition and

$\int_0^{+\infty} r^{d-1}\alpha^p(r)\,dr < \infty$ with $\ p := \min(\delta/(2+\delta), 1/2)$.

$\exists\, \delta > 0 : \ \ \int |Y_0(p)|^{2+\delta}\, \mu_0(Y_0) \leq C < \infty$.

First result

Def. μ_t is the Borel probability measure in $\mathcal{E}^0_\alpha$ given the distribution of the random solution $Y(t)$, $\mu_t(B) = \mu_0(W(-t)B)$, $B \in \mathcal{B}(\mathcal{E}^0_\alpha)$, $t \in \mathbb{R}$.

Theorem. (i) The measures μ_t weakly converge as $t \to \infty$ in the space $\mathcal{E}^s_\beta$ for any $s < 0$, $\beta < \alpha < -d/2$.

The limiting measure μ_∞ is a Gaussian measure concentrated in $\mathcal{E}^0_\alpha$,

$$\widehat{\mu}_\infty(Z) \equiv \int e^{i\langle Y,Z\rangle} \mu_\infty(dY) = e^{-1/2\langle Q_\infty Z,Z\rangle}, \quad \forall Z \in [C_0^\infty(\mathbb{R}^d) \oplus C_0(\mathbb{Z}^d)]^2.$$

(ii) The correlation matrices of μ_t converge to a limit,

$$Q_t(p,p') \equiv \int \Big(Y(p) \otimes Y(p')\Big)\, \mu_t(dY) \to Q_\infty(p,p'), \quad t \to \infty, \quad p,p' \in \mathbb{P}^d.$$

(iii) The measure μ_∞ is stationary in time, i.e., $[W(t)]^*\mu_\infty = \mu_\infty$, $t \in \mathbb{R}$.
The group $W(t)$ satisfies a mixing condition w.r.t. μ_∞, i.e., $\forall f,g \in L^2(\mathcal{E}^0_\alpha, \mu_\infty)$,

$$\int f(W(t)Y)g(Y)\, \mu_\infty(dY) \to \int f(Y)\, \mu_\infty(dY) \int g(Y)\, \mu_\infty(dY), \quad t \to \infty.$$

The limit correlation matrix $Q_\infty(p,p')$

$Q_\infty(p,p')$ is translation-invariant w.r.t. the group $\mathbb{Z}^d$, i.e.,

$$Q_\infty(k+r,k'+r') =: q_\infty(k-k',r,r'), \quad k,k'\in\mathbb{Z}^d, \quad r,r'\in[0,1]^d\cup\{0\}.$$

In the Zak transform,

$$\mathcal{Z}_{p\to(\theta,r)}\mathcal{Z}_{p'\to(-\theta',r')}[Q_\infty(p,p')] = (2\pi)^d\delta(\theta-\theta')\widetilde{q}_\infty(\theta,r,r'), \;\; \theta,\theta'\in[-\pi,\pi]^d,$$

$$\widetilde{q}_\infty(\theta,r,r') = e^{i(r-r')\cdot\theta}\sum_{k\in\mathbb{Z}^d} e^{ik\cdot\theta}q_\infty(k,r,r'), \quad \theta\in[-\pi,\pi]^d, \quad r,r'\in\mathbb{T}_1^d\cup\{0\}.$$

Denote $\widetilde{q}_\infty(\theta)=\mathrm{Op}\left(\widetilde{q}_\infty(\theta,r,r')\right)$ the integral operator with kernel $\widetilde{q}_\infty(\theta,r,r')$. Then

$$\widetilde{q}_\infty(\theta) := \sum_{\sigma=1}^{\infty}\Pi_\sigma(\theta)\,\frac{1}{2}\Big(\widetilde{q}_0(\theta)+C(\theta)\widetilde{q}_0(\theta)C^*(\theta)\Big)\,\Pi_\sigma(\theta),$$

$$C(\theta) := \begin{pmatrix} 0 & \Omega^{-1}(\theta) \\ -\Omega(\theta) & 0 \end{pmatrix}, \qquad \Omega(\theta)=\sqrt{\widetilde{\mathcal{H}}(\theta)}.$$

Note that $\Omega(\theta)=\sum_{\sigma=1}^{\infty}\omega_\sigma(\theta)\Pi_\sigma(\theta)$, where $\omega_\sigma(\theta)$ – eigenvalues of $\Omega(\theta)$ (so-called *Bloch bands*), $\Pi_\sigma(\theta)$ – the corresponding spectral projections.

Problem II: Derivation of the energy transport equation

$\varepsilon > 0$ – a small scale parameter, $\{\mu_0^\varepsilon, \varepsilon > 0\}$ – a family of the initial measures

Conditions on μ_0^ε:

- $\mathbb{E}_0^\varepsilon\big(Y_0(p)\big) \equiv \displaystyle\int Y_0(p)\,\mu_0^\varepsilon(dY_0) = 0.$
- $\forall\varepsilon > 0,\ p, p' \in \mathbb{P}^d,\ \ |Q_\varepsilon(p,p')| \le C(1+|p-p'|)^{-\gamma}, \quad \gamma > d,$

  where $Q_\varepsilon(p,p') := \mathbb{E}_0^\varepsilon\big(Y_0(p)\otimes Y_0(p')\big)$ – correlation matrix of μ_0^ε.
- $Q_\varepsilon([z/\varepsilon]+p, [z/\varepsilon]+p') \to \mathbf{R}(z;p,p'), \quad \varepsilon \to 0, \quad \forall z \in \mathbb{R}^d,\ \ p, p' \in \mathbb{P}^d.$

The matrix-valued function $\mathbf{R}(z;p,p')$ is translation invariant w.r.t. shifts in $\mathbb{Z}^d$, $\mathbf{R}(z;k+r,k'+r') =: R(z;k-k',r,r') \quad k,k' \in \mathbb{Z}^d,\ \ r,r' \in [0,1]^d \cup \{0\}$.
Hence, in the Zak transform,

$$\mathcal{Z}_{p\to(\theta,r)}\mathcal{Z}_{p'\to(-\theta',r')}\left[\mathbf{R}(z;p,p')\right] = (2\pi)^d\delta(\theta-\theta')\widetilde{R}(z;\theta,r,r').$$

Assumption: The operator $\widetilde{R}(z;\theta) = \mathrm{Op}\Big(\widetilde{R}(z;\theta,r,r')\Big)$ is self-adjoint and nonnegative: $\widetilde{R}(z;\theta)^* = \widetilde{R}(z;\theta) \ge 0$ in $[L^2(\mathbb{T}_1^d)\oplus\mathbb{C}^n]^2$, $\forall z \in \mathbb{R}^d$, $\theta \in [-\pi,\pi]^d$.

Example of $Q_\varepsilon(p,p')$ and $\mathbf{R}(z;p,p')$

For simplicity, we assume that the covariance $Q_\varepsilon(p,p')$ has a form

$$Q_\varepsilon(p,p') = T(\varepsilon p)T(\varepsilon p')Q_0(p,p'), \quad p,p' \in \mathbb{P}^d,$$

where

$$T \in C^2(\mathbb{R}^d), \quad T \geq 0, \quad |\widehat{T}(\xi)| \leq C(1+|\xi|)^{-N}, \quad N > d,$$

and the matrix Q_0 satisfies conditions stated in Problem I, in particular,

- $Q_0(p,p')$ is invariant w.r.t. translation in $\mathbb{Z}^d$:
  $Q_0(k+r,k'+r') =: q_0(k-k',r,r'), \quad k,k' \in \mathbb{Z}^d, \quad r,r' \in [0,1]^d \cup \{0\}.$
- $|Q_0(p,p')| \leq C(1+|p-p'|)^{-\gamma}, \ \gamma > d.$

We put $\mathbf{R}(z;p,p') = T^2(z)\,Q_0(p,p')$. Then

$$Q_\varepsilon([z/\varepsilon]+p,[z/\varepsilon]+p') \to \mathbf{R}(z;p,p'), \quad \varepsilon \to 0, \quad \forall z \in \mathbb{R}^d, \quad p,p' \in \mathbb{P}^d.$$

Then, $\mathbf{R}(z;k+r,k'+r') =: R(z;k-k',r,r') = T^2(z)q_0(k-k',r,r')$, and in the Zak transform, the operator $\widetilde{R}(z,\theta) := T^2(z)\,\widetilde{q}_0(\theta)$ is self-adjoint and nonnegative in $[L^2(\mathbb{T}_1^d)\oplus\mathbb{C}^n]^2 \quad \forall z \in \mathbb{R}^d, \ \theta \in [-\pi,\pi]^d$.

Weak convergence

For given $\tau \neq 0$, $z \in \mathbb{R}^d$, let us consider the random field $Y(p,t)$ for

$$p \sim [z/\varepsilon] \in \mathbb{Z}^d, \quad t = \tau/\varepsilon^\kappa, \quad \kappa \in (0,1].$$

Def. μ_t^ε is the distribution of the random solution $Y(\cdot,t) = W(t)Y_0$:

$$\mu_t^\varepsilon(B) = \mu_0^\varepsilon(W(-t)B), \quad B \in \mathcal{B}(\mathcal{E}), \quad t \in \mathbb{R}\,.$$

Given $\tau \neq 0$, $z \in \mathbb{R}^d$, define $\mu^\varepsilon_{\tau/\varepsilon^\kappa, z/\varepsilon}(B) := \mu^\varepsilon_{\tau/\varepsilon^\kappa}(\mathrm{T}_{[z/\varepsilon]}B)$, $B \in \mathcal{B}(\mathcal{E})$, where T_h, $h \in \mathbb{Z}^d$, is the group of space translations: $\mathrm{T}_h Y_0(p) = Y_0(p-h)$.

Theorem. *(i) If $\kappa < 1$, then $\mu^\varepsilon_{\tau/\varepsilon^\kappa, z/\varepsilon} \rightharpoonup \mu_z$, $\varepsilon \to 0$, where μ_z is a Gaussian measure and does not depend on τ.*

(ii) If $\kappa = 1$, then $\mu^\varepsilon_{\tau/\varepsilon, z/\varepsilon} \rightharpoonup \mu^G_{\tau,z}$, $\varepsilon \to 0$ (in the sense of weak convergence). $\mu^G_{\tau,z}$ is a Gaussian measure, which is invariant w.r.t. $W(t)$ and the shifts in $\mathbb{Z}^d$.

Hyperbolic (or Euler) time-space scaling ($\kappa = 1$)

Theorem. *The correlation functions of $\mu^{\varepsilon}_{\tau/\varepsilon, z/\varepsilon}$, $\tau \neq 0$, $z \in \mathbb{R}^d$, converge to a limit,*

$$\lim_{\varepsilon\to 0} Q_{\varepsilon,\tau/\varepsilon}([z/\varepsilon]+p,[z/\varepsilon]+p') = Q_{\tau,z}(p,p'), \quad p,p' \in \mathbb{P}^d.$$

Here $Q_{\tau,z}(k+r,k'+r') =: q_{\tau,z}(k-k',r,r')$. In the Zak transform,

$$\widetilde{q}_{\tau,z}(\theta) = \sum_{\sigma=1}^{\infty} \Pi_\sigma(\theta)\left(\mathrm{L}[\mathbf{R}^+_\sigma(\tau,z;\theta)] + i\,C(\theta)\mathrm{L}[\mathbf{R}^-_\sigma(\tau,z;\theta)]\right)\Pi_\sigma(\theta),\;\; \theta \in [-\pi,\pi]^d,$$

where

$$\mathrm{L}[q] := \tfrac{1}{2}\Big(q(\theta) + C(\theta)q(\theta)C^*(\theta)\Big),\; C(\theta) = \begin{pmatrix} 0 & \Omega^{-1}(\theta) \\ -\Omega(\theta) & 0 \end{pmatrix},\; \Omega(\theta) = \sqrt{\widetilde{\mathcal{H}}(\theta)},$$

$$\mathbf{R}^{\pm}_\sigma(\tau,z;\theta) := \tfrac{1}{2}\left(\widetilde{R}(z+\nabla\omega_\sigma(\theta)\tau;\theta) \pm \widetilde{R}(z-\nabla\omega_\sigma(\theta)\tau;\theta)\right).$$

Recall $\Omega(\theta) = \sum\limits_{\sigma=1}^{\infty} \omega_\sigma(\theta)\Pi_\sigma(\theta)$, where $\omega_\sigma(\theta)$ – eigenvalues of $\Omega(\theta) = \sqrt{\widetilde{\mathcal{H}}(\theta)}$ (so-called *Bloch bands*), $\Pi_\sigma(\theta)$ – the corresponding spectral projections.

Wigner functions

Corollary. $\widetilde{q}_{\tau,z}(\theta)$, $\theta \in [-\pi,\pi]^d$, obeys the (Euler–type) equation

$$\partial_\tau \widetilde{q}_{\tau,z}(\theta) = i\, C(\theta)\, \nabla\Omega(\theta) \cdot \nabla_z \widetilde{q}_{\tau,z}(\theta), \quad z \in \mathbb{R}^d, \quad \tau > 0.$$

We rewrite this result using Wigner functions.

Def. The Wigner matrix-valued function is

$$W^\varepsilon(\tau, z; \theta) = e^{ir\cdot\theta} \sum_{k\in\mathbb{Z}^d} e^{i\theta\cdot k}\, \mathbb{E}^\varepsilon_{\tau/\varepsilon}\big(a^*([z/\varepsilon] + p/2) \otimes a([z/\varepsilon] - p/2)\big) \quad \varepsilon > 0,$$

$\tau \in \mathbb{R}$, $z \in \mathbb{R}^d$, $\theta \in [-\pi,\pi]^d$, $p = k + r \in \mathbb{P}^d$, $k \in \mathbb{Z}^d$, $r \in [0,1]^d \cup \{0\}$,
$a(p) := \dfrac{1}{\sqrt{2}}\Big(\mathcal{H}^{1/4} Y_0^0(p) + i\,\mathcal{H}^{-1/4} Y_0^1(p)\Big) \in \mathbb{C}^{n+1}$.

Lemma. $\lim\limits_{\varepsilon\to 0} W^\varepsilon(0, z; \theta) = W_0(z;\theta)$ (uniformly in $\theta \in \mathrm{K}^d$, $z \in \mathbb{R}^d$), where

$$W_0(z;\theta) := \frac{1}{2}\Big(\Omega^{1/2}(\theta)\tilde{R}^{00}(z;\theta)\Omega^{1/2}(\theta) + \Omega^{-1/2}(\theta)\tilde{R}^{11}(z;\theta)\Omega^{-1/2}(\theta)$$
$$+\, i\,\Omega^{1/2}(\theta)\tilde{R}^{01}(z;\theta)\Omega^{-1/2}(\theta) - i\,\Omega^{-1/2}(\theta)\tilde{R}^{10}(z;\theta)\Omega^{1/2}(\theta)\Big).$$

Energy transport equation

Theorem. *For any* $z \in \mathbb{R}^d$ *and* $\tau > 0$, $W^\varepsilon(\tau; z, \theta) \to W^p(\tau; z, \theta)$ *as* $\varepsilon \to 0$ *(in the sense of distributions).* Here

$$W^{\mathrm{p}}(\tau, z; \theta) := \sum_{\sigma=1}^{+\infty} \Pi_\sigma(\theta)\, W_0(z - \tau \nabla\omega_\sigma(\theta); \theta)\, \Pi_\sigma(\theta)$$
$$= \Omega(\theta)\, \widetilde{q}^{00}_{\tau,z}(\theta) + i\, \widetilde{q}^{01}_{\tau,z}(\theta),$$

where $\omega_\sigma(\theta)$ – eigenvalues of $\Omega(\theta) = \sqrt{\widetilde{\mathcal{H}}(\theta)}$, $\Pi_\sigma(\theta)$ – spectral projections.

Denote by $f_\sigma(\tau, z; \theta)$ the σ-th band of the Wigner function $W^p(\tau, z; \theta)$,

$$f_\sigma(\tau, z; \theta) := \Pi_\sigma(\theta)\, W^{\mathrm{p}}(\tau, z; \theta)\, \Pi_\sigma(\theta), \quad \sigma = 1, 2, \dots$$

Theorem. $f_\sigma(\tau, z; \theta)$ *is a solution of the* **energy transport equation**

$$\partial_\tau f_\sigma(\tau, z; \theta) + \nabla\omega_\sigma(\theta) \cdot \nabla_z f_\sigma(\tau, z; \theta) = 0, \quad \tau > 0,$$
$$f_\sigma(\tau, z; \theta)\Big|_{t=0} = \Pi_\sigma(\theta) W_0(z; \theta) \Pi_\sigma(\theta), \quad z \in \mathbb{R}^d.$$

Application to Gibbs measures

Introduce the Gibbs measures g_β on the space $\mathcal{E}^s_\alpha$, $s, \alpha < -d/2$.
$\beta = T^{-1}$, $T > 0$ is a temperature, $\mathcal{E}^s_\alpha \equiv \mathrm{E}^{s+1}_\alpha \oplus \mathrm{E}^s_\alpha$, $\mathrm{E}^s_\alpha := H^s_\alpha(\mathbb{R}^d) \oplus \ell^2_\alpha(\mathbb{Z}^d)$.

Def. g_β are Gaussian Borel probability measures $g_\beta(dY) = g^0_\beta(dY^0) \times g^1_\beta(dY^1)$ in the spaces $\mathcal{E}^s_\alpha$ with characteristic functionals of the form

$$\hat{g}^0_\beta(Z) = \int \exp\{i\langle Y^0, Z\rangle\}\, g^0_\beta(dY^0) = \exp\left\{-\frac{1}{2\beta}\langle \mathcal{H}^{-1} Z, Z\rangle\right\} \qquad Z \in D_F \oplus D_L$$

$$\hat{g}^1_\beta(Z) = \int \exp\{i\langle Y^1, Z\rangle\}\, g^1_\beta(dY^1) = \exp\left\{-\frac{1}{2\beta}\langle Z, Z\rangle\right\} \qquad D_F := C_0^\infty(\mathbb{R}^d), \quad D_L := C_0(\mathbb{Z}^d)$$

$g^0_\beta(dY^0) \equiv g^0_\beta(d\psi du)$ – Gaussian in E^{s+1}_α with the correlation matrix $Q^{00}_\beta(p, p')$.
In the Zak transform,

$$\widetilde{Q}^{00}_\beta(\theta, \theta') = (2\pi)^d \delta(\theta - \theta')\tilde{q}^{00}_\beta(\theta), \quad \tilde{q}^{00}_\beta(\theta) = \beta^{-1}\widetilde{\mathcal{H}}^{-1}(\theta), \quad \theta \in [-\pi, \pi]^d.$$

$g^1_\beta(dY^1) \equiv g^0_\beta(d\pi dv)$ – Gaussian measure in E^s_α with the correlation matrix

$$Q^{11}_\beta(p, p') = \frac{1}{\beta}\begin{pmatrix} \delta(x - x') & 0 \\ 0 & \delta_{kk'}\mathrm{I} \end{pmatrix}.$$

- Let $\mathbf{R}(z;p,p') = T(z)Q_0(p,p')$ be the correlation matrix of the Gibbs measure $g_{\beta(z)}$ with temperature $\beta^{-1}(z) = T(z) > 0$, $z \in \mathbb{R}^d$.
- Introduce the initial measures g_0^ε, $\varepsilon > 0$, as Gaussian in $\mathcal{E}_\alpha^s$, $s, \alpha < -d/2$, with the correlation matrix $Q_\varepsilon(p,p') = \sqrt{T(\varepsilon p)T(\varepsilon p')}Q_0(p,p')$, $p, p' \in \mathbb{P}^d$. Then

$$Q_\varepsilon([z/\varepsilon]+p, [z/\varepsilon]+p') \to \mathbf{R}(z;p,p'), \quad \varepsilon \to 0.$$

- Denote by g_t^ε the distribution of the random solution $W(t)Y_0$, $t \in \mathbb{R}$.
- $g^\varepsilon_{\tau/\varepsilon^\kappa, z/\varepsilon}(B) := g^\varepsilon_{\tau/\varepsilon^\kappa}(\mathrm{T}_{[z/\varepsilon]}B)$, $B \in \mathcal{B}(\mathcal{E}_\alpha^s)$, $\tau \neq 0$, $z \in \mathbb{R}^d$, $\kappa \in (0,1]$.

Theorem. If $\kappa < 1$, then $\lim\limits_{\varepsilon\to 0} g^\varepsilon_{\tau/\varepsilon^\kappa, z/\varepsilon} = g_{\beta(z)}$ in $\mathcal{E}_\alpha^s$, $s, \alpha < -d/2$.

If $\kappa = 1$, then $g^\varepsilon_{\tau/\varepsilon, z/\varepsilon} \to g_{\tau,z}$, $\varepsilon \to 0$. The limit measure $g_{\tau,z}$ is Gaussian and invariant w.r.t. the translations in $\mathbb{Z}^d$. The limit correlation matrix is $Q_{\tau,z}(k+r, k'+r') =: q_{\tau,z}(k-k', r, r')$, where in the Zak transform,

$$\widetilde{q}_{\tau,z}(\theta) = \sum_{\sigma=1}^{\infty} \begin{pmatrix} \omega_\sigma^{-2}(\theta)\,\mathbf{T}_\sigma^+(\tau,z;\theta) & i\,\omega_\sigma^{-1}(\theta)\,\mathbf{T}_\sigma^-(\tau,z;\theta) \\ -i\,\omega_\sigma^{-1}(\theta)\,\mathbf{T}_\sigma^-(\tau,z;\theta) & \mathbf{T}_\sigma^+(\tau,z;\theta) \end{pmatrix} \Pi_\sigma(\theta),$$

with $\mathbf{T}_\sigma^\pm(\tau,z;\theta) := \left(T(z+\nabla\omega_\sigma(\theta)\tau) \pm T(z-\nabla\omega_\sigma(\theta)\tau)\right)/2.$

Parabolic time-space scaling ($\kappa = 2$)

For $\tau \neq 0$, $z \in \mathbb{R}^d$, let us consider the random field $Y(p,t)$ at

$$p \sim [z/\varepsilon] \in \mathbb{Z}^d, \quad t = \tau/\varepsilon^2.$$

Theorem. *Let $z \in \mathbb{R}^d$, $\tau \neq 0$. Then for any $p, p' \in \mathbb{P}^d$, the correlation functions of $\mu^{\varepsilon}_{\tau/\varepsilon^2, z/\varepsilon}$ have the following asymptotics*

$$\lim_{\varepsilon \to 0} \Big(Q_{\varepsilon, \tau/\varepsilon^2}([z/\varepsilon]+p, [z/\varepsilon]+p') - F_\varepsilon(\tau, z; p-p') \Big) = 0.$$

The explicit formulas for $F_\varepsilon(\tau, z; p)$ are derived.

Set $f_\varepsilon(t,z;\theta) := \widetilde{F}_\varepsilon(\varepsilon t, z; \theta)$.
In the σ-th band ($\sigma = 1, 2, \dots$) the matrix-valued function $f \equiv f_\varepsilon(t,z;\theta)$ evolves according to the following (Navier–Stokes type) equation

$$\partial_t f = i\, C_\sigma(\theta) \left(\nabla\omega_\sigma(\theta) \cdot \nabla_z f + \frac{i\varepsilon}{2} \mathrm{tr} \left[\nabla^2 \omega_\sigma(\theta) \cdot \nabla_z^2 f \right] \right), \quad t > 0,$$

$$\nabla_z^2 f := \left(\frac{\partial^2 f}{\partial z_i \partial z_j} \right)_{i,j=1}^d, \qquad C_\sigma(\theta) := \begin{pmatrix} 0 & \omega_\sigma^{-1}(\theta) \\ -\omega_\sigma(\theta) & 0 \end{pmatrix}.$$

Brief survey of previous results

I. Convergence to equilibrium

Harmonic crystals:

Case $d = 1$ (infinite one-dimensional chain of harmonic oscillators).

- Spohn, Lebowitz (1977) – *for initial measures which have distinct temperatures to the left and to the right*
- Boldrighini, Pellegrinotti, Triolo (1983) – *for a more general class of initial measures which satisfy a mixing condition*
- T.D. (2017) – *infinite harmonic chain in the half-line*
- T.D. (2020) – *non-homogenous chain consisting of two different semi-infinite chains coupled to a "gluing" particle (one defect)*

Case $d \geq 1$.

- Lanford, Lebowitz (1975) – *for initial measures which are absolutely continuous with respect to the canonical Gaussian measure*
- J.L. van Hemmen (1980) – *ergodic properties of the harmonic crystal*
- T.D., A. Komech, H. Spohn (2003) –*for translation-invariant initial measures*
- T.D., A. Komech, N. Mauser (2004) – *for non translation-invariant measures*
- T.D. (2008) – *for harmonic crystals in half-space with zero boundary condition*

Partial differential equations of hyperbolic type in $\mathbb{R}^d$, $d \geq 1$:

- N. Ratanov (1984), E. Kopylova (1986) – *for translation–invariant initial measures*
- T.D., A. Komech, H. Spohn (2002); T.D., A. Komech (2005, 2006);
- T.D. (2021) – *for non translation invariant measures*

Coupled systems:

- Jakšić, Pillet (1998), Rey-Bellet, Thomas (2002) – *ergodic properties of one-dimensional chain of anharmonic oscillators coupled to heat baths*
- T.D., A. Komech (2006) – *the Hamiltonian system consisting of the crystal and the scalar Klein–Gordon field* (translation invariant case)
- T.D. (2010, 2016) – *the Hamiltonian system consisting of a particle and the vector field described by the KG or wave equations with variable coefficients*
- T.D. (2023) – *the "field–crystal" system* (non translation invariant case) (accepted to *Theoret. and Mat. Phys.* 2023)

II. Derivation of hydrodynamic equations (deterministic models)

- Morrey (1955) – *the idea that the Euler equation of fluid dynamics could be derived from microscopic dynamics*
- Boldrighini, Dobrushin, Suhov (1983) – *for one-dimensional hard rods*
- Dobrushin, Pellegrinotti, Suhov, Triolo (1986) – *Euler type equation for one-dimensional chain of harmonic oscillators*
- Dobrushin, Pellegrinotti, Suhov, Triolo (1988) – *Navier–Stokes type equation for one-dimensional chain of harmonic oscillators*
- The survey papers: De Masi, Ianiro, Pellegrinotti, Presutti (1984), Dobrushin, Sinai, Suhov (1985), Spohn (1991)

- D.T., Spohn H. (2006) – *extension of the paper [DPST'86] to any dimension d*
- D.T. (2010–2012) – *lattice dynamics in the half–space, energy transport equation, Navier–Stokes type equation for harmonic crystals in the whole space and in the half–space*
- D.T. (2023) – *local stationarity for Klein–Gordon equation*

Thank you for attention!