Non-Equilibrium States in a Harmonic Crystal coupled to a Klein–Gordon Field

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In the talk, we discuss the long-time behavior of distributions of solutions for infinite-dimensional Hamiltonian systems and the existence of a nonzero heat flux in them. As a model, we consider a linear Hamiltonian system consisting of a real scalar Klein–Gordon field $\psi(x)$ and its momentum $\pi(x)$, $x \in \mathbb{R}^d$, and a harmonic crystal described by the deviations $u(k) \in \mathbb{R}^n$ of the particles (atoms, ions, etc.) and their velocities $v(k) \in \mathbb{R}^n$, $k \in \mathbb{Z}^d$. The Hamiltonian functional of the coupled field–crystal system reads

$$\begin{aligned}\mathrm{H}(\psi,\pi,u,v) =& \frac{1}{2}\int\limits_{\mathbb{R}^d}\Big(|\nabla\psi(x)|^2 + m_0^2|\psi(x)|^2 + |\pi(x)|^2\Big)\,dx \\ &+ \frac{1}{2}\sum_{k\in\mathbb{Z}^d}\Big(\sum_{k'\in\mathbb{Z}^d} u(k)\cdot V(k-k')u(k') + |v(k)|^2\Big) + \sum_{k\in\mathbb{Z}^d}\int\limits_{\mathbb{R}^d} R(x-k)\cdot u(k)\psi(x)\,dx.\end{aligned}$$

Here $m_0 > 0$, the coupled function $R(\cdot) \in \mathbb{R}^n$ is a smooth vector-valued function, exponentially decaying at infinity, "$\cdot$" denotes the inner product in $\mathbb{R}^n$, V is a real interaction matrix, $V(k) \in \mathbb{R}^n \times \mathbb{R}^n$, $d, n \geq 1$. This model 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. Understanding of this motion is one of the central problem of solid state physics.

We study the Cauchy problem with the initial data $Y_0 = (\psi_0, \pi_0, u_0, v_0)$. We assume that Y_0 belong to the phase space $\mathcal{E}_\alpha^s \equiv H_\alpha^{s+1} \oplus H_\alpha^s \oplus \ell_\alpha^2 \oplus \ell_\alpha^2$, where $H_\alpha^s \equiv H_\alpha^s(\mathbb{R}^d)$ denotes the weighted Sobolev space, $\ell_\alpha^2 \equiv \ell_\alpha^2(\mathbb{Z}^d)$ is the Hilbert space of vector-valued sequences $u(k) \in \mathbb{R}^n$, $k \in \mathbb{Z}^d$, with finite norm $\|\langle k\rangle^\alpha u(k)\|_{\ell^2(\mathbb{Z}^d)} < \infty$, $\langle k\rangle := \sqrt{k^2+1}$, $s, \alpha < -d/2$.

We assume that Y_0 is a random function of the form $Y_0(p) = \sum\limits_{\pm} \zeta_\pm(p_1)Y_\pm(p)$, where $p = (p_1, \ldots, p_d) \in \mathbb{P}^d \equiv \mathbb{R}^d \cup \mathbb{Z}^d$, $\zeta_\pm$ are nonnegative cut-off functions equal to one for $\pm p_1 > a$ and zero for $\pm p_1 < -a$ with some $a > 0$, the random functions $Y_\pm(p)$ have Gibbs distributions $g_{\beta_\pm}$, $\beta_\pm = T_\pm^{-1}$, with temperatures $T_\pm > 0$. Given $t \in \mathbb{R}$, denote by μ_t the probability Borel measure in $\mathcal{E}_\alpha^s$ that gives the distribution of the random solution $Y(t) \equiv (\psi(\cdot,t), \pi(\cdot,t), u(\cdot,t), v(\cdot,t))$ with the random initial data Y_0. The main result is the following theorem.

Theorem. *The measures μ_t weakly converge to a Gaussian measure μ_∞ as $t \to \infty$ on the space $\mathcal{E}_\alpha^s$, $s, \alpha < -d/2$. The correlation matrix of μ_∞ is translation-invariant w.r.t. shifts in $\mathbb{Z}^d$. The explicit formulas for the limiting correlation functions are given.*

In non-equilibrium statistical mechanics, the heat flux is often calculated in models, which are an open system coupled to at least two reservoirs with different temperatures. These models differ in the description of the system, reservoirs and the type of interaction between them, see, e.g., [1]. Similar to these models, our system can be represented as a "system + two heat reservoirs", where "reservoirs" are described by the solutions $Y(p,t)$ with coordinates lying in two regions with $p_1 \leq -a$ and $p_1 \geq a$, and an "open system" by the solutions with coordinates from the remaining part of the space. Initially, the reservoirs are assumed to be in thermal equilibrium with different temperatures T_- and T_+. The limiting energy current density is

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$J = -c\,(T_+ - T_-, 0, \dots, 0)$, $c > 0$, i.e., the heat flows (on average) from the "hot reservoir" to the "cold" one. Thus, we prove that there exist stationary non-equilibrium states, i.e., the probability limiting measures μ_∞, in which there is a non-zero heat flux in the model under consideration.

For initial measures which are translation-invariant w.r.t. shifts in $\mathbb{Z}^d$, the weak convergence of μ_t was proved in [2]. The similar results were obtained in [3, 4] for the Klein–Gordon fields and in [5, 6] for the harmonic crystals.

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