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Macroscopic behavior of microscopic oscillations in harmonic lattices via Wigner-Husimi transforms

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Abstract

We consider the dynamics of infinite harmonic lattices in the limit of the lattice distance ε tending to 0. We allow for general polyatomic crystals but assume exact periodicity such that the system can be solved in principle by Fourier transform and linear algebra.

Our aim is to derive macroscopic continuum limit equations for $\varepsilon \to 0$. For the weak limit of displacements and velocities we find the equation of linear elastodynamics, where the elasticity tensor is obtained as a Γ-limit. The weak limit of the local energy density can be described by generalizations of the Wigner-Husimi measure which satisfies a transport equation on the product of physical space and Fourier space. The concepts are illustrated via several examples and via a comparison to Whitham's modulation equation.

1 Introduction

This paper is devoted to the problem of deriving macroscopic, continuum models from microscopic, discrete systems. More precisely, we start from the atomistic model for a crystal which consists of periodically spaced mass points whose motion is governed by linear interaction forces. The aim is to provide exact mathematical links between this microscopic system and its macroscopic limits arising when the atomic distance ε tends to 0. In fact, we will obtain one equation which describes the evolution of the macroscopic displacement and another equation which allows us to calculate the transport of energy in the crystal.

The analysis of discrete systems attracted a lot of attention over the last decades. However, most work is restricted to the one-dimensional oscillator chain

$$\ddot{x}_\gamma = \sum_{\alpha=1}^{M} \Big(V'_\alpha(x_{\gamma+\alpha} - x_\gamma) - V'_\alpha(x_\gamma - x_{\gamma-\alpha}) \Big) - W'(x_\gamma), \qquad \gamma \in \mathbb{Z}, \tag{1.1}$$

where V_α is the interaction potential with the neighbors at distance α and W the on-site potential which couples the atoms to a background. Apart from methods for completely integrable systems like the Toda lattices (with $V(y) = \mathrm{e}^y$ and $W \equiv 0$, see, e.g., [DKKZ96, DKV95]) the analysis is restricted either to stationary problems [FJ00, FT02, Bla01] or they concern very special types of solutions like solitons, breathers or wave trains [FW94, MA94, FP99, FV99, IK00, Ioo00, AMM00, Jam01, Jam02]. Another series of papers tries to characterize the response of a lattice to a simple initial disturbance [BCS01] or to

Riemann initial data. In the latter case either a semi-infinite chain is pulled at the end [DKKZ96, DKV95] or a double-infinite chain has initial data which jumps at one point [DK00]. An interesting model studying the interaction of traveling and standing waves is proposed and analyzed in [BCS01].

Rigorous justifications of macroscopic PDEs for the oscillator chain are provided in [FP99, SW00] where the Korteweg-de Vries equation is obtained as the macroscopic model for describing the evolution of long-wave interactions. In [GM04b, GM04a] the nonlinear Schrödinger equation is derived to describe macroscopic evolution of pulses which modulate a periodic pattern on the microscopic scale. Similar work, which is even more nonlinear, concerns the modulation of large-amplitude traveling waves. In [HLM94] the discrete, nonlinear Schrödinger equation $\mathrm{i}\dot{A}_\gamma + c_1(A_{\gamma-1} - 2A_\gamma + A_{\gamma+1}) + c_2|A_\gamma|^2 A_\gamma = 0$ with $A_\gamma(t) \in \mathbb{C}$ is studied. It has exact traveling waves of the form $A_\gamma(t) = \rho \mathrm{e}^{\mathrm{i}(\theta\gamma+\omega t)}$ where $\omega = \Omega(\rho, \theta) := c_2\rho^2 - 2c_1(1 - \cos\theta)$ and it is studied via a formal two-scale ansatz how solutions with initial conditions of the form

$$A_\gamma^\varepsilon(0) = \widetilde{\rho}(\varepsilon\gamma)\mathrm{e}^{\mathrm{i}(\widetilde{\theta}(\varepsilon\gamma)\gamma + \widetilde{\omega}(\varepsilon\gamma)t)} \quad \text{with } \widetilde{\omega}(y) = \Omega(\widetilde{\rho}(y), \widetilde{\theta}(y))$$

evolve. It is shown there via numerical experiments, that the functions $\widetilde{r}$ and $\widetilde{\theta}$ evolve on the macroscopic time scale $\tau = \varepsilon t$ according to the following system:

$$\partial_\tau(\widetilde{\rho}^2) = -\partial_y(2c_1\widetilde{\rho}^2 \sin\widetilde{\theta}), \quad \partial_\tau\widetilde{\theta} = \partial_y(c_2\widetilde{\rho} + 2c_1\cos\widetilde{\theta}).$$

For the oscillator chain (1.1) with $W \equiv 0$ similar results have been derived in [FV99, DHM04]. Here, the problem leads to a system of four coupled equations, since the additional Galileian invariance leads to macroscopic deformations as well. Let the family $\mathbb{X}(r, \theta, \omega; \cdot)$ of 2π–periodic functions be such that for all r, θ and ω the function $x_\gamma(t) = r\gamma + \mathbb{X}(r, \theta, \omega; \theta\gamma + \omega t)$ is an exact traveling-wave solution for (1.1). Now consider initial conditions for (1.1) in the form

$$\begin{aligned} x_\gamma(0) &= \tfrac{1}{\varepsilon}\widetilde{X}(\varepsilon\gamma) + \mathbb{X}(\widetilde{r}(\varepsilon\gamma), \widetilde{\theta}(\varepsilon\gamma), \widetilde{\omega}(\varepsilon\gamma); \tfrac{1}{\varepsilon}\widetilde{\phi}(\varepsilon\gamma)), \\ \dot{x}_\gamma(0) &= \widetilde{v}(\varepsilon\gamma) + \widetilde{\omega}(\varepsilon\gamma)\tfrac{\partial}{\partial\phi}\mathbb{X}(\widetilde{r}(\varepsilon\gamma), \widetilde{\theta}(\varepsilon\gamma), \widetilde{\omega}(\varepsilon\gamma); \tfrac{1}{\varepsilon}\widetilde{\phi}(\varepsilon\gamma)), \end{aligned}$$

where $\widetilde{X}(y) = \int_0^y \widetilde{r}(z)\,\mathrm{d}z$ and $\widetilde{\phi}(y) = \int_0^y \widetilde{\theta}(z)\,\mathrm{d}z$.

The question is, whether the solutions of (1.1) remain in such a form on the macroscopic time scale $\tau = \varepsilon t$. If yes then the macroscopic functions $\widetilde{r}, \widetilde{v}, \widetilde{\theta}$ and $\widetilde{\omega}$ will evolve according to the so-called Whitham modulation equation

$$\begin{array}{rcll} \partial_\tau\widetilde{r} &=& \partial_y\widetilde{v} & \text{(continuity equation for mass)} \\ \partial_\tau\widetilde{v} &=& -\partial_y\big[\frac{\partial}{\partial\widetilde{r}}F(\widetilde{r}, \widetilde{\theta}, \widetilde{\omega})\big] & \text{(conservation of momentum)} \\ \partial_\tau\widetilde{\theta} &=& \partial_y\widetilde{\omega} & \text{(continuity equation for phase)} \\ \partial_\tau\big[\frac{\partial}{\partial\widetilde{\omega}}F(\widetilde{r}, \widetilde{\theta}, \widetilde{\omega})\big] &=& \partial_y\big[\frac{\partial}{\partial\widetilde{\theta}}F(\widetilde{r}, \widetilde{\theta}, \widetilde{\omega})\big] & \text{(conservation of energy)} \end{array} \tag{1.2}$$

where the macroscopic constitutive function F can explicitly be calculated from (1.1) and $\mathbb{X}$. In [DHM04] the validity of (1.2) is discussed in detail and for special cases a rigorous convergence results are obtained (see also Section 6.6).

The purpose of this work aims in a similar direction, however it is different in the methodology. We restrict ourselves completely to the linear setting and thus are free to generalize in many other directions. First, we are able to study very general lattices in any dimension. Second, we are able to investigate the dynamics of solutions for much more general initial data. Finally, our results will be more detailed. As a side effect we will obtain a justification of the Whitham equation in the linear case. In a certain sense our work is closer to the statistical approaches for harmonic lattices, see e.g., [DPST86, DPST88, DPS90, SL03]. In particular, the latter work also derives an energy-transport equation. However, we stay fully in the deterministic setting.

To be more specific, consider a d–dimensional Bravais lattice $\Gamma \subset \mathbb{R}^d$ and the set of coupled ODEs

$$M\ddot{x}_\gamma = -\textstyle\sum_{\beta\in\Gamma} A_\beta x_{\gamma+\beta} \quad \text{for } \gamma \in \Gamma, \tag{1.3}$$

which will be our basic microscopic system. Here, the vector $x_\gamma \in \mathbb{R}^m$ may contain the displacements of several atoms in the cell associated with the lattice point γ. The mass matrix $M \in \mathbb{R}^{m\times m}$ is symmetric and positive definite and the interaction matrices satisfy $A_\beta = A_{-\beta}^{\mathsf{T}}$ and $\|A_\beta\| \leq C\mathrm{e}^{-b|\beta|}$.

An essential feature of such harmonic lattices is the presence of many traveling wave solutions in the form

$$x_\gamma(t) = \mathrm{e}^{\mathrm{i}(\theta\cdot\gamma+\omega t)}\Phi \quad \text{where } \theta \in \mathbb{R}^d_* \text{ and } (\mathbb{A}(\theta) - \omega^2 M)\Phi = 0. \tag{1.4}$$

The wave vectors θ are taken from the torus $\mathcal{T}_{\Gamma_*}$, which is obtained by factoring $\mathbb{R}^d_* = \mathrm{Lin}(\mathbb{R}^d)$ with respect to the dual lattice. The symbol matrix $\mathbb{A}(\theta)$ reads

$$\mathbb{A}(\theta) = \textstyle\sum_{\beta\in\Gamma} \mathrm{e}^{\mathrm{i}\theta\cdot\beta} A_\beta \in \mathbb{C}^{m\times m} \qquad \text{for } \theta \in \mathcal{T}_{\Gamma_*}.$$

Hence, $\mathbb{A}(\theta)$ is Hermitian, and we always impose the basic assumption of stability in the form $\mathbb{A}(\theta) \geq 0$ for all $\theta \in \mathbb{R}^d_*$.

First, we derive a continuum-limit equation for the displacements in the case of the atomic distance ε tending to 0. To this end we define the interpolation operator

$$\mathcal{S}_\varepsilon : \begin{cases} \ell^2(\Gamma, \mathbb{R}^m) & \to \qquad \mathrm{L}^2(\mathbb{R}^d, \mathbb{R}^m), \\ x = (x_\gamma)_{\gamma\in\Gamma} & \mapsto \quad c_\varepsilon \sum_\Gamma x_\gamma \mathrm{sinc}_\Gamma(\frac{\cdot}{\varepsilon} - \gamma), \end{cases}$$

where sinc_Γ is a function satisfying $\mathrm{sinc}_\Gamma(\beta - \gamma) = \delta_{\beta,\gamma}$ and other useful features. We will use $y = \varepsilon\gamma \in \mathbb{R}^d$ as the macroscopic space variable and $\tau = \varepsilon t$ as the macroscopic time variable. Using the Fourier transform $\mathcal{F}$, eqn. (1.3) can be written in terms of $X^\varepsilon(\tau, \cdot) = \varepsilon\mathcal{S}_\varepsilon x(\tau/\varepsilon)$ as follows:

$$\frac{\partial^2}{\partial\tau^2} X^\varepsilon + \mathcal{A}_\varepsilon X^\varepsilon = 0 \quad \text{with } \mathcal{A}_\varepsilon = \frac{1}{\varepsilon^2}\mathcal{F}^{-1}\mathbb{A}(\varepsilon\cdot)\mathcal{F}. \tag{1.5}$$

Macroscopic behavior is associated with large wave length and hence with small wave vectors $\theta = \varepsilon\eta$. Denoting by $V \subset \mathbb{R}^m$ the kernel of $\mathbb{A}(0)$ we construct a polynomial $\mathbb{Q} : V \to \mathbb{R}$ which is homogeneous of degree 2 and satisfies

$$\langle \mathbb{Q}(\eta)v, v\rangle = \inf\{ \liminf_{\varepsilon\to 0} \frac{1}{\varepsilon^2}\langle \mathbb{A}(\varepsilon\eta)w_\varepsilon, w_\varepsilon\rangle \mid \operatorname*{w-lim}_{\varepsilon\to 0} w_\varepsilon = v \}.$$

Then, $\mathbb{Q}$ defines the second order differential operator $\mathcal{A}_0 = \mathbb{Q}(\mathrm{i}\nabla_y)$ and we obtain the partial differential equation

$$M_V \frac{\partial^2}{\partial \tau^2} Z + \mathcal{A}_0 Z = 0 \quad \text{for } (\tau, y) \in \mathbb{R}\times\mathbb{R}^d, \tag{1.6}$$

where M_V is the restriction of M to V.

In Theorem 4.2 we show that (1.6) is a macroscopic limit equation for (1.3) in an exact mathematical sense. In particular, we show that the limit $\varepsilon \to 0$ commutes with the time evolution, which means the following. Assume we have a family $(x_0^\varepsilon, x_1^\varepsilon)_{\varepsilon>0}$ of initial data for the microscopic problem (1.3) such that $\mathcal{S}_\varepsilon(\varepsilon x_0^\varepsilon, x_1^\varepsilon)$ converges weakly to the macroscopic initial data (Z_0, Z_1). Then, we have two choices. First, we may consider the solutions $t \mapsto x^\varepsilon(t)$ of (1.3) with initial data $(x_0^\varepsilon, x_1^\varepsilon)$. For fixed $\tau = \varepsilon t$ we may then consider the macroscopic limits $(\varepsilon x^\varepsilon(\tau/\varepsilon), \dot{x}^\varepsilon(\tau/\varepsilon)) \rightharpoonup (Z_0(\tau), Z_1(\tau))$. Second, we may use the macroscopic initial data for the macroscopic equation (1.6) and obtain the solution $\tau \mapsto Z(\tau)$. The theorem now states that both ways provide the same result, namely $Z_0(\tau) = Z(\tau)$ and $Z_1(\tau) = \partial_\tau Z(\tau)$. This means that in the following abstract diagram the time evolution commutes with the coarse graining:

$$\begin{array}{cccc} & \textbf{microscopic} & \xrightarrow{\mathcal{S}_\varepsilon} & \textbf{macroscopic} \\ \text{initial data } t=0 & (\varepsilon x_0^\varepsilon, x_1^\varepsilon) & \xrightarrow{\varepsilon \to 0} & (Z_0, Z_1) \\ \boxed{\textbf{time evolution}} & \big\downarrow t>0 & & \tau>0 \big\downarrow \\ & (\varepsilon x^\varepsilon(\tau/\varepsilon), \dot{x}^\varepsilon(\tau/\varepsilon)) & \xrightarrow{\varepsilon \to 0} & (Z(\tau), \partial_\tau Z(\tau)) \\ & \text{discrete, atomistic} & \boxed{\textbf{coarse graining}} & \text{continuum} \end{array}$$

The static operator $\mathcal{A}_0$ may be considered as a Gamma limit of the operators $\mathcal{A}_\varepsilon$, when looking at their quadratic forms. It is interesting to note that doing the Gamma limit in the static part and simply projecting the kinetic part to V already suffices to obtain the correct dynamical limit equation. We do not know under which general conditions such a procedure works. Similar ideas have been used in [BB04] where general unstructured networks are considered. Under suitable structure conditions on the network geometry and the interaction forces a space-dependent wave equation is derived.

In Section 5 we study the transport of energy which occurs according to the group velocity of the microscopic wave pattern. The classical WKB method (cf. [Bri60]) shows that macroscopically modulated pulses of the harmonic traveling waves (1.4) propagate with the group velocity $c_{\text{group}} = \nabla_\theta \omega(\theta)$. For studying macroscopic energy transport we have to know how much energy is located at which point, in which wave length and in which energy band, i.e., in which of the $2m$ eigenpairs (ω, Φ) associated with θ.

For this purpose it is convenient to reformulate the Fourier transformed version of (1.5) as a first order system in diagonal form:

$$\frac{\partial}{\partial\tau}\widehat{U}^\varepsilon(\tau,\eta)=\frac{\mathrm{i}}{\varepsilon}\widehat{\Omega}(\varepsilon\eta)\widehat{U}^\varepsilon(\tau,\eta),\quad \text{with } \widehat{\Omega}(\theta)=\mathrm{diag}(\omega_1(\theta),\ldots,\omega_{2m}(\theta)),\tag{1.7}$$

where $\omega_{j+m}=-\omega_j$ for $j=1,\ldots,m$.

The relevant tools for studying the macroscopic spatial distribution of microscopic oscillations is the Wigner transform $W^\varepsilon[U^\varepsilon(\tau;\cdot)]$ or the Husimi transform $H^\varepsilon[U^\varepsilon(\tau;\cdot)]$ and their limits, the matrix-valued Wigner measure $\mu(\tau)$. This theory is recalled in Section 5.2 and in Section 5.4 we derive the energy-transport equation for the diagonal entries $\mu_j(\tau)=\lim_{\varepsilon\to0}W^\varepsilon[U_j^\varepsilon(\tau)]$, $j=1,\ldots,2m$, of the Wigner measure:

$$\partial_\tau\mu_j(\tau;y,\theta)=\nabla_\theta\omega_j(\theta)\cdot\partial_y\mu(\tau;y,\theta)\quad\text{for } (\tau,y,\theta)\in\mathbb{R}\times\mathbb{R}^d\times\mathcal{T}_{\Gamma_*}.\tag{1.8}$$

The energy density $e(\tau,y)$ at a macroscopic point y at time τ is then recovered via

$$e(\tau,y)=\int_{\mathcal{T}_{\Gamma_*}}\sum_{j=1}^{2m}\mu_j(\tau;y,\mathrm{d}\theta)=\int_{\mathcal{T}_{\Gamma_*}}\sum_{j=1}^{2m}\mu_j(0;y+\tau\nabla_\theta\omega_j(\theta),\mathrm{d}\theta).$$

energy-transport equations of this type are well established in the theory of propagation of oscillations in partial differential equations, see [GL93, MMP94, RPK96, GMMP97, TP04], however, their usage for discrete system has not yet been explored systematically. In [Mac02, Mac04] some results in this direction are obtained. One problem with the above transport equation is that it only holds if the group-velocity mapping is $\theta\mapsto\nabla_\theta\omega_j(\theta)$ differentiable. If $\nabla_\theta\omega_j$ is not continuous on a singular set $\mathbb{S}\subset\mathcal{T}_{\Gamma_*}$, then (1.8) can still be derived under the additional restriction that there is no energy located in $\mathbb{S}$, i.e., $\mu_j(\tau,\mathbb{R}^d\times\mathbb{S})=0$ for all τ, see Theorem 5.6. As in our situation of a perfect periodic crystal there is no transport between different wave vectors, it is sufficient to have this condition for the initial data at $\tau=0$. Such singularities occur generically in all crystal models, as near the wave vector $\theta=0$ the acoustic branches of the dispersion relation have expansions $\omega_j(\theta)=(\langle Q_j\theta,\theta\rangle+O(|\theta|^3))^{1/2}$ for some positive definite matrix $Q_j\in\mathbb{R}^{d\times d}$.

In Section 5.3 we provide a generalization of the Wigner measure which we call *Husimi measure*. This generalization allows us to generalize the transport equation (1.8) to situations where the group velocity is only continuous. As the Husimi transform has the major advantage that it maps functions from $\mathrm{L}^2(\mathbb{R}^d)$ into nonnegative functions on $\mathrm{L}^1(\mathbb{R}^d\times\mathcal{T}_{\Gamma_*})$ there is the possibility to test with arbitrary continuous functions. We show in Section 3 that all the functions ω_j are Lipschitz and piecewise analytic. Hence, the singular sets $\mathbb{S}_j$ have Lebesgue measure 0 and so has $\mathbb{S}=\cup_1^{2m}\mathbb{S}_j$. Finally, there exists a compactification $\mathbb{K}$ of $\mathcal{T}_{\Gamma_*}\backslash\mathbb{S}$ such that all $\nabla_\theta\omega_j$ have continuous extensions $\widetilde{\nabla_\theta}\omega_j:\mathbb{K}\to\mathbb{R}^d$.

In Theorem 5.7 we show that (1.8) can be generalized to an energy-transport equation on $\mathbb{R}^d\times\mathbb{K}$ under the following two conditions: First, the functions $\nabla_\theta\omega_j$ must behave nicely near $\mathbb{S}$, for instance it is sufficient when $|\mathrm{D}^2\omega_j(\theta)|\le C/\mathrm{dist}(\theta,\mathbb{S})$ for all $\theta\in\mathcal{T}_{\Gamma_*}\backslash\mathbb{S}$. Second, because the Husimi transform is less precise in locating the energy in terms of the

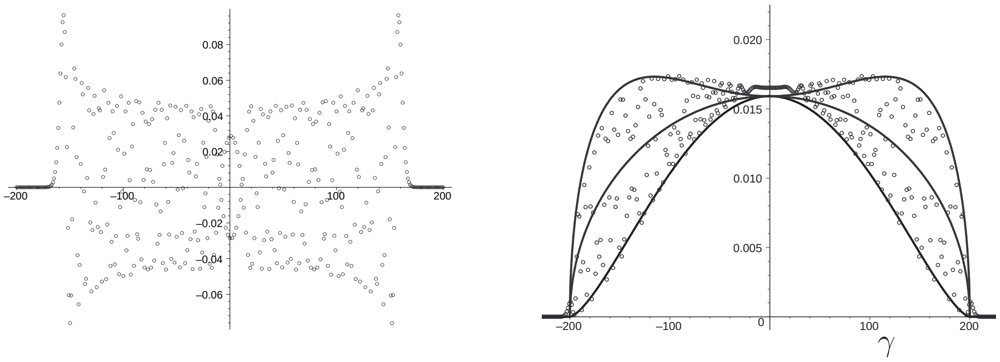


Figure 1.1: Green's function for t=200: displacements x_γ (left) and energies e_γ (right).

corresponding wave vectors, we have to assume that the energy does not concentrate as fast as $\varepsilon^{1/2}$ on $\mathbb{S}$, i.e., for all $R > 0$ we need

$$\int_{\operatorname{dist}(\theta,\mathbb{S})<\varepsilon^{1/2}R} \tfrac{1}{(2\varepsilon\pi)^d} |\widehat{U}^\varepsilon(\theta/\varepsilon)|^2 \,\mathrm{d}\theta \;\longrightarrow 0 \quad \text{for } \varepsilon \to 0.$$

In Section 6 we underpin and illustrate the abstract theory via several examples. Section 6.1 discusses the question of the convergence of Husimi and Wigner measures for a simple one-dimensional problem with dispersion relation $\omega(\theta) = 2|\sin(\theta/2)|$ for $\theta \in \mathbb{R}_{/2\pi\mathbb{Z}}$. We show that the for initial conditions which concentrate at $\theta = 0$, the corresponding transport equation may not be satisfied. Moreover, if we take out $\mathbb{S} = \{0\}$, compactify by introducing the left and right limits at 0^+ and 0^- and extend $\nabla\omega$ by $+1$ and -1, respectively, we find that the corresponding Wigner and Husimi measures may be different.

In Section 6.2 we show some simulations for the linear harmonic chain

$$\ddot{x}_\gamma = x_{\gamma-1} - 2x_\gamma + x_{\gamma+1}, \quad \gamma \in \mathbb{Z},$$

which was studied also in [Fri03] by completely different methods, namley the explicit representation of the solution via oscillatory integrals. The left picture in Figure 1.1 shows the displacements x_γ for the Green's function (with intial condtions $x_\gamma(0) = \delta_\gamma$ and $\dot{x}(t)_\gamma = 0$ at time $t = 200$). The right picture displays the energies $e_\gamma = \frac{1}{2}\dot{x}_\gamma^2 + \frac{1}{4}(x_\gamma - x_{\gamma+1})^2 + \frac{1}{4}(x_\gamma - x_{\gamma-1})^2$ for the same solution. The middle line shows the distribution predicted by the Wigner measure, namely the semicircle law $e(\tau, y) = \frac{1}{\tau\pi}\sqrt{1-(y/\tau)^2}$. It turns out that the convergence towards the Wigner measure is weak and that the fluctuations around the local mean value satisfy an arcsin distribution.

In Section 6.4 we analyze the standard discretization

$$\ddot{x}_\gamma = -4x_\gamma + x_{\gamma+(0,1)} + x_{\gamma+(0,-1)} + x_{\gamma+(1,0)} + x_{\gamma+(-1,0)}$$

for the wave equation $\partial_\tau^2 u = \Delta_y u$ and show that the macroscopic energy distribution $e(\tau,\cdot) : \mathbb{R}^2 \to [0,\infty)$ for the Green's function is singular along a closed curve strictly inside its support which is the circle obtain from the macroscopic wave speeds c with $|c| = 1$, see Figures 6.4 and 6.5.

In Section 6.6 we finally compare the energy-transport equation obtained via the Wigner measure with Whitham's modulation equation (1.2). A formal calculation shows that in the intersection of their applicability both theories lead to the same partial differential equation for the transport of the microscopic wave-vector and the energy.

2 Fourier transform and lattices

We introduce our conventions and notations concerning Fourier transforms and lattices. In particular, we give all the normalizing constants. For $u \in \mathrm{L}^2(\mathbb{R}^d)$ we define the Fourier transformation $\mathcal{F} = \mathcal{F}_{y\to\eta}$ via

$$\widehat{u}(\eta) = (\mathcal{F}u)(\eta) \stackrel{\text{def}}{=} \int_{y\in\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}y\cdot\eta} u(y)\,\mathrm{d}y,\ \eta \in \mathbb{R}^d_* = \mathrm{Lin}(\mathbb{R}^d, \mathbb{R})$$

implying $\|\mathcal{F}u\|_* = (2\pi)^{d/2}\|u\|$. The inverse Fourier transform $\mathcal{F}^{-1} = \mathcal{F}^{-1}_{\eta\to y}$ then reads

$$u(y) = (\mathcal{F}^{-1}\widehat{u})(y) = (2\pi)^{-d} \int_{\eta\in\mathbb{R}^d_*} \mathrm{e}^{\mathrm{i}y\cdot\eta} \widehat{u}(\eta)\,\mathrm{d}\eta,\ y \in \mathbb{R}^d,$$

with the norm relation $\|\mathcal{F}^{-1}\widehat{u}\| = (2\pi)^{-d/2}\|\widehat{u}\|_*$.

A d–dimensional lattice $\Gamma \subset \mathbb{R}^d$ is an additive subgroup of $\mathbb{R}^d$ which has the form

$$\Gamma = \{\, \gamma = k_1 g_1 + \cdots + k_d g_d \mid k = (k_1, \ldots, k_d) \in \mathbb{Z}^d \,\}$$

where $\{g_1, \ldots, g_d\}$ is a set of linearly independent vectors. The dual lattice Γ_* is defined via

$$\Gamma_* := \{\, \theta \in \mathbb{R}^d_* \mid \forall \alpha \in \Gamma : \theta \cdot \alpha \in 2\pi\mathbb{Z} \,\},$$

For the primal lattice Γ the unit cell U_Γ is given by

$$U_\Gamma := \{\, \gamma = k_1 g_1 + \cdots + k_d g_d \mid k_j \in [0, 1) \text{ for } j = 1, \ldots, d) \,\}.$$

While this definition of U_Γ depends on the choice of the generating vectors $\{g_1, \ldots, g_d\}$, the volume $V_\Gamma := \mathrm{vol}(U_\Gamma)$ of the unit cell of Γ depends on Γ alone.

For the dual lattice it is common to a use the Brillouin zone B_{Γ_*} as the unit cell,

$$B_{\Gamma_*} = \{\, \eta \in \mathbb{R}^d_* \mid \forall \gamma_* \in \Gamma_* \setminus \{0\} : |\eta| < |\eta - \gamma_*| \,\} \subset \mathbb{R}^d_*.$$

Hence, B_{Γ_*} is an open bounded subset of $\mathbb{R}^d_*$ which contains $\eta = 0$ in its interior. Moreover, for the volume we have the relation

$$\mathrm{vol}(U_\Gamma)\,\mathrm{vol}(B_{\Gamma_*}) = (2\pi)^d.$$

The dual torus $\mathcal{T}_{\Gamma_*}$ associated with the lattice Γ is defined as the compact manifold

$$\mathcal{T}_{\Gamma_*} := \mathbb{R}^d_*/_{\Gamma_*} = \{\, \theta := (\eta + \Gamma_*) \subset \mathbb{R}^d_* \mid \eta \in \mathbb{R}^d \,\}.$$

For each lattice $\mathcal{T}_{\Gamma_*}$ is a d–dimensional torus diffeomorphic to $\mathbb{T}^d := (\mathbb{S}^1)^d$. It is important to distinguish the dual torus $\mathcal{T}_{\Gamma_*}$ from the Brillouin zone B_{Γ_*}, the first being a compact manifold without boundary and the latter being a subset of $\mathbb{R}^d_*$. However, $\mathcal{T}_{\Gamma_*}$ can be obtained from the closure of the Brillouin zone by identifying the boundary hypersurfaces with their opposites.

For $x = (x_\gamma)_{\gamma\in\Gamma} \in \ell^2(\Gamma)$ we define the periodic function $\widetilde{X} = \mathcal{F}_{\Gamma_*}x$ via

$$\widetilde{X}(\theta) = (\mathcal{F}_{\Gamma_*}x)(\theta) \stackrel{\text{def}}{=} c_{\Gamma_*} \textstyle\sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}\theta\cdot\gamma} x_\gamma$$

for $\theta \in \mathcal{T}_{\Gamma_*} = \mathbb{R}^d_*/\Gamma_*$. The minus sign in $\mathrm{e}^{-\mathrm{i}\theta\cdot\gamma}$ is chosen for later consistency with the continuous Fourier transform. Choosing $c_{\Gamma_*} = \mathrm{vol}(\mathcal{T}_{\Gamma_*})^{-1/2}$ we obtain

$$\|\widetilde{X}\|^2_{\mathrm{L}^2(\mathcal{T}_{\Gamma_*})} = \textstyle\sum_{\gamma\in\Gamma} |x_\gamma|^2 = \|x\|_{\ell^2}.$$

Using the length scale parameter $\varepsilon > 0$ we may associate with each $x \in \ell^2(\Gamma)$ a function $\widehat{X} = \mathcal{B}_\varepsilon x \in \mathrm{L}^2(\mathbb{R}^d_*)$ via

$$\widehat{X}(\eta) = (\mathcal{B}_\varepsilon x)(\eta) \stackrel{\text{def}}{=} \begin{cases} \varepsilon^{d/2}\widetilde{X}(\varepsilon\eta) & \text{for } \eta \in \frac{1}{\varepsilon}B_{\Gamma_*}, \\ 0 & \text{else.} \end{cases}$$

Again, we have $\|\mathcal{B}_\varepsilon x\|_{\mathrm{L}^2(\mathbb{R}^d_*)} = \|x\|_{\ell^2}$. Later on we will use θ to denote the microscopic wave vectors in $\mathcal{T}_{\Gamma_*}$ and we use $\eta \in \mathbb{R}^d_*$ to denote the macroscopic wave vectors which are dual to the macroscopic space variable $y = \varepsilon\gamma \in \mathbb{R}^d$.

The function $\widehat{X}$ can be transformed into a function $X = \mathcal{S}_\varepsilon x \in \mathrm{L}^2(\mathbb{R}^d)$ by inverse Fourier transform

$$X = \mathcal{S}_\varepsilon x = (2\pi)^{2/d}\mathcal{F}^{-1}(\mathcal{B}_\varepsilon x). \tag{2.1}$$

By construction, $\mathcal{S}_\varepsilon : \ell^2(\Gamma) \to \mathrm{L}^2(\mathbb{R}^d)$ has the following useful properties

$$\begin{aligned} &\|\mathcal{S}_\varepsilon x\|_{\mathrm{L}^2(\mathbb{R}^d)} = \|x\|_{\ell^2(\Gamma)}, \\ &(\mathcal{S}_\varepsilon x)(y) = \mathrm{vol}(B_{\Gamma_*})^{-1/2}\big(\tfrac{2\pi}{\varepsilon}\big)^{d/2} \textstyle\sum_{\gamma\in\Gamma} x_\gamma \mathrm{sinc}_\Gamma(\tfrac{y}{\varepsilon}-\gamma), \end{aligned} \tag{2.2}$$

where sinc_Γ is the "sinc function" associated with the lattice Γ. It is defined via $\mathrm{sinc}_\Gamma := \frac{(2\pi)^d}{\mathrm{vol}(B_{\Gamma_*})}\mathcal{F}^{-1}\mathcal{X}_{B_{\Gamma_*}}$, where $\mathcal{X}$ is the indicator function. In particular, it satisfies the relations

$$\mathrm{sinc}_\Gamma(\gamma) = \delta_\gamma \quad \text{and} \quad \int_{\mathbb{R}^d} \mathrm{sinc}_\Gamma(y-\gamma)\mathrm{sinc}_\Gamma(y-\beta)\,\mathrm{d}y = \frac{(2\pi)^d}{\mathrm{vol}(B_{\Gamma_*})}\,\delta_{\gamma-\beta} \tag{2.3}$$

for all $\beta, \gamma \in \Gamma$.

Thus, we have defined the four equivalent descriptions $x \in \ell^2(\Gamma)$, $\widetilde{X} = \mathcal{F}_{\Gamma_*}x \in \mathrm{L}^2(\mathcal{T}_{\Gamma_*})$, $\widehat{X} = \mathcal{B}_\varepsilon x \in \mathrm{L}^2(\mathbb{R}^d_*)$ and $X = \mathcal{S}_\varepsilon x \in \mathrm{L}^2(\mathbb{R}^d)$. The definition of the transformations are such that they are norm invariant. The first two representations $x \in \ell^2(\Gamma)$ and $\widetilde{X} \in \mathrm{L}^2(\mathcal{T}_{\Gamma_*})$ are more useful for extracting microscopic information, whereas the other two representiations $\widehat{X} \in \mathrm{L}^2(\mathbb{R}^d_*)$ and $X \in \mathrm{L}^2(\mathbb{R}^d)$ are more useful to study macroscopic properties. We illustrate the four equivalent descriptions in Figure 2.1.

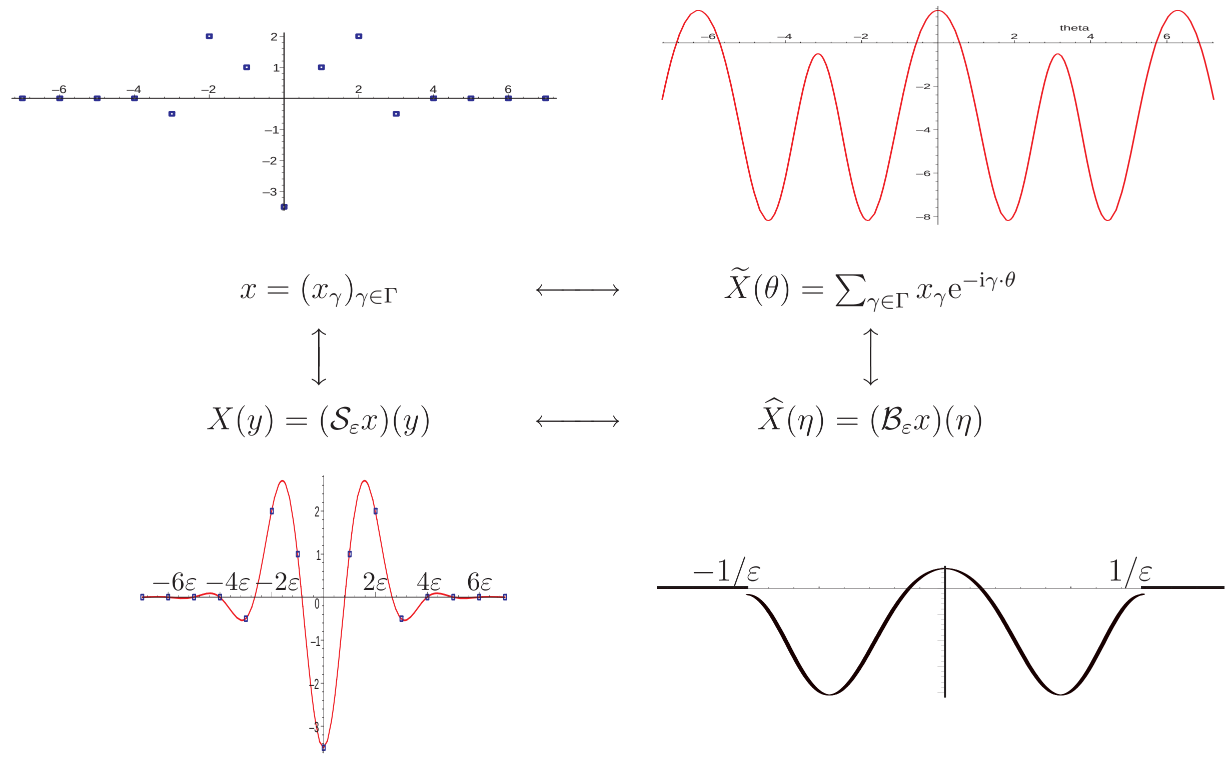


Figure 2.1: The four equivalent descriptions of a sequence on a lattice: $x \in \ell^2(\Gamma)$, $\widetilde{X} = \mathcal{F}_{\Gamma_*}x \in \mathrm{L}^2(\mathcal{T}_{\Gamma_*})$, $X = \mathcal{S}_\varepsilon x \in \mathrm{L}^2(\mathbb{R}^d)$ and $\widehat{X} = \mathcal{B}_\varepsilon x \in \mathrm{L}^2(\mathbb{R}^d_*)$.

3 Harmonic lattice dynamics

We consider a d-dimensional polycrystal whose atoms are placed at lattice sites in the discrete set $\widetilde{\Gamma} \subset \mathbb{R}^d$. The atoms at $\widetilde{\alpha} \in \widetilde{\Gamma}$ have the mass $m_{\widetilde{\alpha}}$ and interact with the neighboring atoms via linearized interaction forces such that the atomistic, Newtonian model for the displacement $u_{\widetilde{\gamma}} \in \mathbb{R}^n$ takes the form

$$m_{\widetilde{\gamma}}\ddot{u}_{\widetilde{\gamma}} = -\sum_{\widetilde{\alpha}\in\widetilde{\Gamma}} \widetilde{A}_{\widetilde{\gamma},\widetilde{\alpha}} u_{\widetilde{\alpha}}.$$

Usually $n = d$ but we may also assume $n < d$ for problems where motion only occurs in subspaces. Also $n > d$ might be relevant if further order parameters are taken into account.

Throughout we assume that the crystal is periodic with respect to a lattice group Γ. Note that in general $\Gamma \subset \widetilde{\Gamma}$ where Γ is an additive group (Bravais lattice), while $\widetilde{\Gamma}$ is the set of positions of atoms, which need not have a group structure. Associated with the lattice is the semi-closed unit cell U_Γ. The periodicity of the crystal is expressed by the fact that the masses and the interactions of the atoms are the same after translating by a lattice vector $\gamma \in \Gamma$:

$$m_{\widetilde{\alpha}+\gamma} = m_{\widetilde{\alpha}}, \qquad \widetilde{A}_{\widetilde{\alpha}+\gamma,\widetilde{\beta}+\gamma} = \widetilde{A}_{\widetilde{\alpha},\widetilde{\beta}} \tag{3.1}$$

for all $\widetilde{\alpha}, \widetilde{\beta} \in \widetilde{\Gamma}$ and all $\gamma \in \Gamma$.

Thus, by factoring the lattice sites $\widetilde{\Gamma}$ with respect to the lattice group we obtain an elementary cell $C = \widetilde{\Gamma}/_{\Gamma}$ which is assumed to consist of finitely many points, let us say $k \in \mathbb{N}$. We identify C with the mass points in the unit cell U_Γ, i.e., $C \approx C_0 \overset{\text{def}}{=} \widetilde{\Gamma} \cap U_\Gamma$. In particular, we have $C_0 = \{\widetilde{\alpha}_1, \dots, \widetilde{\alpha}_k\} \subset \widetilde{\Gamma}$ and $\widetilde{\Gamma}$ decomposes into a disjoint union of cells $C_\gamma = \gamma + C$.

For each cell C_γ we define the displacement vector $x_\gamma \in \mathbb{R}^{kn}$, a mass matrix $M_\gamma \in \mathbb{R}^{kn\times kn}$ and interaction matrices $A_{\gamma,\widehat{\gamma}} =\in \mathbb{R}^{kn\times kn}$ via

$$x_\gamma = (u_{\widetilde{\alpha}_j+\gamma})_{j=1,\dots,k}, \quad M_\gamma = \operatorname{diag}(m_{\widetilde{\alpha}_j+\gamma})_{j=1,\dots,k}, \quad \widehat{A}_{\gamma,\widehat{\gamma}} = (\widetilde{A}_{\widetilde{\alpha}_i+\gamma,\widetilde{\alpha}_j+\widehat{\gamma}})_{i,j=1,\dots,k}.$$

By periodicity we have $M_\gamma = M$ with $M \overset{\text{def}}{=} M_0$ and $\widehat{A}_{\gamma,\widehat{\gamma}} = A_{\gamma-\widehat{\gamma}}$ with $A_\gamma \overset{\text{def}}{=} \widehat{A}_{0,\gamma}$.

Using $m = kn$ we arrive at the following general system

$$M\ddot{x}_\gamma = -\sum_{\beta\in\Gamma} A_{\gamma-\beta}x_\beta = -\sum_{\alpha\in\Gamma} A_\alpha x_{\gamma+\alpha} \quad \text{for } \gamma \in \Gamma. \tag{3.2}$$

Note that the mass matrix $M \in \mathbb{R}^{m\times m}$ is the symmetric and positive definite. If the interaction matrices A_α satisfy $A_\alpha = 0$ for all $\alpha \in \Gamma$ with $|\alpha| > R$ we say that the system has finite-range interaction. In the case of infinite interaction we assume sufficiently rapid decay, e.g. $\|A_\alpha\| \le C_0 \mathrm{e}^{-b|\alpha|}$ with $b > 0$.

If the interaction matrices $\widetilde{A}_{\widetilde{\alpha},\widetilde{\gamma}} \in \mathbb{R}^{d\times d}$ satisfy $\widetilde{A}_{\widetilde{\alpha},\widetilde{\gamma}} = \widetilde{A}^{\mathsf{T}}_{\widetilde{\gamma},\widetilde{\alpha}}$, then we also have $A_\alpha^{\mathsf{T}} = A_{-\alpha} \in \mathbb{R}^{m\times m}$. This will be taken for granted from now on. Then, our system is in an infinite-dimensional Hamiltonian system with kinetic energy $\mathcal{K}(\dot{x})$ and potential energy $\mathcal{U}(x)$ given by

$$\mathcal{K}(\dot{x}) = \tfrac{1}{2}\sum_{\gamma\in\Gamma}\langle \dot{x}_\gamma, M\dot{x}_\gamma\rangle \ \text{ and } \ \mathcal{U}(x) = \tfrac{1}{2}\sum_{\gamma\in\Gamma}\sum_{\alpha\in\Gamma}\langle x_\gamma, A_\alpha x_{\alpha+\gamma}\rangle,$$

where $\langle\,\cdot\,,\,\cdot\,\rangle$ denotes the scalar product in $\mathbb{R}^m$ (or $\mathbb{C}^m$). Clearly, the total energy $\widehat{\mathcal{H}} \overset{\text{def}}{=} \mathcal{K}+\mathcal{U}$ is conserved and (3.2) has the Lagrangian form

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial}{\partial \dot{x}_\gamma}\mathcal{K}(\dot{x})\Big) + \frac{\partial}{\partial x_\gamma}\mathcal{U}(x) = 0.$$

Introducing the momenta $p_\gamma = M\dot{x}_\gamma$ we also have the Hamiltonian form

$$\dot{x}_\gamma = \frac{\partial}{\partial p_\gamma}\mathcal{H}(x,p), \quad \dot{p}_\gamma = -\frac{\partial}{\partial x_\gamma}\mathcal{H}(x,p),$$

where $\mathcal{H}(x,p) = \mathcal{K}(M^{-1}p) + \mathcal{U}(x)$.

The linear system (3.2), which is translationally invariant with respect to Γ, admits special solutions in the form of plane waves

$$x_\gamma(t) = \mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}\theta\cdot\gamma}\Phi \text{ with } \Phi \in \mathbb{C}^m, \tag{3.3}$$

where $\theta \in \mathbb{R}^d_*$ is the wave vector, ω is the frequency, and "$\cdot$" denotes the dual pairing between $\mathbb{R}^d_*$ and $\mathbb{R}^d$. Clearly, x_γ in (3.3) solves (3.2) if and only if

$$(\omega^2 M - \mathbb{A}(\theta))\Phi = 0 \text{ where } \mathbb{A}(\theta) = \sum_{\alpha\in\Gamma} A_\alpha \mathrm{e}^{\mathrm{i}\theta\cdot\alpha}.$$

We call $\mathbb{A}$ the dispersion matrix, and later on the symbol. We always have the symmetries $\mathbb{A}(\theta) = \mathbb{A}(\theta)^* = \mathbb{A}(-\theta)^\mathsf{T}$ (where * denotes complex conjugation together with transposition $^\mathsf{T}$).

There may be further symmetries in the crystal which we do not formalize here. For instance, reflection symmetries of the lattice are given by two linear operators $R_d \in \mathbb{R}^{d\times d}$ and $R_m \in \mathbb{R}^{m\times m}$, which are involutions (i.e., $R_d^2 = \mathbf{1}_{\mathbb{R}^d}$, $R_m^2 = \mathbf{1}_{\mathbb{R}^m}$), R_d maps Γ onto itself, and the mass and the interaction matrices satisfy

$$R_m M R_m = M, \quad R_m A_\gamma R_m = A_{R_d\gamma}.$$

Then, the dispersion matrix satisfies $R_m \mathbb{A}(R_d^*\theta) R_m = \mathbb{A}(\theta)$.

Using the dual lattice Γ_*, it is immediate that $\mathbb{A}$ is periodic with $\mathbb{A}(\theta+\zeta) = \mathbb{A}(\theta)$ for all $\theta \in \mathbb{R}^d_*$ and $\zeta \in \Gamma_*$. Hence, $\mathbb{A}$ should be considered as a mapping from the torus $\mathcal{T}_{\Gamma_*} = \mathbb{R}^d_*/_{\Gamma_*}$ into $\mathbb{H}(\mathbb{C}^m)$, where for any linear complex space $V \subset \mathbb{C}^m$ we let $\mathbb{H}(V) \overset{\text{def}}{=} \{ A \in \mathrm{Lin}(V,V) \mid A = A^* \}$.

We now make the first essential assumption, namely the **stability condition**:

$$\begin{aligned} &\mathbb{A}(\theta) \text{ is positive semidefinite for all } \theta \in \mathcal{T}_{\Gamma_*}, \\ &\exists\, c > 0\, \forall\, \theta \in B_{\Gamma_*}: \ \mathbb{A}(\theta) \geq c|\theta|^2, \\ &\dim\ker \mathbb{A}(0) = d_0 \in \{0, 1, ..., m\}. \end{aligned} \tag{3.4}$$

From this it follows that for each $\theta \in \mathcal{T}_{\Gamma_*}$ there exists m pairs $\pm\omega_j(\theta)$, $j = 1, \ldots, m$, of frequencies. Throughout this paper, we will order the nonnegative frequencies such that $0 \leq \omega_1(\theta) \leq \ldots \leq \omega_j(\theta) \leq \ldots \leq \omega_m(\theta)$. The frequencies ω_j for $j = 1, \ldots, d_0$ will correspond to macroscopic behavior, since they satisfy $\omega_j(\theta) = O(|\theta|)$. These frequencies are called “acoustic” in contrast to the “optical” or “photonic” frequencies ω_j with $j = d_0{+}1, \ldots, m$. For the usual crystal model with $n = d$ the dimension d_0 usually equals the space dimension d, since the rigid translation $u_{\widetilde{\gamma}} \equiv u^\circ \in \mathbb{R}^d$ is a solution which implies $\sum_{\widetilde{\alpha}\in\widetilde{\Gamma}} \widetilde{A}_{\widetilde{\gamma},\widetilde{\alpha}} u^\circ = 0$. Thus, for each $u^\circ \in \mathbb{R}^d$ the vector $v = (u^\circ, \ldots, u^\circ) \in \mathbb{R}^{kd} = \mathbb{R}^m$ lies in the kernel of $\mathbb{A}(0) = \sum_{\gamma\in\Gamma} A_\gamma$.

For $V \overset{\text{def}}{=} \ker \mathbb{A}(0)$ and $V^\perp \overset{\text{def}}{=} \{ w \in \mathbb{C}^m \mid \langle v, w\rangle = 0 \text{ for all } v \in V \}$ we have $\dim V = d_0$ and denote by $P_V \in \mathbb{H}(\mathbb{C}^m)$ the orthogonal projection onto V. Usually, the subspace V corresponds to the translational degrees of freedom of the cells as a whole, whereas the subspace $V^\perp$ corresponds to the internal degree of freedoms of the cells.

Using the fundamental stability assumption (3.4) we obtain the following result.

Lemma 3.1 *Assume that* $\mathbb{A} \in \mathrm{C}^2(\mathcal{T}_{\Gamma_*}, \mathbb{H}(\mathbb{C}^m))$ *and that* (3.4) *holds. Using the decomposition* $\mathbb{C}^m = V \oplus V^\perp$ *the dispersion matrix* $\mathbb{A}(\theta)$ *has the block structure*

$$\mathbb{A}(\theta) = \begin{pmatrix} \mathbb{A}_{11}(\theta) & \mathbb{A}_{12}(\theta) \\ \mathbb{A}_{12}^*(\theta) & \mathbb{A}_{22}(\theta) \end{pmatrix} = \begin{pmatrix} O(|\theta|^2) & O(|\theta|) \\ O(|\theta|) & O(1) \end{pmatrix} \textit{ for } \theta \to 0 \textit{ in } B_{\Gamma_*}.$$

Moreover, there exists $C_V > 0$ such that for all $w \in V^\perp$, $v \in V$ and $\theta \in B_{\Gamma_*}$ we have

$$\tfrac{1}{C_V}(|\theta|^2|v|^2 + |w|^2) \leq \langle \mathbb{A}(\theta)(v{+}w), v{+}w\rangle \leq C_V(|\theta|^2|v|^2 + |w|^2). \tag{3.5}$$

Proof: From $V = \ker \mathbb{A}(0)$ we conclude $\mathbb{A}_{11}(0) = \mathbb{A}_{12}(0) = 0$. However, (3.4) implies $\mathbb{A}(\theta) \geq 0$ for all $\theta \in B_{\Gamma_*}$, which gives $\mathrm{D}_\theta \mathbb{A}_{11}(0) = 0$.

For $v \in V$, $w \in V^\perp$, and $\theta \in B_{\Gamma_*}$ we have now $|\langle \mathbb{A}(\theta)v, w\rangle| \leq |\mathbb{A}_{12}(\theta)^* v|\,|w| \leq C_{12}|\theta|\,|v|\,|w|$ and $\langle \mathbb{A}_{22}(\theta)w, w\rangle \geq c_{22}|w|^2$ for suitable constants $c_{22}, C_{12} > 0$. For $\alpha \in (0,1)$ we estimate

$$\begin{aligned}
&\langle \mathbb{A}(\theta)(v{+}w), v{+}w\rangle = (1{-}\alpha)\langle \mathbb{A}(\theta)(v{+}w), v{+}w\rangle + \alpha\langle \mathbb{A}(\theta)(v{+}w), v{+}w\rangle\\
&\geq (1{-}\alpha)c|\theta|^2(|v|^2{+}|w|^2) + \alpha\Big[\langle \mathbb{A}_{11}(\theta)v, v\rangle{+}2\,\mathrm{Re}\langle \mathbb{A}_{12}(\theta)w, v\rangle{+}\langle \mathbb{A}_{22}(\theta)w, w\rangle\Big]\\
&\geq c|\theta|^2|v|^2 + \alpha\Big[\langle \mathbb{A}_{11}(\theta)v, v\rangle - c|\theta|^2|v|^2\Big] - 2\alpha C_{12}|\theta||v||w| + \Big[(1{-}\alpha)|\theta|^2 + \alpha c_{22}\Big]|w|^2\\
&\geq c|\theta|^2|v|^2 - 2\alpha C_{12}|\theta||v||w| + \alpha c_{22}|w|^2.
\end{aligned}$$

Choosing $\alpha < c_{22}c/C_{12}^2$ we obtain the desired result. ■

The appearance of the nontrivial kernel is often due to the Galileian invariance which leads to $d_0 = d$. For a monoatomic system with $m = d$ the variables $x_\gamma \in \mathbb{R}^d$ simply denotes the displacement of the particle with position $\gamma \in \Gamma \subset \mathbb{R}^d$. Galileian invariance then means $V = \mathbb{C}^m$ and we have

$$\begin{aligned}
&\mathbb{A}(0) = \textstyle\sum_{\gamma\in\Gamma} A_\gamma = 0, \quad \mathbb{A}_1[\eta] = \sum_{\gamma\in\Gamma} \gamma{\cdot}\eta A_\gamma = 0,\\
&\text{and} \quad \mathbb{A}_2[\eta] = \textstyle\sum_{\gamma\in\Gamma}(\gamma{\cdot}\eta)^2 A_\gamma \geq c > 0 \text{ for all } \eta \in \mathbb{R}^d,
\end{aligned} \tag{3.6}$$

where $\mathbb{A}_1[\eta] = \mathrm{D}\mathbb{A}(0)[\eta]$ and $\mathbb{A}_2[\eta] = \mathrm{D}^2\mathbb{A}(0)[\eta, \eta]$.

Because of $\|A_\beta\| \leq C\mathrm{e}^{-b|\beta|}$ the symbol matrix $\mathbb{A}$ depends smoothly on $\theta \in \mathcal{T}_{\Gamma_*}$, but this does not imply that all ω_j are smooth functions, since multiple eigenvalues may occur. General spectral theory for Hermitian matrices implies that $\theta \mapsto \omega_j(\theta)^2$ is always Lipschitz continuous. We now show that in fact $\theta \mapsto \omega_j(\theta)$ is Lipschitz which is nontrivial for $\theta \approx 0$, since $\omega_j(\theta) = O(|\theta|)$ for $j = 1, \ldots, d_0$.

Choose θ such that ω_j is smooth in this point and choose a direction $\eta \in \mathbb{R}^d_*$. Then we let $\mathbb{A}'(\theta) = \mathrm{D}\mathbb{A}(\theta)[\eta]$ and $\omega_j'(\theta) = \mathrm{D}\omega_j(\theta)[\eta]$. With $\Phi_j' = \mathrm{D}\Phi_j(\theta)[\eta]$ we have

$$(\mathbb{A}{-}\omega_j^2 M)\Phi_j = 0 \quad \text{ and } \quad (\mathbb{A} - \omega_j^2 M)\Phi_j' = (\mathbb{A}'{-}2\omega_j\omega_j' M)\Phi_j.$$

Taking the scalar product with Φ_j in both equations gives

$$|\omega_j'|^2 \leq \frac{\langle \mathbb{A}'\,\Phi_j, \Phi_j\rangle^2}{4\langle \mathbb{A}\Phi_j, \Phi_j\rangle\,\langle \mathbb{M}\Phi_j, \Phi_j\rangle}.$$

Our assumptions on $\mathbb{A}(\theta)$ imply

$$\begin{aligned}\langle \mathbb{A}(\theta)(v{+}w), v{+}w\rangle &\geq \frac{1}{C_V}(|\theta|^2|v|^2 + |w|^2),\\ \langle M(v{+}w), v{+}w\rangle &\geq \frac{1}{C_M}(|v|^2 + |w|^2),\\ \langle \mathbb{A}'(\theta)(v{+}w), v{+}w\rangle &\leq C'(|\theta||v|^2 + |v||w| + |w|^2).\end{aligned}$$

Hence, we conclude $|\omega_j'|^2 \leq \frac{3}{4}(C')^2 C_M C_V$ and obtain Lipschitz continuity.

In the special case of a mono-atomic crystal with $m = d$ we have $V = \mathbb{R}^d$ and $\mathbb{A}(0) = \sum_{\beta\in\Gamma} A_\eta = 0$. If additionally $A_\beta = A_\beta^\top \leq 0$ holds for $\beta \neq 0$ (which is the case for attracting potentials), we can show that $\sup\{\,|\nabla\omega_j(\theta)| \mid \theta \in \mathcal{T}_{\Gamma_*}\,\}$ is approached near $\theta = 0$, i.e., the macroscopic group velocities have maximal modulus. With

$$\mathbb{A}'(\theta) = \mathrm{D}\mathbb{A}(\theta)[\eta] = \textstyle\sum_{\beta\neq 0}(\beta\cdot\eta)\sin(\beta\cdot\theta)(-A_\beta)$$

and $(\sin\alpha)^2 \leq 2(1-\cos\alpha)$ we obtain

$$\begin{aligned}\langle \mathbb{A}'(\theta)\Phi, \Phi\rangle^2 &= \textstyle\sum_{\beta\neq 0}(\beta\cdot\eta)\sin(\beta\cdot\theta)\langle -A_\beta\Phi, \Phi\rangle)^2\\ &\leq (\textstyle\sum(\beta\cdot\eta)^2\langle -A_\beta\Phi, \Phi\rangle)(\sum 2[1-\cos(\phi\cdot\beta)]\langle -A_\beta\Phi, \Phi\rangle)\\ &= \langle \mathrm{D}^2\mathbb{A}(0)[\eta,\eta]\Phi, \Phi\rangle 2\langle \mathbb{A}(\theta)\Phi, \Phi\rangle.\end{aligned}$$

With the above discussion this implies

$$|\mathrm{D}\omega_j(\theta)[\eta]|^2 \leq \frac{1}{2}\,\frac{\langle \mathrm{D}^2\mathbb{A}(0)[\eta,\eta]\Phi_j, \Phi_j\rangle}{\langle M\Phi_j, \Phi_j\rangle}$$

and we will see later, that the right-hand side is achieved in the long-wave limit $\theta \to 0$.

Including repelling interaction forces (i.e., $A_\beta \not\leq 0$), we may have group velocities with $|\nabla\omega_j(\theta_*)| > \limsup_{\theta\to 0}|\nabla\omega_j(\theta)|$. As an example consider $m = d = 1$ with

$$\omega(\theta)^2 = \sum_{m=1}^{5} a_m 2(1-\cos(m\theta)), \text{ where } a_1 = 0,\ a_2 = 3,\ a_3 = 5,\ a_4 = -2,\ a_5 = 1.$$

We find $\lim_{\theta\to 0}|\omega'(\theta)| = 5\sqrt{2} \approx 7.071 < \omega'(\theta^*) \approx 7.132$ for $\theta^* = 2.59$.

4 Weak convergence to a wave equation

We will associate with our lattice model a macroscopic partial differential equation. It relates to linear elasto-dynamics in most cases, namely when $V = \ker\mathbb{A}(0)$ has dimension $d_0 = d$ and is given by the rigid translations of the unit cell. However, in certain degenerate cases we might also have $\dim V > d$.

We define macroscopic spatial and temporal variables

$$y = \varepsilon\gamma \in \mathbb{R}^d \quad \text{and} \quad \tau = \varepsilon t \in \mathbb{R}$$

and use the norm preserving isomorphism $\mathcal{S}_\varepsilon$ defined in Section 2 between $\ell^2(\Gamma,\mathbb{R}^m)$ and $\mathcal{P}_\varepsilon \mathrm{L}^2(\mathbb{R}^d,\mathbb{R}^m)$ where $\mathcal{P}_\varepsilon$ is the orthogonal projection defined via

$$\mathcal{F}(\mathcal{P}_\varepsilon Z)(\eta) = \mathcal{X}_{\frac{1}{\varepsilon}B_{\Gamma_*}}(\eta)\mathcal{F}Z(\eta). \tag{4.1}$$

Thus, a function $x:\mathbb{R}\to\ell^2(\Gamma,\mathbb{R}^m)$ solves the microscopic problem (1.3) if and only if $Z:\mathbb{R}\to\mathrm{L}^2(\mathbb{R}^d,R^m)$ with $Z(\tau)=\varepsilon(\mathcal{S}_\varepsilon x)(\tau/\varepsilon)$ solves

$$MZ''+\mathcal{A}_\varepsilon Z=0 \quad\text{and}\quad Z(\tau)\in\mathcal{P}_\varepsilon\mathrm{L}^2(\mathbb{R}^d,\mathbb{R}^m), \tag{4.2}$$

where $' = \frac{\mathrm{d}}{\mathrm{d}\tau}$ and $\mathcal{A}_\varepsilon\in\mathrm{Lin}(\mathrm{L}^2(\mathbb{R}^d,\mathbb{R}^m)$ is defined via Fourier transform and the rescaled symbol $\mathbb{A}^\varepsilon$ through

$$\mathcal{F}(\mathcal{A}_\varepsilon Z)(\eta)=\mathbb{A}^\varepsilon(\eta)(\mathcal{F}Z)(\eta) \quad\text{and}\quad \mathbb{A}^\varepsilon(\eta)\overset{\text{def}}{=}\begin{cases}\varepsilon^{-2}\mathbb{A}(\varepsilon\eta) & \text{for } \varepsilon\eta\in B_{\Gamma_*},\\ 0 & \text{else.}\end{cases}$$

Note that the scalings were done such that the energies are preserved, i.e.,

$$\textstyle\sum_\Gamma\Big(\langle\dot{x}_\gamma,M\dot{x}_\gamma\rangle+\sum_\Gamma\langle x_\gamma,A_\alpha x_{\gamma+\alpha}\rangle\Big)=\int_{\mathbb{R}^d}\langle Z',MZ'\rangle+\langle Z,\mathcal{A}_\varepsilon Z\rangle\,\mathrm{d}y.$$

Clearly, $\mathcal{A}_\varepsilon$ is again a pseudo-differential operator, and it is obtained by the Fourier symbol $\mathbb{A}^\varepsilon$. We now want to study to which limit this operator converges under the assumption that we are looking at solutions with finite energy.

According to our stability assumption (3.4) the splitting $\mathbb{C}^m=V\oplus V^\perp$ with $V=\ker\mathbb{A}(0)$ gives rise to the block structure $\mathbb{A}=\left(\begin{smallmatrix}\mathbb{A}_{11} & \mathbb{A}_{12}\\ \mathbb{A}_{12}^* & \mathbb{A}_{22}\end{smallmatrix}\right)$, such that the Schur complement

$$\mathbb{B}(\theta)\overset{\text{def}}{=}\mathbb{A}_{11}(\theta)-\mathbb{A}_{12}(\theta)^*\mathbb{A}_{22}(\theta)^{-1}\mathbb{A}_{12}(\theta)\in\mathbb{H}(V) \tag{4.3}$$

is well-defined. Then, Lemma 3.1 implies that $\mathbb{B}^\varepsilon(\eta)\overset{\text{def}}{=}\varepsilon^{-2}\mathbb{B}(\varepsilon\eta)$ converges to $\mathbb{Q}^{(2)}(\eta,\eta)=\frac{1}{2}\mathrm{D}^2\mathbb{B}(0)[\eta,\eta]$ for $\varepsilon\to 0$, uniformly on compact sets in $\mathbb{R}^d_*$, where

$$\mathbb{Q}^{(2)}(\eta_1,\eta_2)=\frac{1}{2}\mathrm{D}^2\mathbb{A}_{11}(0)[\eta_1,\eta_2]-\mathrm{D}\mathbb{A}_{12}(0)^*[\eta_1]\mathbb{A}_{22}(0)^{-1}\mathrm{D}\mathbb{A}_{12}(0)^*[\eta_2]\in\mathbb{H}(V)$$

is a bilinear mapping which satisfies $\mathbb{Q}^{(2)}(\eta_1,\eta_2)=\mathbb{Q}^{(2)}(\eta_2,\eta_1)^*$. Hence, $\mathbb{Q}^{(2)}$ corresponds to a second order differential operator for functions $Z:\mathbb{R}^d\to V$:

$$\mathcal{A}_0 Z\overset{\text{def}}{=}-\mathbb{Q}^{(2)}(\nabla,\nabla)Z=-\mathrm{div}(\mathbb{E}\,[\mathrm{D}Z]),$$

where the fourth order tensor $\mathbb{E}\in\mathrm{Lin}(\mathrm{Lin}(\mathbb{R}^d,V),\mathrm{Lin}(\mathbb{R}^d,V))$ is defined via

$$\mathbb{E}(a\otimes\eta_1)\eta_2=\mathbb{Q}^{(2)}(\eta_1,\eta_2)a \text{ for all } \eta_1,\eta_2\in\mathbb{R}^d_* \text{ and } a\in V. \tag{4.4}$$

Our aim is to show that the macroscopic equation associated to (4.2) is the hyperbolic system

$$M_V Z'' + \mathcal{A}_0 Z = 0 \text{ with } Z(\tau, y) \in V, \tag{4.5}$$

where $M_V = P_V M|_V \in \mathrm{Lin}(V, V)$. Assuming that the kernel of $\mathbb{A}(0)$ is given just by Galileian invariance (see (3.6)) this equation is exactly the wave equation of linearized elasticity.

The definition of the operator $\mathcal{A}_0$ does not just use the quadratic part of the projection $\mathbb{A}_{11} = P_V \mathbb{A}|_V$. The Schur complement $\mathbb{B}(\theta) \leq \mathbb{A}_{11}(\theta)$ leads to a weakening. This weakening is well known as the effective macroscopic properties of a crystal are obtained by minimization with respect to the internal microscopic degrees of freedom lying in $V^\perp$. In fact, we have

$$\langle \mathbb{B}(\theta)v, v\rangle = \min\{\, \langle \begin{pmatrix} \mathbb{A}_{11}(\theta) & \mathbb{A}_{12}(\theta) \\ \mathbb{A}_{12}^*(\theta) & \mathbb{A}_{22}(\theta) \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix}, \begin{pmatrix} v \\ w \end{pmatrix} \rangle \mid w \in V^\perp \,\}.$$

This result can also be phrased in terms of Gamma convergence for the associated potential energies. Define the quadratic form

$$\mathcal{U}_\varepsilon : \mathrm{L}^2(\mathbb{R}^d, \mathbb{R}^m) \to [0, \infty]; Z \mapsto \begin{cases} \int_{\mathbb{R}^d} \frac{1}{2}\langle Z, \mathcal{A}_\varepsilon Z\rangle \,\mathrm{d}y & \text{for } Z \in \mathbb{L}_\varepsilon, \\ \infty & \text{else,} \end{cases}$$

and set $\mathcal{U}_0(Z) = \int_{\mathbb{R}^d} \frac{1}{2}\langle Z, \mathcal{A}_0 Z\rangle \,\mathrm{d}y = \int_{\mathbb{R}^d} \frac{1}{2}\langle \mathrm{D}Z, \mathbb{E}\mathrm{D}Z\rangle \,\mathrm{d}y$ for $Z \in \mathrm{H}^1(\mathbb{R}^d, V)$ and $\mathcal{U}_0(Z) = \infty$ else.

Proposition 4.1 *For $\varepsilon \to 0$ we have the Gamma convergence $\mathcal{U}_\varepsilon \xrightarrow{\text{Gamma}} \mathcal{U}_0$, i.e., for each sequence $(Z_\varepsilon)_\varepsilon$ with $Z_\varepsilon \rightharpoonup Z$ we have $\liminf_{\varepsilon\to 0} \mathcal{U}_\varepsilon(Z_\varepsilon) \geq \mathcal{U}_0(Z)$ and for each $Z \in \mathrm{L}^2(\mathbb{R}^d, \mathbb{R}^m)$ there exists a recovery sequence $\widehat{z}_\varepsilon$ with $\widehat{z}_\varepsilon \rightharpoonup Z$ and $\mathcal{U}_\varepsilon(\widehat{z}_\varepsilon) \to \mathcal{U}_0(Z)$.*

Proof: The result is immediate if we transform all functionals into Fourier variables. Note that $\mathcal{F}$ is linear and hence preserves weak converge. Then, it is sufficient to consider each $\eta \in \mathbb{R}^d_*$ separately. But now it is easy to see that on the finite dimensional space $\mathbb{C}^m$ the quadratic functional $U_\varepsilon : z \mapsto \frac{1}{2}\langle \mathbb{A}^\varepsilon(\eta)z, z\rangle$ Gamma converges to U_0 with $U_0(z) = \frac{1}{2}\mathbb{Q}^{(2)}(z, z)$ for $z \in V$ and ∞ else. ∎

In this special situation where the dynamical part of the problem is given by the simple multiplication operator M it can now be shown that the Gamma limit of the static part is in fact enough to go to the limit also in the dynamical situation.

Theorem 4.2 *Let $(x_0^\varepsilon, x_1^\varepsilon)_{\varepsilon>0}$ be a sequence of initial data for (1.3) in $(\ell^2(\Gamma, \mathbb{R}^m))^2$ with corresponding solutions $x^\varepsilon : \mathbb{R} \to \ell^2(\Gamma, \mathbb{R}^m)$ of (1.3) with $(x^\varepsilon(0), \dot{x}^\varepsilon(0)) = (x_0^\varepsilon, x_1^\varepsilon)$. Assume that there exists $C^* > 0$ such that*

$$\varepsilon\|x_0^\varepsilon\|_{\ell^2} + e^\varepsilon \leq C^* \text{ for } \varepsilon \in (0, \varepsilon_0), \text{ where } e^\varepsilon = \mathcal{K}(x_1^\varepsilon) + \mathcal{U}(x_0^\varepsilon).$$

Then, the transformed initial data

$$(Z_0^\varepsilon, Z_1^\varepsilon) \overset{\text{def}}{=} (\varepsilon \mathcal{S}_\varepsilon x_0^\varepsilon, \mathcal{S}_\varepsilon x_1^\varepsilon) \textit{ are bounded in } \mathrm{H}^1(\mathbb{R}^d, \mathbb{R}^m) \times \mathrm{L}^2(\mathbb{R}^d, \mathbb{R}^m).$$

If the stability condition (3.4) *holds and the initial data converge weakly, i.e.,*

$$Z_0^\varepsilon \rightharpoonup Z_0 \textit{ in } \mathrm{H}^1(\mathbb{R}^d, \mathbb{R}^m) \quad \textit{and} \quad Z_1^\varepsilon \rightharpoonup Z_1 \textit{ in } \mathrm{L}^2(\mathbb{R}^d, \mathbb{R}^m) \quad \textit{for } \varepsilon \to 0, \tag{4.6}$$

then $(Z_0, Z_1) \in \mathrm{H}^1(\mathbb{R}^d, V) \times \mathrm{L}^2(\mathbb{R}^d, V)$ *and the following holds:*
If $Z \in \mathrm{C}^0(\mathbb{R}, \mathrm{H}^1(\mathbb{R}^d, V)) \cap \mathrm{C}^1(\mathbb{R}, \mathrm{L}^2(\mathbb{R}^d, V))$ *is the unique solution of* (4.5) *with* $Z(0) = Z_0$ *and* $Z'(0) = Z_1$*, then for all* $\tau \in \mathbb{R}$ *we have*

$$\left.\begin{array}{rcll} \varepsilon \mathcal{S}_\varepsilon x^\varepsilon(\tau/\varepsilon) & \rightharpoonup & Z(\tau) & \textit{in } \ \mathrm{H}^1(\mathbb{R}^d, V), \\ \mathcal{S}_\varepsilon \dot{x}^\varepsilon(\tau/\varepsilon) & \rightharpoonup & Z'(\tau) & \textit{in } \ \mathrm{L}^2(\mathbb{R}^d, V). \end{array}\right\} \textit{for } \varepsilon \to 0.$$

Moreover, the limiting energy $\widetilde{e} = \frac{1}{2}\langle\!\langle M\widetilde{Z}'(\tau), \widetilde{Z}'(\tau)\rangle\!\rangle + \frac{1}{2}\langle\!\langle \mathbb{E}[\mathrm{D}\widetilde{Z}], \mathrm{D}\widetilde{Z}\rangle\!\rangle$*, which is independent of* τ*, satisfies* $\widetilde{e} \le \liminf_{\varepsilon\to 0} e^\varepsilon \le C^*$*.*

We continue to use the notation $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ for the scalar product on $\mathrm{L}^2(\mathbb{R}^d, \mathbb{C}^m)$, i.e., $\langle\!\langle Z_1, Z_2\rangle\!\rangle \overset{\text{def}}{=} \int_{\mathbb{R}^d} \langle Z_1(y), Z_2(y)\rangle \,\mathrm{d}y$.

Proof: We consider the solutions Z^ε of (4.2) which are given via $Z^\varepsilon(\tau) = \varepsilon \mathcal{S}_\varepsilon x^\varepsilon(\tau/\varepsilon)$ and satisfy (cf. (2.2))

$$\|Z^\varepsilon(\tau)\| = \varepsilon \|x^\varepsilon(\tau/\varepsilon)\| \text{ and } \tfrac{1}{2}\langle\!\langle M\partial_\tau Z^\varepsilon, \partial_\tau Z^\varepsilon\rangle\!\rangle + \tfrac{1}{2}\langle\!\langle \mathcal{A}_\varepsilon Z^\varepsilon, Z^\varepsilon\rangle\!\rangle = e^\varepsilon.$$

Note that $\widehat{Z}^\varepsilon(\tau) = \mathcal{F}Z^{(\varepsilon)}(\tau)$ has support in $\frac{1}{\varepsilon}B_{\Gamma_*}$ and that (3.5) implies

$$\tfrac{1}{C_V}(|\eta|^2|v{+}w|^2 + \varepsilon^{-2}|w|^2) \le \langle \mathbb{A}^\varepsilon(\eta)(v{+}w), v{+}w\rangle \le C_V(|\eta|^2|v{+}w|^2 + \varepsilon^{-2}|w|^2)$$

for all $v \in V, w \in V^\perp$ and $\eta \in \frac{1}{\varepsilon}B_{\Gamma_*}$. Together with

$$\langle\!\langle \mathcal{A}_\varepsilon Z^\varepsilon, Z^\varepsilon\rangle\!\rangle = (2\pi)^{-d}\int_{\varepsilon\eta\in B_{\Gamma_*}} \langle \mathbb{A}^\varepsilon(\eta)\widehat{Z}^\varepsilon(\eta), \widehat{Z}^\varepsilon(\eta)\rangle \,\mathrm{d}\eta$$

we find a constant $C_2 > 0$ such that

$$\tfrac{e^\varepsilon}{C_2} \le \|\partial_\tau Z^\varepsilon(\tau)\|^2 + \|\mathrm{D}Z^\varepsilon(\tau)\|^2 + \tfrac{1}{\varepsilon^2}\|(I{-}P_V)Z^\varepsilon\|^2 \le C_2 e^\varepsilon \le C_* C^*.$$

As $(\varepsilon x_0^\varepsilon)_{\varepsilon\in(0,\varepsilon_0)}$ is bounded $(Z^\varepsilon(0))_{\varepsilon\in(0,\varepsilon_0)}$ is bounded as well. By $\|\partial_\tau Z^\varepsilon(\tau)\|^2 \le C_* C^*$ we conclude $\|Z^\varepsilon(\tau)\| \le C_3(1{+}|\tau|)$, independently of $\varepsilon \in (0, \varepsilon_0)$. This establishes the boundedness of $(Z^\varepsilon(\tau), \partial_\tau Z^\varepsilon(\tau))$ in $\mathrm{H}^1(\mathbb{R}^d, \mathbb{R}^m) \times \mathrm{L}^2(\mathbb{R}^d, \mathbb{R}^m)$. Moreover, every weak limit $Z^{(0)}(\tau)$ must satisfy $(I{-}P_V)Z^{(0)}(\tau) = 0$ as $\|(I{-}P_V)Z^\varepsilon(\tau)\| \le C_4\varepsilon$.

The weak limit exists for all $\tau \in \mathbb{R}$ if it exists for $\tau = 0$, since the evolution operator $(x^\varepsilon(0), \dot{x}^\varepsilon(0)) \mapsto (x^\varepsilon(\tau), \dot{x}^\varepsilon(\tau))$ is a bounded, linear operator, and hence is weakly continuous.

Thus, it remains to be shown that the function $\tau \mapsto Z^{(0)}(\tau)$ satisfies the limit equation (4.5). For this purpose we consider the weak form of (4.2), namely

$$0 = \int_{\tau\in\mathbb{R}} \langle\!\langle Z^\varepsilon(\tau), M\partial_\tau^2\varphi(\tau) + \mathcal{A}_\varepsilon\varphi(\tau)\rangle\!\rangle \,\mathrm{d}\tau \tag{4.7}$$

for all $\varphi \in \mathrm{C}^2_\mathrm{c}(\mathbb{R}, \mathrm{H}^2(\mathbb{R}^d, \mathbb{R}^m))$. To study the limit $\varepsilon \to 0$ we choose special testfunctions φ^ε as follows. For $\psi \in \mathrm{C}^2_\mathrm{c}(\mathbb{R}, \mathrm{H}^2(\mathbb{R}^d, V))$ let $\varphi^\varepsilon(\tau) = \psi(\tau) + K^\varepsilon\psi(\tau)$ with $K^\varepsilon : \mathrm{H}^2(\mathbb{R}^d, V) \to \mathrm{H}^{(2)}(\mathbb{R}^d, V^\perp)$ defined via

$$(\mathcal{F}K^\varepsilon\psi)(\eta) = -\mathbb{A}_{22}(\varepsilon\eta)^{-1}\mathbb{A}_{12}^*(\varepsilon\eta)\mathcal{X}_{B_{\Gamma_*}}(\varepsilon\eta)(\mathcal{F}\psi)(\eta).$$

By construction we obtain $(I{-}P_V)\mathcal{A}_\varepsilon(\psi{+}K^\varepsilon\psi) \equiv 0$ as well as

$$\|P_V\mathcal{A}_\varepsilon(\psi{+}K^\varepsilon\psi) - \mathcal{A}_0\psi\|_{\mathrm{H}^{-1}(\mathbb{R}^d)} \to 0. \tag{4.8}$$

The latter convergence is easily checked by Fourier transform. It is equivalent to

$$\int_{\mathbb{R}^d_*} \mathcal{X}_{B_{\Gamma_*}}(\varepsilon\eta)(1{+}|\eta|^2)^{-1}|B(\varepsilon,\eta)(\mathcal{F}\psi)(\eta)|^2\,\mathrm{d}\eta \to 0,$$

where $B(\varepsilon,\eta) = \frac{1}{\varepsilon^2}\mathbb{B}(\varepsilon\eta) - \mathbb{Q}^{(2)}(\eta,\eta)$, see (4.3). Since $B(\varepsilon,\eta) \to 0$ for η fixed and $\varepsilon \to 0$, $|B(\varepsilon,\eta)| \le C|\eta|^2$ for $\varepsilon\eta \in B_{\Gamma_*}$ and $\psi \in \mathrm{H}^2(\mathbb{R}^d, V)$, Lebesgue's dominated convergence theorem gives (4.8).

Now we are able to pass to the limit $\varepsilon \to 0$ in (4.7) and find

$$0 = \int_{\tau\in\mathbb{R}} \langle\!\langle Z^{(0)}(\tau), M\partial_\tau^2\psi(\tau) + \mathcal{A}_0\psi(\tau)\rangle\!\rangle \,\mathrm{d}\tau.$$

Since ψ was an arbitrary testfunction, this implies (4.5). ■

5 Energy transport via the group velocity

In dispersive wave equations one has to distinguish the local phase velocity of a oscillatory wave and its group velocity. For plane waves with $x_\gamma(t) = \mathrm{e}^{\mathrm{i}(\omega_j t+\theta\cdot\gamma)}\Phi_j$ the vector $c_\mathrm{phase} = \frac{\omega_j}{\theta^2}\theta$ is called the *phase velocity* as we may rewrite the wave in the form $x_\gamma(t) = \mathrm{e}^{\mathrm{i}(c_\mathrm{phase}t+\gamma)\cdot\theta}$.

The *group velocity* is defined as $c_\mathrm{group} = \nabla_\theta\omega_j(\theta)$. For slowly modulated pulses of the form $x_\gamma(t) = A(\varepsilon t, \varepsilon\gamma)\mathrm{e}^{\mathrm{i}(\omega_j t+\theta\cdot\gamma)}\Phi_j$ with a smooth profile $A : \mathbb{R} \to \mathbb{C}$ it is known that A satisfies the transport equation $\partial_\tau A = c_\mathrm{group}\cdot\nabla_y A$ to lowest order in ε. Hence, the energy which is macroscopically localized in the pulse via $|A(\tau,y)|^2$ is transported with the group velocity. On the time scale $t = \tau/\varepsilon$ there will be no dispersive effects which take place only on time of the order $1/\varepsilon^2$, see [SW00, GM04b]. Our task here is to make this picture rigorous for arbitrary initial conditions which may contain energy in all kind of microscopic wave vectors and without any smoothness assumptions on envelopes.

Of course the problem is linear and these waves do not interact. However, the local energy is a quadratic function of the local state. Hence, we lose many nice tools of linear functional analysis, in particular the weak-convergence property.

5.1 Local energy densities

For general lattice models it is not obvious how to associate for a given solution to each particle the current local energy. The first naive choice would be

$$e_\gamma(t) = \tfrac{1}{2}\langle M\dot{x}_\gamma(t), \dot{x}_\gamma(t)\rangle + \tfrac{1}{2}\langle A_0 x_\gamma(t), x_\gamma(t)\rangle + \tfrac{1}{4}\textstyle\sum_{\beta\neq 0}\langle A_\beta x_{\gamma+\beta}(t), x_\gamma(t)\rangle,$$

but it is not clear that this term is always nonnegative. Of course, if the interactions in the crystal are composed from attracting springs (pair interactions), such that the static energy is $\mathcal{U}(x) = \frac{1}{2}\sum_\Gamma \sum_{\beta\in I} |B_\beta(x_\gamma - x_{\gamma-\beta})|^2$ with $I \subset \Gamma$ finite, we may define the energy at the lattice point γ as the kinetic energy plus half of the energy in each interacting spring in $\gamma+I$.

More generally, we may assume that the operator $A : x \mapsto (\sum_\beta A_\beta x_{\gamma+\beta})_{\gamma\in\Gamma}$ can be written in the form $A = L^*L$, where $L : \ell^2(\Gamma, \mathbb{R}^m) \to \ell^2(\Gamma, \mathbb{R}^m)^p$ is again given in the form $(Lx)_\gamma = (\sum_\beta L^1_\beta x_{\gamma+\beta}, \ldots, \sum_\beta L^p_\beta x_{\gamma+\beta})$, where all sums are supposed to be finite (or with exponentially decaying kernels). The relation $A = L^*L$ then means $A_\beta = \sum_{j=1}^p \sum_{\delta\in\Gamma} (L^j_{\beta-\delta})^\mathsf{T} L^j_\delta$. Then, we can set

$$e_\gamma(t) = \tfrac{1}{2}\langle M\dot{x}_\gamma(t), \dot{x}_\gamma(t)\rangle + \tfrac{1}{2}|(Lx)_\gamma|^2. \tag{5.1}$$

It is not clear, whether every stable interaction operators A can be written in the form L^*L with a finite number p of components L^j with exponentially decaying kernels. For pairwise interaction attractive springs with $(B_\gamma)_{\beta\in I}$ as above, this factorization works with $(Lx)_\gamma = \big(B_\beta(x_\gamma - x_{\gamma-\beta})\big)_{\beta\in I}$.

Similarly, we may associate with the rescaled macroscopic function $Z^\varepsilon : \tau \mapsto \varepsilon\mathcal{S}_\varepsilon x(\tau/\varepsilon)$ a continuous energy density

$$\begin{aligned}
&E^\varepsilon(\tau, y) = \mathcal{E}^\varepsilon_2((Z^\varepsilon(\tau), \partial_\tau Z^\varepsilon(\tau)), (Z^\varepsilon(\tau), \partial_\tau Z^\varepsilon(\tau)))(y) \;\geq\; 0 \text{ with}\\
&\mathcal{E}^\varepsilon_2((z_0, z_1), (v_0, v_1))(y) = \tfrac{1}{2}\langle M^{1/2} z_1(y), M^{1/2} v_1\rangle + \tfrac{1}{2}\langle (\mathcal{A}^{1/2}_\varepsilon z_0)(y), (\mathcal{A}^{1/2}_\varepsilon v_0)(y)\rangle.
\end{aligned}$$

where $\mathcal{A}^{1/2}_\varepsilon$ is defined as positive semi-definite square root of $\mathcal{A}_\varepsilon$, e.g., $\mathcal{F}(\mathcal{A}^{1/2}_\varepsilon Z)(\eta) = \mathbb{A}^\varepsilon(\eta)^{1/2}\mathcal{F}Z(\eta)$. Note that $E^\varepsilon : \mathbb{R}^d \to [0, \infty)$ will have spatial oscillations on the length scale ε, but again $E^\varepsilon(\tau, \cdot) \in \mathrm{L}^1(\mathbb{R}^d) \subset \mathcal{M}(\mathbb{R}^d)$ is bounded.

As there is a problem that $\mathbb{A}(\cdot)^{1/2}$ is in general no longer smooth, one may also use the decomposition $A = L^*L$, if available. We associate to L the symbol $\mathbb{L}(\theta) = \sum_\beta \mathrm{e}^{-\mathrm{i}\gamma\cdot\theta} L_\beta \in \mathbb{C}^{pm\times m}$ such that $\mathbb{A}(\theta) = \mathbb{L}(\theta)^*\mathbb{L}(\theta)$. Using the Fourier transform and $\mathbb{L}^\varepsilon(\eta) = \frac{1}{\varepsilon}\mathbb{L}(\varepsilon\eta)$ we define $\mathcal{L}_\varepsilon$ via $\mathcal{F}(\mathcal{L}_\varepsilon Z) = \mathbb{L}^\varepsilon\mathcal{F}Z$. Now the analog of the discrete energy in (5.1) can be defined as

$$\widetilde{E}^\varepsilon(\tau, y) = \tfrac{1}{2}\langle M\partial_\tau Z^\varepsilon, \partial_\tau Z^\varepsilon\rangle + \tfrac{1}{2}|\mathcal{L}_\varepsilon Z^\varepsilon|^2.$$

However, none of the two above constructions leads to a direct control over the energy transport. Instead, we will use the theory of Wigner and Husimi transforms to control the energy transport. Before developing this theory we decompose the sequence of solutions

Z^ε into one part which converges strongly to the weak limit $\widetilde{Z}$ and a fluctuating part U^ε which converges weakly to 0, namely

$$Z^\varepsilon(\tau) = S^\varepsilon(\tau) + T^\varepsilon(\tau) \quad \text{with } S^\varepsilon(\tau) = \mathcal{P}_\varepsilon \widetilde{Z}(\tau),$$

with $\mathcal{P}_\varepsilon$ from (4.1). Clearly we have

$$S^\varepsilon(\tau) \to \widetilde{Z}(\tau) \in \mathrm{H}^1(\mathbb{R}^d, \mathbb{R}^m) \quad \text{and} \quad T^\varepsilon(\tau) \rightharpoonup 0 \in \mathrm{H}^1(\mathbb{R}^d, \mathbb{R}^m).$$

If we insert this splitting into the energy density E^ε as defined above we obtain for fixed τ

$$\begin{aligned} E^\varepsilon(\cdot) &= A^\varepsilon_{SS} + 2A^\varepsilon_{ST} + A^\varepsilon_{TT} \ \in \mathrm{L}^1(\mathbb{R}^d) \text{ with} \\ A^\varepsilon_{SS} &= \mathcal{E}^\varepsilon((S^\varepsilon, \partial_\tau S^\varepsilon), (S^\varepsilon, \partial_\tau S^\varepsilon)) \\ A^\varepsilon_{ST} &= \mathcal{E}^\varepsilon((S^\varepsilon, \partial_\tau S^\varepsilon), (T^\varepsilon, \partial_\tau T^\varepsilon)) \\ A^\varepsilon_{TT} &= \mathcal{E}^\varepsilon((T^\varepsilon, \partial_\tau T^\varepsilon), (T^\varepsilon, \partial_\tau T^\varepsilon)). \end{aligned}$$

With the techniques used in the proof of Theorem 4.2 we easily obtain

$$\mathcal{A}_\varepsilon^{1/2} S^\varepsilon \to \mathcal{A}_0^{1/2} \widetilde{Z} \text{ in } \mathrm{L}^2(\mathbb{R}^d, \mathbb{R}^m) \quad \text{and} \quad \mathcal{A}_\varepsilon^{1/2} T^\varepsilon \rightharpoonup 0 \text{ in } \mathrm{L}^2(\mathbb{R}^d, \mathbb{R}^m).$$

Using the definition of $\mathcal{A}_0$ and $\mathbb{E}$ this yields

$$A^\varepsilon_{SS} \to \tfrac{1}{2}\langle \partial_\tau \widetilde{Z}, M \partial_\tau \widetilde{Z}\rangle + \tfrac{1}{2}\langle \mathrm{D}\widetilde{Z}, \mathbb{E}\mathrm{D}\widetilde{Z}\rangle \ \text{ in } \mathrm{L}^1(\mathbb{R}^d).$$

This density is the energy distribution which associates with the macroscopic kinetic energy and the macroscopic deformation. Second, since $f_n \rightharpoonup 0$ and $g_n \to g$ in $\mathrm{L}^2(\mathbb{R}^d)$ implies $f_n g_n \overset{*}{\rightharpoonup} 0$ in $\mathrm{L}^1(\mathbb{R}^d)$, we conclude $A^\varepsilon_{ST} \overset{*}{\rightharpoonup} 0$. Hence, to understand the limit of the total energy distribution it is sufficient to study the energy associated with the fluctuation part T^ε which is due to pure microscopic behavior.

A similar splitting of the energy holds if we consider $\widetilde{E}^\varepsilon$ instead of E^ε. Thus, in the sequel we restrict to the fluctuation part which converges weakly to 0.

5.2 Wigner and Husimi transforms and measures

The Wigner and Husimi transforms apply to a vector-valued function and they measure correlations between the components on a scale of microscopic wave lengths. The Wigner measure associated with a family $(f^\varepsilon)_\varepsilon$ of functions is a limit object which measures how much oscillations occur at a given macroscopic point $y \in \mathbb{R}^d$ with a given microscopic wave vector $\theta \in \mathbb{R}^d_*$. We refer to [GL93, MMP94, RPK96, GMMP97, TP04, Mac04] for general references on this subject. Here, we just recall the main definitions, properties and formulae.

We define the matrix-valued Wigner transform of $f \in \mathrm{L}^2(\mathbb{R}^d, \mathbb{C}^m)$ via

$$W^\varepsilon[f](y,\theta) \overset{\text{def}}{=} \frac{1}{(2\pi)^d} \int_{v \in \mathbb{R}^d} f(y - \frac{\varepsilon}{2} v) \otimes \overline{f}(y + \frac{\varepsilon}{2} v)\, \mathrm{e}^{\mathrm{i} v\cdot\theta}\, \mathrm{d}v \ \in \mathbb{C}^{m\times m}, \tag{5.2}$$

where $\otimes$ denotes the tensor product of two vectors. We mention explicitly here that here $y \in \mathbb{R}^d$ stands for the macroscopic space variable in $\mathbb{R}^d$, whereas $\theta \in \mathbb{R}^d$ denotes the microscopic wave vector as it is dual to the integration variable v which is multiplied by ε. Later on θ will be restricted to lie in $\mathcal{T}_{\Gamma_*}$.

Note that $W^\varepsilon[f]$ is in general not $\mathrm{L}^1(\mathbb{R}^d \times \mathbb{R}^d_*, \mathbb{C}^{m\times m})$, but it is well-defined as a distribution. For instance, the Fourier transform with respect to y leads to

$$\widehat{W^\varepsilon}[f](\eta,\theta) \stackrel{\text{def}}{=} \mathcal{F}_{y\to\eta} W^\varepsilon[f](\eta,\theta) = \tfrac{1}{(2\pi\varepsilon)^d} (\mathcal{F}f)(\tfrac{\theta}{\varepsilon}+\tfrac{\eta}{2}) \otimes \overline{\mathcal{F}f}(\tfrac{\theta}{\varepsilon}-\tfrac{\eta}{2}). \tag{5.3}$$

This formula is the basis of most of the energy-transport theory for Wigner measures. It also gives the nice estimate

$$\sup\{ \, \|\widehat{W^\varepsilon}[f](\eta,\cdot)\|_{\mathrm{L}^1(\mathbb{R}^d_*)} \mid \eta \in \mathbb{R}^d_* \} \leq \|f\|^2_{\mathrm{L}^2(\mathbb{R}^d)}, \tag{5.4}$$

which can be used to show that $W^\varepsilon[f]$ is a well-defined distribution.

The next two relations show that the Wigner transform is a kind of measure on $\mathbb{R}^d \times \mathbb{R}^d_*$ whose marginal distributions are just the classical ones. Integration (in a certain principal sense) with respect to $\eta \in \mathbb{R}^d_+$ or $y \in \mathbb{R}^d$ gives the identities

$$\begin{aligned} &\textstyle\int_{\theta\in\mathbb{R}^d_*} W^\varepsilon[f](y,\theta)\,\mathrm{d}\theta = f(y) \otimes \overline{f}(y) && \text{for a.e. } y \in \mathbb{R}^d, \\ &\textstyle\int_{y\in\mathbb{R}^d} W^\varepsilon[f](y,\theta)\,\mathrm{d}y = \frac{1}{(2\varepsilon\pi)^d}\, (\mathcal{F}f)(\theta/\varepsilon) \otimes \overline{\mathcal{F}f}(\theta/\varepsilon) && \text{for a.e. } \theta \in \mathbb{R}^d_*. \end{aligned} \tag{5.5}$$

The major disadvantage of the Wigner transform is that it is not integrable. In contrast, the Husimi transform leads to true matrix-valued measures, but it loses the exact energy location as expressed in (5.5). The Husimi transform is based on the wave packets (cf. [CF78])

$$\mathcal{H}^\varepsilon[f](y,\theta) \stackrel{\text{def}}{=} \tfrac{1}{2^{d/2}(\varepsilon\pi)^{3d/4}} \textstyle\int_{\mathbb{R}^d} f(z) \mathrm{e}^{-|y-z|^2/(2\varepsilon)}\, \mathrm{e}^{-\mathrm{i}z\cdot\theta/\varepsilon}\,\mathrm{d}z = \frac{1}{(\varepsilon\pi)^{d/4}} \mathcal{F}\big[f\, G^{2\varepsilon}(\cdot - y)\big]\big(\tfrac{\theta}{\varepsilon}\big),$$

where the Gaussian kernel G^α is defined via $G^\alpha(y) = (\alpha\pi)^{-d/2}\,\mathrm{e}^{-|y|^2/\alpha}$. The Husimi transform is simply the tensor product of these wave packet with itself and takes the form

$$H^\varepsilon[f](y,\theta) \stackrel{\text{def}}{=} \mathcal{H}^\varepsilon[f](y,\theta) \otimes \overline{\mathcal{H}^\varepsilon[f]}(y,\theta).$$

By its definition it is obvious that $H^\varepsilon[f]$ takes values in $\mathbb{C}^{m\times m}_{\geq 0}$. Moreover, some elementary manipulations show the identity

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d_*} \mathrm{tr} H^\varepsilon[f](y,\theta)\,\mathrm{d}\theta\,\mathrm{d}y = \|\mathcal{H}^\varepsilon[f]\|^2_{\mathrm{L}^2(\mathbb{R}^d\times\mathbb{R}^d_*)} = \|f\|^2_{\mathrm{L}^2(\mathbb{R}^d)}.$$

From $H^\varepsilon[f](y,\theta) \in \mathbb{C}^{m\times m}_{\geq 0}$ we know $|(H^\varepsilon[f])_{l,n}| \leq (H^\varepsilon[f])^{1/2}_{n,n} |(H^\varepsilon[f])^{1/2}_{l,l}$ almost everywhere in $\mathbb{R}^d \times \mathbb{R}^d_*$. Hence, by the Cauchy-Bunyakovski-Schwarz inequality we conclude

$$\int_{\mathbb{R}^d\times\mathbb{R}^d_*} \sum_{l,n=1}^m |(H^\varepsilon[f])_{l,n}(y,\theta)|\,\mathrm{d}\theta\,\mathrm{d}y \leq m\|f\|^2_{\mathrm{L}^2(\mathbb{R}^d,\mathbb{C}^m)}. \tag{5.6}$$

Thus, the major advantage of the Husimi transform is that it defines a bounded quadratic mapping from $\mathrm{L}^2(\mathbb{R}^d, \mathbb{C}^m)$ into $\mathrm{L}^1(\mathbb{R}^d\times\mathbb{R}^d_*, \mathbb{C}^{m\times m}_{\geq 0})$.

However, this advantage leads to a smearing out of the information in physical and wave-vector space. In fact, the Husimi transform can be obtained from the Wigner transform via convolution by suitable Gauss kernels, viz.,

$$\begin{aligned} H^\varepsilon[f] &= W^\varepsilon[f] * G^\varepsilon_y * G^\varepsilon_\theta \quad \text{ i.e.,} \\ H^\varepsilon[f](y,\theta) &= \tfrac{1}{(\varepsilon\pi)^d} \int_{z\in\mathbb{R}^d} \int_{\vartheta\in\mathbb{R}^d_*} W^\varepsilon[f](z,\vartheta) \mathrm{e}^{-(|y-z|^2+|\theta-\vartheta|^2)/\varepsilon} \,\mathrm{d}\vartheta\,\mathrm{d}z. \end{aligned} \tag{5.7}$$

The Gauss kernels have a width of $\sqrt{\varepsilon}$ and thus, the localized information in $W^\varepsilon[f]$ is slightly smeared out in physical space $\mathbb{R}^d_y$ and in the microscopic wave-vector space $\mathbb{R}^d_{*,\theta}$. The corresponding counterparts to (5.3) and (5.5) read

$$\begin{aligned} \widehat{H^\varepsilon}[f](\eta,\theta) &\stackrel{\text{def}}{=} \mathcal{F}_{y\to\eta} H^\varepsilon[f](\cdot,\theta)(\eta) = \mathcal{F}_{y\to\eta}\Big(W^\varepsilon[f] * G^\varepsilon_y * G^\varepsilon_\theta\Big)(\eta,\theta) \\ &= \widehat{G^\varepsilon_y}(\eta)\Big[\widehat{W^\varepsilon}[f](\eta,\cdot) * G^\varepsilon_\theta\Big](\theta) \\ &= \tfrac{\mathrm{e}^{-\varepsilon|\eta|^2/4}}{(2\varepsilon\pi)^d} \int_{\vartheta\in\mathbb{R}^d_*} \mathcal{F}f(\tfrac{\vartheta}{\varepsilon}+\tfrac{\eta}{2}) \otimes \overline{\mathcal{F}f}(\tfrac{\vartheta}{\varepsilon}-\tfrac{\eta}{2}) G^\varepsilon(\vartheta-\theta)\,\mathrm{d}\vartheta. \end{aligned} \tag{5.8}$$

Moreover, for almost all $y \in \mathbb{R}^d$ and $\theta \in \mathbb{R}^d_*$ we have

$$\begin{aligned} \int_{\theta\in\mathbb{R}^d_*} H^\varepsilon[f](y,\theta)\,\mathrm{d}\theta &= \int_{\mathbb{R}^d} f(z)\otimes\overline{f}(z)\, G^\varepsilon(z-y)\,\mathrm{d}z, \\ \int_{y\in\mathbb{R}^d} H^\varepsilon[f](y,\theta)\,\mathrm{d}y &= \int_{\mathbb{R}^d_*} \tfrac{1}{(2\varepsilon\pi)^d} (\mathcal{F}f)(\vartheta/\varepsilon)\otimes\overline{\mathcal{F}f}(\vartheta/\varepsilon)\, G^\varepsilon(\vartheta-\theta)\,\mathrm{d}\vartheta. \end{aligned} \tag{5.9}$$

Note that $\mathrm{L}^1(\mathbb{R}^d\times\mathbb{R}^d_*, \mathbb{C}^{m\times m})$ is a weak$*$ dense subspace of the matrix-valued Radon measures $\mathcal{M}(\mathbb{R}^d\times\mathbb{R}^d_*, \mathbb{C}^{m\times m})$. The set of these measures forms exactly the dual space of $\mathrm{C}^0_0(\mathbb{R}^d\times\mathbb{R}^d_*, \mathbb{C}^{m\times m})$, the set of continuous functions which decay at infinity. Thus, by the Banach-Alaoglu theorem every bounded sequence in $\mathrm{L}^1(\mathbb{R}^d\times\mathbb{R}^d_*, \mathbb{C}^{m\times m})$ has a weak$*$ convergent subsequence and the limit is called the Wigner measure associated with the sequence. While the existence of limit objects is easy for the Husimi transform, the same result for the Wigner transform is nontrivial. The major result on the Wigner transform W^ε is that for all bounded sequences $(f^\varepsilon)_{\varepsilon\in(0,\varepsilon_0)}$ in $\mathrm{L}^2(\mathbb{R}^d)$ there exists a subsequence (ε_k) such that $W^{(\varepsilon_k)}[f^{(\varepsilon_k)}]$ has a limit which is called *Wigner measure*. It can be shown (cf. [GL93, GMMP97]) that all limit points of the two families $(W^\varepsilon[f^\varepsilon])_\varepsilon$ and $(H^\varepsilon[f^\varepsilon])_\varepsilon$ lie in $\mathcal{M}(\mathbb{R}^d\times\mathbb{R}^d_*, \mathbb{C}^{m\times m}_{\geq 0})$ and are the same.

To formulate the following result we define the notions of a tight family and an ε–oscillatory family. A bounded family $(f^\varepsilon)_\varepsilon$ is called *tight for* $\varepsilon \to 0$, if

$$\limsup_{\varepsilon\to 0} \int_{|y|>R} |f^\varepsilon(y)|^2\,\mathrm{d}y \quad \xrightarrow{R\to\infty} \quad 0. \tag{5.10}$$

The bounded family $(f^\varepsilon)_\varepsilon$ is called ε*–oscillatory for* $\varepsilon \to 0$, if for each continuous, compactly supported $\varphi : \mathbb{R}^d \to \mathbb{C}$ we have

$$\limsup_{\varepsilon\to 0} \int_{|\eta|>R/\varepsilon} |\mathcal{F}(\varphi f^\varepsilon)(\eta)|^2\,\mathrm{d}\eta \quad \xrightarrow{R\to\infty} \quad 0. \tag{5.11}$$

Hence, tightness means that no mass escapes to ∞ in physical space, and ε–oscillatoryness means that no mass escapes to ∞ in Fourier space faster than $1/\varepsilon$.

We will use the following precise statement on the existence of Wigner measures.

Theorem 5.1 *Let $(f^\varepsilon)_{\varepsilon\in(0,\varepsilon_0)}$ be a bounded family in $\mathrm{L}^2(\mathbb{R}^d,\mathbb{C}^m)$. Then, there exists a subsequence $(\varepsilon_k)_{k\in\mathbb{N}}$ with $\varepsilon_k \to 0$ for $k\to\infty$ and a matrix-valued, bounded Radon measure $\mu \in \mathcal{M}(\mathbb{R}^d\times\mathbb{R}^d_*,\mathbb{C}^{m\times m})$ such that the following holds:*

1. *$\forall\, B \subset \mathbb{R}^d\times\mathbb{R}^d_*$ measurable: $\mu(B)\in\mathbb{C}^{m\times m}_{\geq 0}$,*
2. *$W^{(\varepsilon_k)}[f^{(\varepsilon_k)}] \xrightarrow{\mathcal{D}} \mu$ (in the sense of distributions) and $H^{(\varepsilon_k)}[f^{(\varepsilon_k)}] \overset{*}{\rightharpoonup} \mu$ in $\mathcal{M}(\mathbb{R}^d\times\mathbb{R}^d_*,\mathbb{C}^{m\times m})$,*
3. *$f^{(\varepsilon_k)}\otimes\overline{f^{(\varepsilon_k)}} \overset{*}{\rightharpoonup} \nu_{\mathrm{phys}} = \int_{\mathbb{R}^d_*}\mu(\cdot,\mathrm{d}\eta)$ in $\mathcal{M}(\mathbb{R}^d,\mathbb{C}^{m\times m})$ and $\frac{1}{(2\varepsilon\pi)^d}\mathcal{F}f^{(\varepsilon_k)}(\frac{\cdot}{\varepsilon})\otimes\overline{\mathcal{F}f^{(\varepsilon_k)}(\frac{\cdot}{\varepsilon})} \overset{*}{\rightharpoonup} \nu_{\mathrm{Fourier}} = \int_{\mathbb{R}^d}\mu(\mathrm{d}y,\cdot)$ in $\mathcal{M}(\mathbb{R}^d_*,\mathbb{C}^{m\times m})$.*

If in addition the sequence $(f^\varepsilon)_\varepsilon$ is tight and ε–oscillatory, then

$$\int_{\mathbb{R}^d}\nu_{\mathrm{phys}}(\mathrm{d}y) = \int_{\mathbb{R}^d_*}\nu_{\mathrm{Fourier}}(\mathrm{d}\theta) = \lim_{\varepsilon\to 0}\|f^\varepsilon\|^2_{\mathrm{L}^2(\mathbb{R}^d,\mathbb{C}^m)}.$$

For a proof of these results we refer to the above-mentioned references.

This condition of ε–oscillatoryness roughly means that the oscillations do not occur on scales finer than that of order ε. For our lattice problem this condition is satisfied by construction. In particular, the Fourier transforms of our solutions $Z^\varepsilon = \varepsilon\mathcal{S}_\varepsilon x^\varepsilon$ have a compact support lying in $\frac{1}{\varepsilon}B_{\Gamma_*}\subset\frac{1}{\varepsilon}B_{R_*}(0)$ for some $R_*>0$.

Lemma 5.2 *Let Z^ε be a bounded sequence in $\mathrm{L}^2(\mathbb{R}^d,\mathbb{C}^k)$ with $\mathrm{sppt}(\mathcal{F}Z^\varepsilon)\subset\frac{1}{\varepsilon}B_{R_*}(0)$, then* (5.11) *is satisfied, i.e. Z^ε is ε–oscillatory.*

If $\mathrm{sppt}(\mathcal{F}Z^\varepsilon)\subset\frac{1}{\varepsilon}B_{\Gamma_*}$ then any Wigner measure $\mu\in\mathcal{M}(\mathbb{R}^d\times\mathbb{R}^d_*,\mathbb{C}^{m\times m}_{\geq 0})$ has support in $\mathbb{R}^d\times B_{\Gamma_*}$.

Proof: Let $R>R_*$ and $C_* = \limsup_{\varepsilon\to 0}\|\mathcal{F}Z^\varepsilon\|^2<\infty$. For $\varphi\in\mathrm{C}^0_{\mathrm{c}}(\mathbb{R}^d)$ we have

$$\begin{aligned}&\int_{|\eta|>R/\varepsilon}|\mathcal{F}(\varphi Z^\varepsilon)(\eta)|^2\,\mathrm{d}\eta = \int_{|\eta_1+\eta_2|>R/\varepsilon}|\mathcal{F}\varphi(\eta_1)|^2|\mathcal{F}Z^\varepsilon(\eta_2)|^2\,\mathrm{d}(\eta_1,\eta_2)\\ &\leq \int_{|\eta_1|>(R-R_*)/\varepsilon}|\mathcal{F}\varphi(\eta_1)|^2\,\mathrm{d}\eta_1\int_{|\eta_2|<R_*/\varepsilon}|\mathcal{F}Z^\varepsilon(\eta_2)|^2\,\mathrm{d}\eta_2,\end{aligned}$$

where we used $\mathcal{F}Z^\varepsilon(\eta)=0$ for $|\eta|\geq R_*/\varepsilon$. The first factor tends to 0 for $\varepsilon\to 0$ due to $\mathcal{F}\varphi\in\mathrm{L}^2(\mathbb{R}^d_*)$, and the second factor is bounded by C_*. This proves the first assertion.

For the second assertion we use the representation (5.3) for $\widehat{W^\varepsilon}[Z^\varepsilon,Z^\varepsilon]$. For $\varepsilon\eta\notin B_{\Gamma_*}$ and any ζ and ε at least one of the two vectors $\eta/\varepsilon+\zeta/2$ and $\eta/\varepsilon-\zeta/2$ does not lie in B_{Γ_*}, since this set is convex. This shows that $\widehat{W^\varepsilon}[Z^\varepsilon]$ has support in $\mathbb{R}^d_*\times B_{\Gamma_*}$ and hence

$\mathrm{sppt}W^\varepsilon[Z^\varepsilon] \subset \mathbb{R}^d \times B_{\Gamma_*}$. Clearly, this support property is preserved in the limit $\varepsilon \to 0$, which proves the second assertion. ∎

Because of the second part of the previous lemma we consider the Wigner and the Husimi transform as functions on $\mathbb{R}^d \times \mathcal{T}_{\Gamma_*}$. We use the notation $W^\varepsilon_\Gamma[f]$ if we want to emphasize the fact, that $W^\varepsilon[f]$ is considered to be a periodic function of $\theta \in \mathcal{T}_{\Gamma_*}$. Because of convolution with G^ε_θ the same support property does not hold for the Husimi transform. However, we define the periodic variant by replacing the Gaussian kernel by its periodic counterpart. Thus, we set

$$H^\varepsilon_\Gamma[f](y,\theta) \stackrel{\text{def}}{=} \sum_{\beta\in\Gamma_*} H^\varepsilon[f](y,\theta+\beta) \quad \text{and} \quad G^\varepsilon_\Gamma(\theta) \stackrel{\text{def}}{=} \sum_{\beta\in\Gamma_*} G^\varepsilon(\theta+\beta).$$

Then, we also have the formula $H^\varepsilon_\Gamma[f] = W^\varepsilon_\Gamma[f] * G^\varepsilon_y * G^\varepsilon_\Gamma$, where the convolution with G^ε_Γ is now done on the additive group $\mathcal{T}_{\Gamma_*}$. Moreover, $H^\varepsilon_\Gamma[f]$ remains a measure with values in $\mathbb{C}^{m\times m}_{\geq 0}$ and $\int_{\mathbb{R}^d\times\mathcal{T}_{\Gamma_*}} \operatorname{tr} H^\varepsilon_\Gamma[f](y,\theta)\,\mathrm{d}\theta\,\mathrm{d}y = \|f\|^2_{\mathrm{L}^2(\mathbb{R}^d)}$.

5.3 Concentrations on singular sets and Husimi measures

Below we need to control the speed with which the energy is concentrated at certain singular sets $S \subset \mathcal{T}_{\Gamma_*}$. We say that the sequence $\rho^\varepsilon \in \mathcal{M}(\mathcal{T}_{\Gamma_*})$ *concentrates on* S *in the order* ε^α with $\alpha > 0$, if there exists $R > 0$ such that

$$\limsup_{\varepsilon\to 0} \rho^\varepsilon(\{\,\theta \mid \operatorname{dist}(x,S) \leq \varepsilon^\alpha R\,\}) > 0,$$

where "dist" denotes the standard distance on the torus $\mathcal{T}_{\Gamma_*}$. Of course, concentration in the order ε^α implies concentration in the order ε^β if $0 < \beta < \alpha$.

For Wigner transforms $W^\varepsilon[f^\varepsilon]$ and Husimi transforms $H^\varepsilon[f^\varepsilon]$ we say that they concentrate on S in the order ε^α if the measures $\rho^\varepsilon_{\mathrm{W}}$ and $\rho^\varepsilon_{\mathrm{H}}$, respectively, concentrate in the sense above, where $\rho^\varepsilon_{\mathrm{W}}$ and $\rho^\varepsilon_{\mathrm{H}}$ are defined through the densities $\delta^\varepsilon : \theta \mapsto \frac{1}{(2\varepsilon\pi)^d}|\mathcal{F}f^\varepsilon(\theta/\varepsilon)|^2$ and $\delta^\varepsilon * G^\varepsilon$, respectively.

As an example consider a sequence $(f^\varepsilon)_{\varepsilon>0}$ which has a nontrivial weak limit $f^0 \neq 0$ in $\mathrm{L}^2(\mathbb{R}^d)$, then the sequence $W^\varepsilon[f^\varepsilon]$ concentrates on $S = \{0\}$ in the order ε^1. To see this we argue as in Section 5.1 to obtain $\mathcal{F}f^\varepsilon \rightharpoonup \mathcal{F}f^0$ and $|\mathcal{F}f^\varepsilon|^2 \stackrel{*}{\rightharpoonup} |\mathcal{F}f^0|^2 + g$ where $|\mathcal{F}(f^\varepsilon - f^0)|^2 \stackrel{*}{\rightharpoonup} g \geq 0$. Thus for each $R > 0$ we find

$$\rho^\varepsilon_{\mathrm{W}}(\{\,\theta \mid |\theta| \leq \varepsilon R\,\}) = \int_{|\theta|\leq\varepsilon R} \tfrac{1}{(2\varepsilon\pi)^d} |(\mathcal{F}f^\varepsilon)(\theta/\varepsilon)|^2\,\mathrm{d}\theta = \tfrac{1}{(2\pi)^d}\int_{|\eta|\leq R} |(\mathcal{F}f^\varepsilon)(\eta)|^2\,\mathrm{d}\eta,$$

which implies $\limsup_{\varepsilon\to 0} \rho^\varepsilon_{\mathrm{W}}(\{|\theta| \leq \varepsilon R\}) \geq \frac{1}{(2\pi)^d}\int_{|\eta|\leq R} |(\mathcal{F}f^0)(\eta)|^2\,\mathrm{d}\eta > 0$ for sufficiently large R.

Lemma 5.3 *Let $\alpha \in (0, \frac{1}{2}]$, $S \subset \mathcal{T}_{\Gamma_*}$, take a bounded sequence $\rho^\varepsilon_{\mathrm{W}}$ in $\mathcal{M}(\mathcal{T}_{\Gamma_*})$ and define $\rho^\varepsilon_{\mathrm{H}} = \rho^\varepsilon_{\mathrm{W}} * G^\varepsilon_\Gamma$. Then, $\rho^\varepsilon_{\mathrm{W}}$ concentrates on S in the order ε^α if and only if $\rho^\varepsilon_{\mathrm{H}}$ does so.*

If $\rho^\varepsilon_{\mathrm{W}}$ concentrates on S in the order ε^β for some $\beta > 1/2$, then, in general, $\rho^\varepsilon_{\mathrm{H}}$ concentrates on S in the order $\varepsilon^{1/2}$ only. Just consider $\rho^\varepsilon_{\mathrm{W}} = \delta_s$ for some $s \in S$.

Proof: Let $S^\varepsilon_R = \{\,\theta \mid \mathrm{dist}(x,S) \leq \varepsilon^\alpha R\,\}$ and $a^\varepsilon(r) = \int_{\mathrm{dist}(0,\theta)>r} G^\varepsilon_\Gamma(\theta)\,\mathrm{d}\theta$, then

$$\rho^\varepsilon_{\mathrm{H}}(S^\varepsilon_R) = \int_{\mathcal{T}_{\Gamma_*}} \mathcal{X}_{S^\varepsilon_R}\rho^\varepsilon_{\mathrm{H}}(\mathrm{d}\theta) = \int_{\mathcal{T}_{\Gamma_*}} \Xi^\varepsilon_R(\theta)\rho^\varepsilon_{\mathrm{W}}(\mathrm{d}\theta) \text{ with } \Xi^\varepsilon_R = \mathcal{X}_{S^\varepsilon_R} * G^\varepsilon_\Gamma.$$

Using the triangle inequality for "dist" we find the estimates

$$1 - a^\varepsilon(\mathrm{dist}(\theta, \mathcal{T}_{\Gamma_*}\backslash S^\varepsilon_R)) \leq \Xi^\varepsilon_R(\theta) \leq a^\varepsilon(\mathrm{dist}(\theta, S^\varepsilon_R)).$$

For $\theta \in S^\varepsilon_{R/2}$ we have $\mathrm{dist}(\theta, \mathcal{T}_{\Gamma_*}\backslash S^\varepsilon_R) \geq \varepsilon^\alpha R/2$ and $\Xi^\varepsilon_R(\theta) \geq 1-a^\varepsilon(\varepsilon^\alpha R/2)$ implying

$$\rho^\varepsilon_{\mathrm{H}}(S^\varepsilon_R) \geq (1-a^\varepsilon(\varepsilon^\alpha R/2))\rho^\varepsilon_{\mathrm{W}}(S^\varepsilon_{R/2}).$$

Because of $\alpha \leq 1/2$ we have $a^\varepsilon(\varepsilon^\alpha r) \to c(r) \in [0,1)$ for $\varepsilon \to 0$ (in fact $c(r) = 0$ if $\alpha < 1/2$). This implies $\limsup_{\varepsilon\to 0} \rho^\varepsilon_{\mathrm{H}}(S^\varepsilon_R) \geq (1-c(R/2)), \limsup_{\varepsilon\to 0} \rho^\varepsilon_{\mathrm{W}}(S^\varepsilon_{R/2})$. Hence, $\rho^\varepsilon_{\mathrm{H}}$ concentrates if $\rho^\varepsilon_{\mathrm{W}}$ does.

Similarly for $\theta \notin S^\varepsilon_{R_1}$ with $R_1 > R$ we have $\mathrm{dist}(\theta, S^\varepsilon_R) \geq \varepsilon^\alpha(R_1-R)$ and obtain

$$\begin{aligned}\rho^\varepsilon_{\mathrm{H}}(S^\varepsilon_R) &\leq \int_{S^\varepsilon_{R_1}} 1\rho^\varepsilon_{\mathrm{W}}(\mathrm{d}\theta) + \int_{\mathcal{T}_{\Gamma_*}\backslash S^\varepsilon_{R_1}} a^\varepsilon(\varepsilon^\alpha(R_1-R))\rho^\varepsilon_{\mathrm{W}}(\mathrm{d}\theta)\\ &\leq \rho^\varepsilon_{\mathrm{W}}(S^\varepsilon_{R_1}) + a^\varepsilon(\varepsilon^\alpha(R_1-R))\rho^*,\end{aligned}$$

with $\rho^* = \sup\{\,\rho^\varepsilon_{\mathrm{W}}(\mathcal{T}_{\Gamma_*}) \mid \varepsilon > 0\,\}$. Thus, we conclude $\delta^R_{\mathrm{H}} = \limsup_{\varepsilon\to 0}\rho^\varepsilon_{\mathrm{H}}(S^\varepsilon_R) \leq \delta^W_{R_1} + c(R_1-R)\rho^*$ with $\delta^W_{R_1} = \limsup_{\varepsilon\to 0}\rho^\varepsilon_{\mathrm{W}}(S^\varepsilon_{R_1})$. For $\alpha < 1/2$ we have $c(R_1-R) = 0$ and the desired result $\delta^W_{R_1} \geq \delta^H_R$ is immediate. In the case $\alpha = 1/2$ we use that $c(r) \to 0$ for $r \to \infty$. Hence, we choose R_1 so large that $c(R_1-R)\rho^* < \delta^H_R/2$ and conclude $\delta^W_{R_1} \geq \delta^H_R/2$. In both cases we see that concentration of $\rho^\varepsilon_{\mathrm{H}}$ implies that of $\rho^\varepsilon_{\mathrm{W}}$ ■

The need of the study of concentrations near singular sets arises from the fact that the dispersion relations $\omega \mapsto \omega_j(\theta)$ are in general not smooth. To handle the problem we use the following properties. Each $\omega_j : \mathcal{T}_{\Gamma_*} \to \mathbb{R}$ is Lipschitz continuous, but in general not in $\mathrm{C}^1(\mathcal{T}_{\Gamma_*}, \mathbb{R})$. However, differentiability can be lost only at smooth subsurfaces (points, lines, surfaces), see [Hag98]. Let $\mathbb{T}_j \subset \mathcal{T}_{\Gamma_*}$ be the open subset of differentiability points of ω_j and set

$$\mathbb{T} \stackrel{\mathrm{def}}{=} \cap_{j=1}^k \mathbb{T}_j \subset \mathcal{T}_{\Gamma_*} \quad \text{and} \quad \mathbb{S} \stackrel{\mathrm{def}}{=} \mathcal{T}_{\Gamma_*} \setminus \mathbb{T}.$$

Then, each $\mathbb{T}_j$, and hence $\mathbb{T}$, are open and have full measure in $\mathcal{T}_{\Gamma_*}$. In particular, the singular set $\mathbb{S}$ consists of finitely many lower-dimensional analytic surfaces.

On $\mathbb{T}$ the functions $\nabla_\theta\omega_j$ are defined and bounded. Hence, there exists a compactification $\mathbb{K}$ such that all functions $\nabla_\theta\omega_j$, $j = 1,\ldots,k$ can be extended continuously to $\mathbb{K}$. We denote these continuations by $\widetilde{\nabla_\theta}\omega_j$. Below, we illustrate this construction by two examples.

The main advantage of the Husimi transform is that we are able interprete functions in $\mathrm{L}^1(\mathcal{T}_{\Gamma_*})$ (which is the same as $\mathrm{L}^1(\mathbb{T})$ as $\mathbb{S}$ has measure 0) as measures on $\mathbb{K}$. To this end let $\phi : \mathbb{T} \to \mathbb{K}$ be the continuous, injective, and dense embedding. Now every testfunction $\Psi \in \mathrm{C}^0(\mathbb{K})$ defines via $\psi = \Psi \circ \phi$ a continuous, bounded function on $\mathbb{T}$, in particular $\psi \in \mathrm{L}^\infty(\mathbb{T})$. Thus, we can embed $\mathrm{L}^1(\mathbb{R}^d \times \mathcal{T}_{\Gamma_*}, \mathbb{C}^{k\times k})$ into $\mathcal{M}(\mathbb{R}^d \times \mathbb{K}, \mathbb{C}^{k\times k})$ via the linear mapping Φ defined by

$$\langle \Phi h, \Psi\rangle = \int_{\mathbb{R}^d\times\mathbb{K}} \Psi(y,\kappa){:}(\Phi h)(\mathrm{d}y,\mathrm{d}\kappa) \overset{\text{def}}{=} \int_{\mathbb{R}^d\times\mathbb{T}} \Psi(y,\phi(\theta)){:}h(y,\theta)\,\mathrm{d}y\,\mathrm{d}\theta,$$

where $h \in \mathrm{L}^1(\mathbb{R}^d \times \mathcal{T}_{\Gamma_*}, \mathbb{C}^{k\times k})$, $\Psi \in \mathrm{C}^0_0(\mathbb{R}^d \times \mathbb{K}, \mathbb{C}^{k\times k})$, and ":" denotes the scalar product in $\mathbb{C}^{k\times k}$. The last integral could also be taken over $\mathbb{R}^d \times \mathcal{T}_{\Gamma_*}$, as the difference has Lebesgue measure 0.

Thus, our final Husimi measures will be defined on $\mathcal{M}(\mathbb{R}^d \times \mathbb{K}, \mathbb{C}^{k\times k})$ as limit of the embedded Husimi transforms, i.e., $\Phi H^\varepsilon[f^\varepsilon] \overset{*}{\rightharpoonup} \mu_{\mathrm{H}}$. We call the latter measure a *Husimi measure*.

Example 5.4 In Section 6.3 we consider the bi-atomic chain. Using the parameters $m = 6$, $\widetilde{m} = 10$, $k = \kappa = 1, \widetilde{\kappa} = 2$ (see Figure 6.3, right), the eigenvalues ω_1 and ω_2 touch at $\theta = 0$ and $\theta = \pm\pi$. Thus, $\mathbb{T}_1 = \mathbb{T}_2 = \mathbb{T} = (-\pi, 0) \cup (0, \pi)$ and $\mathbb{S} = \{0, \pi = -\pi\}$. As compactification we may take $\mathbb{K} = [-\pi, 0^-] \cup [0^+, \pi]$ which is the disjoint union of two compact intervals. Clearly, the group velocities $\nabla\omega_j$ have continuous extensions to this compactifications.

Example 5.5 In two or higher-dimensional problems the singularity at $\theta = 0$ becomes worse. In Section 6.5 we consider the square lattice, where $\mathcal{T}_{\Gamma_*} = (\mathbb{S}^1)^2$ which is the two-torus. For $k = 1/2$ we obtain the explicit dispersion relations

$$\omega_1(\theta) = \sqrt{2 - \cos\theta_1 - \cos\theta_2} \quad \text{and} \quad \omega_2(\theta) = \sqrt{4 - \cos\theta_1 - \cos\theta_2 - 2\cos\theta_1\cos\theta_2}.$$

Obviously, $\mathbb{T}_1 = \mathbb{T}_2 = \mathbb{T} = \mathcal{T}_{\Gamma_*} \setminus \{0\}$ and $\mathbb{S} = \{0\}$ and the frequencies have the expansions $\omega_j = \sqrt{(1{+}2j)/2}\,|\theta| + O(|\theta|^3)$. Thus, $\mathbb{K}$ is obtained by inserting a small circle instead of $\theta = 0$. More precisely, one introduces polar coordinates near $\theta = 0$; e.g., for $0 < |\theta| \le 1$ we write $\theta = r(\cos\rho, \sin\rho)$ with $r \in (0, 1]$ and $\rho \in \mathbb{S}^1$. Then, $\mathbb{K}$ is obtained by adding the points $(r, \rho) = (0, \rho)$ for $\rho \in \mathbb{S}^1$. In particular, the gradients satisfy $\nabla_\theta\omega_j(\theta) = \sqrt{(1{+}2j)/2}\,\frac{1}{|\theta|}\,\theta + O(|\theta|^2)$ for $\theta \to 0$. Obviously, there are unique extensions onto $\mathbb{K}$ with $\widetilde{\nabla_\theta}\omega_j((r, \rho)) \to \sqrt{(1{+}2j)/2}(\cos\rho, \sin\rho)$ for $r \to 0$.

5.4 Energy transport via Wigner and Husimi measures

In this section we present two versions of the energy-transport equation. The first result concerns the classical Wigner measures and is formulated on $\mathbb{R}^d \times \mathcal{T}_{\Gamma_*}$, but has the additional assumption that the Husimi or Wigner transforms do not concentrate on the singular set $\mathbb{S}$ at all. This is a simple adaption of the theory developed in [GMMP97]. In the second result we use the Husimi measure introduced above and thus we are able to allow for some concentration of the energy on the singular set $\mathbb{S}$. The order of concentration must be slower than $\varepsilon^{1/2}$ and the functions $\nabla_\theta \omega_j$ need to behave suitably well near $\mathbb{S}$.

To study the energy associated with the solutions $(Z^\varepsilon(\tau), \partial_\tau Z^\varepsilon(\tau))$ it is advantageous to transform the system into diagonal form, when written in Fourier space:

$$\partial_\tau \widehat{U}(\tau,\eta) = \frac{\mathrm{i}}{\varepsilon}\widehat{\Omega}(\varepsilon\eta)\widehat{U}(\tau,\eta), \quad \widehat{U}(0,\cdot) = \widehat{U}_0 \in \mathrm{L}^2(\mathbb{R}^d, \mathbb{C}^{2m}) \tag{5.12}$$

with $\widehat{\Omega}(\theta) = \mathrm{diag}(\omega_1(\theta), \ldots, \omega_{2m}(\theta)) \in \mathbb{R}^{2m\times 2m}$. This is obtained from (4.2) written in Fourier space as

$$M\partial_\tau^2 \widehat{Z}(\tau,\eta) + \mathbb{A}^\varepsilon(\eta)\widehat{Z}(\tau,\eta) = 0. \tag{5.13}$$

Since $\omega_j(\theta)^2$, $j = 1, \ldots, m$ are the eigenvalues of $M^{-1/2}\mathbb{A}_{\mathrm{per}}(\theta)M^{-1/2}$, we let $\Omega(\theta) = \mathrm{diag}(\omega_1(\theta), \ldots, \omega_m(\theta))$ and find a family of unitary matrices $(Q(\theta))_{\theta\in\mathcal{T}_{\Gamma_*}}$ such that

$$M^{-1/2}\mathbb{A}(\theta)M^{-1/2} = Q(\theta)^*\Omega(\theta)^2 Q(\theta).$$

Hence, (5.13) transforms into (5.12) with

$$\widehat{U}(\tau,\eta) = \begin{pmatrix} 1/2 & -\mathrm{i}/2 \\ 1/2 & \mathrm{i}/2 \end{pmatrix} \begin{pmatrix} \Omega(\varepsilon\eta)Q(\varepsilon\eta)M^{1/2}\widehat{Z}(\tau,\eta) \\ Q(\varepsilon\eta)M^{1/2}\partial_\tau\widehat{Z}(\tau,\eta) \end{pmatrix} \text{ and } \widehat{\Omega}(\theta) = \begin{pmatrix} \Omega(\theta) & 0 \\ 0 & -\Omega(\theta) \end{pmatrix}.$$

The transformation was done such that

$$|\widehat{U}(\tau,\eta)|^2 = \tfrac{1}{2}\langle M\partial_\tau\widehat{Z}(\tau,\eta), \partial_\tau\widehat{Z}(\tau,\eta)\rangle + \tfrac{1}{2}\langle \mathbb{A}^\varepsilon(\eta)\widehat{Z}(\tau,\eta), \widehat{Z}(\tau,\eta)\rangle,$$

which shows that $|U|^2$ is an energetic quantity. Applying the Wigner transform to $U(\tau) = \mathcal{F}^{-1}\widehat{U}(\tau,\cdot)$, we see that $W^\varepsilon[U^\varepsilon]$ allows us to control the energy located in physical space via

$$e^\varepsilon_{\mathrm{W}}(\tau,y) = |U^\varepsilon(\tau,y)|^2 = \int_{\mathcal{T}_{\Gamma_*}} \mathrm{tr}\Big(W^\varepsilon[U^\varepsilon(\tau)](y,\theta)\Big)\,\mathrm{d}\theta.$$

This energy distribution is a replacement for E^ε or $\widetilde{E}^\varepsilon$ defined in Section 5.1.

The difference between E^ε, $\widetilde{E}^\varepsilon$ and $e^\varepsilon_{\mathrm{W}}$ arises because of the transformation via $Q(\theta)$ in Fourier space. This gives rise to pseudo differential operators which lead to a certain nonlocality on the microscopic level which disappears in the limit $\varepsilon \to 0$. In the case that $\mathbb{A}(\theta) = \mathbb{L}(\theta)^*\mathbb{L}(\theta)$ with smooth $\mathbb{L}$ holds, the connection between the energies can be made more exact. For solutions Z^ε we define the vectors

$$V^\varepsilon = \begin{pmatrix} M^{1/2}\partial_\tau Z^\varepsilon \\ \mathcal{L}_\varepsilon Z^\varepsilon \end{pmatrix} \in \mathrm{L}^2(\mathbb{R}^d, \mathbb{R}^m)^{1+p}, \tag{5.14}$$

then we have $\widetilde{E}^\varepsilon(\tau,y) = \frac{1}{2}|V^\varepsilon(t,y)|^2$, $\widehat{V}^\varepsilon = \mathcal{F}V^\varepsilon = \left(\begin{smallmatrix} M^{1/2}\partial_\tau\widehat{Z}^\varepsilon \\ \frac{1}{\varepsilon}\mathbb{L}(\varepsilon\eta)\widehat{Z}^\varepsilon \end{smallmatrix}\right)$ and $|\widehat{V}^\varepsilon|^2 = 2|\widehat{U}^\varepsilon|^2$.

We now state our first result which is based on the Wigner measure. Recall that $\mathbb{S} \subset \mathcal{T}_{\Gamma_*}$ is the singular set where $\nabla_\theta \omega_j$ is not defined.

Theorem 5.6 *Let $(U^\varepsilon)_{\varepsilon>0}$ be a family of solutions of (5.12) such that sppt$(\widehat{U}^\varepsilon) \subset \frac{1}{\varepsilon} B_{\Gamma_*}$, that $U^\varepsilon \rightharpoonup 0$ in $\mathrm{L}^2(\mathbb{R}^d, \mathbb{C}^{2m})$ and that there is no concentration on the singluar set $\mathbb{S}$, i.e.,*

$$\limsup_{\varepsilon\to 0} \int_{\mathrm{dist}(\theta,\mathbb{S})<r} \tfrac{1}{(2\varepsilon\pi)^d} |\widehat{U}^\varepsilon(\theta/\varepsilon)|^2 \,\mathrm{d}\theta \quad \longrightarrow 0 \quad \textit{for } r \to 0.$$

Further, assume that for all $j = 1, \ldots, 2m$ the Wigner transforms $W^\varepsilon_\Gamma[U^\varepsilon_j(0,\cdot)]$ of the initial data converge to the Wigner measure $\mu^0_j \in \mathcal{M}(\mathbb{R}^d \times \mathcal{T}_{\Gamma_*})$.

Then, for all $\tau \in R$ and all $j = 1, \ldots, 2m$ we have the convergence

$$W^\varepsilon_\Gamma[U^\varepsilon_j(0,\cdot)] \xrightarrow{\mathcal{D}} \mu_j(\tau;\cdot) \in \mathcal{M}(\mathbb{R}^d \times \mathcal{T}_{\Gamma_*}),$$

where μ_j satisfies (in the sense of distributions) the transport equation

$$\partial_\tau \mu_j(\tau) = \nabla_\theta \omega_j(\theta) \cdot \partial_y \mu_j(\tau) \quad \textit{and} \quad \mu_j(0) = \mu^0_j. \tag{5.15}$$

Remarks

1. Note that all $\mu_j(\tau)$ satisfy $\int_{\mathbb{R}^d \times \mathbb{S}} \mu_j(\tau; \mathrm{d}y, \mathrm{d}\theta) = \mu(\tau; \mathbb{R}^d \times \mathbb{S}) = 0$, such that it is irrelevant that $\nabla \omega_j$ is not defined on $\mathbb{S}$.

2. The same statement of the theorem holds also for the Husimi transform. Then, the convergence is better, namely weak$*$ in $\mathcal{M}(\mathbb{R}^d \times \mathbb{S})$. We keep the formulation of the result in terms of the Wigner transform to conform with [GMMP97] and to provide a simple proof. Of course, Theorem 5.7 includes the present result as a special case.

3. The solution of (5.15) is uniquely defined via transport in y with speed $\nabla_\theta \omega_j(\theta)$, i.e., $\mu_j(\tau, y, \theta) = \mu^0_j(y + \nabla_\theta \omega_j(\theta), \theta)$. More precisely, this means that for all $\Psi \in C^0_0(\mathbb{R}^d \times \mathcal{T}_{\Gamma_*})$ we have

$$\int_{\mathbb{R}^d \times \mathcal{T}_{\Gamma_*}} \Psi(y,\theta) \mu_j(\tau; \mathrm{d}y, \mathrm{d}\theta) = \int_{\mathbb{R}^d \times \mathbb{T}} \Psi(y - \tau \nabla_\theta \omega_j(\theta), \theta) \mu^0_j(\mathrm{d}y, \mathrm{d}\theta).$$

Integration over $\mathcal{T}_{\Gamma_*}$ can be replaced by one over $\mathbb{T} = \mathcal{T}_{\Gamma_*} \backslash \mathbb{S}$ because of $\mu^0_j(\mathbb{R}^d \times \mathbb{S}) = 0$.

4. If we additionally assume that the sequence $(U^\varepsilon)_\varepsilon$ is tight, then we know that $\int_{\mathbb{R}^d \times \mathbb{T}} \sum_{j=1}^{2m} \mu_j(\tau; \mathrm{d}y, \mathrm{d}\theta) = \lim_{\varepsilon\to 0} \int_{\mathbb{R}^d} |U^\varepsilon(y)|^2 \,\mathrm{d}y$.

Proof: We sketch the main arguments of this comparable simple proof. The exact details are given in the proof of the following theorem.

Via (5.3) and (5.13) we obtain the differential equation

$$\begin{aligned} &\partial_\tau \widehat{w}^\varepsilon(\tau,\zeta,\theta) = \mathrm{i}\Delta_\varepsilon(\theta,\zeta)\, \widehat{w}^\varepsilon(\tau,\zeta,\theta) \\ &\text{with } \Delta_\varepsilon(\theta,\zeta) \stackrel{\text{def}}{=} \tfrac{1}{\varepsilon} \left[\omega_j(\theta + \tfrac{\varepsilon}{2}\zeta)) - \omega_j(\theta - \tfrac{\varepsilon}{2}\zeta) \right] \end{aligned} \tag{5.16}$$

where $\widehat{w}^\varepsilon = \mathcal{F}_{y\to\zeta} W^\varepsilon[U^\varepsilon_j(\tau,\cdot)]$. The explicit solution reads

$$\widehat{w}^\varepsilon(\tau,\zeta,\theta) = \mathrm{e}^{\mathrm{i}\Delta_\varepsilon(\zeta,\theta)\tau} \widehat{w}^\varepsilon(0,\zeta,\theta) \quad \text{for } (\tau,\eta,\theta) \in \mathbb{R} \times \mathbb{R}^d_* \times \mathcal{T}_{\Gamma_*}.$$

By (5.4) we know that $(w^\varepsilon(\tau))_\varepsilon$ is uniformly bounded in $\mathrm{L}^\infty(\mathbb{R}^d_*, \mathrm{L}^1(\mathcal{T}_{\Gamma_*}))$. We choose testfunctions $\psi \in \mathrm{L}^1(\mathbb{R}^d_*, \mathrm{C}^0(\mathcal{T}_{\Gamma_*}))$ with the additional property $\psi \in \mathrm{C}^0_\mathrm{c}(\mathbb{R}^d_* \times \mathbb{T})$. On the compact support $\mathrm{sppt}(\psi) \subset \mathbb{R}^d_* \times \mathbb{T}$ the convergence

$$\Delta_\varepsilon(\zeta, \theta) \;\longrightarrow \zeta \cdot \nabla_\theta \omega_j(\theta) \quad \text{for } \varepsilon \to 0,$$

is uniform as ω_j is twice differentiable on $\mathbb{T}$ and as ζ is bounded. Define

$$\widehat{g}^\varepsilon(\tau, \zeta, \theta) = \mathrm{e}^{\mathrm{i}\zeta\cdot\nabla_\theta \omega_j(\theta)\,\tau}\,\widehat{w}^\varepsilon(0, \zeta, \theta)$$

as an intermediate approximation. Then, with (5.4) we have, for $\varepsilon \to 0$,

$$\begin{aligned}&\big|\textstyle\int_{\mathbb{R}^d_*\times\mathbb{T}} \psi(\zeta, \theta)\mathrm{e}^{\mathrm{i}\Delta_\varepsilon(\theta,\zeta)\,\tau}\widehat{w}^\varepsilon(0, \zeta, \theta)\,\mathrm{d}\zeta\,\mathrm{d}\theta - \int_{\mathbb{R}^d_*\times\mathbb{T}} \psi(\zeta, \theta)\widehat{g}^\varepsilon(\tau, \zeta, \theta)\,\mathrm{d}\zeta\,\mathrm{d}\theta\big| \\ &\le |\tau| \sup_{(\theta,\zeta)\in\mathrm{sppt}(\psi)} |\Delta_\varepsilon(\theta, \zeta) - \zeta\cdot\nabla_\theta \omega_j(\theta)| \;\textstyle\int_{\mathbb{R}^d_*} \|\psi(\zeta)\|_{\mathrm{C}^0_\mathrm{c}(\mathbb{T})} \|\widehat{w}^\varepsilon(0, \zeta)\|_{\mathrm{L}^1(\mathcal{T}_{\Gamma_*})}\,\mathrm{d}\zeta \to 0.\end{aligned}$$

Moreover, since $(\zeta, \theta) \mapsto \psi(\zeta, \theta)\mathrm{e}^{\mathrm{i}\zeta\cdot\nabla_\theta \omega_j(\theta)\,\tau}$ is in the set of admissible testfunctions for the convergence of Wigner transforms (see [GMMP97, Rem.1.3]), the convergence $\widehat{w}^\varepsilon(0) \xrightarrow{\mathcal{D}} \mu^0_j$ implies

$$\int_{\mathbb{R}^d_*\times\mathbb{T}} \psi(\zeta, \theta)\widehat{g}^\varepsilon(\tau, \eta, \theta)\,\mathrm{d}\zeta\,\mathrm{d}\theta \;\xrightarrow{\varepsilon\to 0}\; \int_{\mathbb{R}^d_*\times\mathbb{T}} \psi(\zeta, \theta)\mathrm{e}^{\mathrm{i}\zeta\cdot\nabla_\theta \omega_j(\theta)\,\tau}\mu^0_j(\mathrm{d}\eta, \mathrm{d}\theta).$$

If we define $\mu_j(\tau)$ through the right-hand side we first see that the transport equation (5.15) holds and with the above estimate we have

$$\int_{\mathbb{R}^d_*\times\mathbb{T}} \psi(\zeta, \theta)\mathrm{e}^{\mathrm{i}\Delta_\varepsilon(\theta,\zeta)\,\tau}\widehat{w}^\varepsilon(0, \zeta, \theta)\,\mathrm{d}\zeta\,\mathrm{d}\theta \;\xrightarrow{\varepsilon\to 0}\; \int_{\mathbb{R}^d_*\times\mathbb{T}} \psi(\zeta, \theta)\mu_j(\tau; \mathrm{d}\eta, \mathrm{d}\theta).$$

Finally we remark that the set of testfunctions ψ, we have considered so far, is dense in the set of all necessary testfunctions. This establishes the desired result. ∎

As a consequence of the above result we obtain an exact characterization of the weak$*$ limit of e^ε_W defined as $e^\varepsilon_\mathrm{W}(\tau, y) = |U^\varepsilon(\tau, y)|^2$. Starting with the Wigner measures $\mu_j(0) \in \mathcal{M}(\mathbb{R}^d\times\mathbb{T})$ of the initial data, the energy $e^\varepsilon_\mathrm{W}(\tau)$ is obtained by

$$\textstyle\int_{\mathbb{R}^d} \Psi(y) e^\varepsilon_\mathrm{W}(\tau; \mathrm{d}y) = \int_{\mathbb{R}^d\times\mathbb{T}} \sum_{j=1}^{2m} \Psi(y - \tau\nabla_\theta \omega_j(\theta))\mu^0_j(\mathrm{d}y, \mathrm{d}\theta). \tag{5.17}$$

Before we turn to the second result we want to highlight a general feature of the above proof and of the proof to come. In showing convergence of the approximations $f^\varepsilon(\tau) = W^\varepsilon_\Gamma[U^\varepsilon_j(\tau)]$ or $f^\varepsilon(\tau) = H^\varepsilon_\Gamma[U^\varepsilon_j(\tau)]$ towards the limit $\mu_j(\tau)$ it is advantageous to introduce an intermediate approximation $g^\varepsilon(\tau)$ which is a solution of the limit equation, initially derived for μ_j only, with the ε-dependent initial data $f^\varepsilon(0)$. As the limit equation does not depend on ε and we know that the initial data converge, i.e., $f^\varepsilon(0) \rightsquigarrow \mu_i(0)$, it is easy to conclude $g^\varepsilon(\tau) \rightsquigarrow \mu_j(\tau)$, where the converge is in general as weak as the convergence of the initial data. In a second step, one then shows $f^\varepsilon(\tau) - g^\varepsilon(\tau) \to 0$, where one needs to exploit the convergence of the Fourier symbols, i.e., $\Delta_\varepsilon(\zeta, \theta) \to \zeta \cdot \nabla_\theta \omega_j(\theta)$. This convergence is usually more explicit and error bounds can be obtained in suitable weak function spaces, see [TP04].

Our second result involves the Husimi measure and allows for certain energy concentrations on the singular set $\mathbb{S}$. Thus, the above result is not applicable for our lattice models if energy is concentrated in mesoscopic wave lengths of order $\sqrt{\varepsilon}$, since the point $\theta = 0$ always lies in the singular set because of the acoustic waves. The following result shows, that in certain cases we can still go to the limit if we use the compactification $\mathbb{K}$ of $\mathbb{T} = \mathcal{T}_{\Gamma_*} \backslash \mathbb{S}$. Recall that we consider Husimi transforms $H^\varepsilon_\Gamma[U^\varepsilon_j]$ as measures in $\mathcal{M}(\mathbb{R}^d \times \mathbb{K})$ via the identification Φ. To emphasize this embedding we set $H^\varepsilon_\mathbb{K}[f] = \Phi H^\varepsilon_\Gamma[f] \in \mathcal{M}(\mathbb{R}^d \times \mathbb{K})$ and recall the definition

$$\int_{\mathbb{R}^d \times \mathbb{K}} \Psi(y, \kappa)(H^\varepsilon_\mathbb{K}[U^\varepsilon_j])(\mathrm{d}y, \mathrm{d}\kappa) = \int_{\mathbb{R}^d \times \mathbb{T}} \Psi(y, \phi(\theta)) H^\varepsilon_\Gamma[U^\varepsilon_j](y, \theta)\, \mathrm{d}y\, \mathrm{d}\theta,$$

where $\Psi \in \mathrm{C}^0_0(\mathbb{R}^d \times \mathbb{K})$ is a testfunction and $\phi : \mathbb{T} \to \mathbb{K}$ is the continuous, injective embedding with dense range.

Theorem 5.7 *Assume that $\mathbb{K}$ is a compactification of $\mathbb{T}$ such that all $\nabla_\theta \omega_j$ have continuous extensions $\widetilde{\nabla_\theta} \omega_j$. Moreover, assume*

$$\begin{aligned} &\exists\, C_* > 0\; \exists\, \sigma \in (0, 1]\; \forall\, j \in \{1, ..., m\}\; \forall\, \theta_1, \theta_2 \in \mathbb{T} : \\ &\qquad |\nabla_\theta \omega_j(\theta_1) - \nabla_\theta \omega_j(\theta_2)| \le C \Big(\frac{\mathrm{dist}(\theta_1, \theta_2)}{\min\{\mathrm{dist}(\theta_1, \mathbb{S}), \mathrm{dist}(\theta_2, \mathbb{S})\}} \Big)^\sigma. \end{aligned} \tag{5.18}$$

Let $(U^\varepsilon)_{0<\varepsilon<1}$ be a family of solutions of (5.12) such that $U^\varepsilon \rightharpoonup 0$ in $\mathrm{L}^2(\mathbb{R}^d, \mathbb{C}^{2m})$, sppt$(\widehat{U}^\varepsilon) \subset \frac{1}{\varepsilon} B_{\Gamma_*}$ and that it does not concentrate on the singular set $\mathbb{S}$ in the order $\varepsilon^{1/2}$, i.e, for all $R > 0$ we have

$$\int_{\mathrm{dist}(\theta, \mathbb{S}) < \varepsilon^{1/2} R} \tfrac{1}{(2\varepsilon\pi)^d} |\widehat{U}^\varepsilon(\theta/\varepsilon)|^2\, \mathrm{d}\theta \;\longrightarrow 0 \quad \text{for } \varepsilon \to 0.$$

Further, assume that for all $j = 1, \dots, 2m$ the Husimi transforms $H^\varepsilon_\mathbb{K}[U^\varepsilon_j(0, \cdot)]$ of the initial data converge to the Husimi measure $\mu^0_j \in \mathcal{M}(\mathbb{R}^d \times \mathbb{K})$.

Then, for all $\tau \in \mathbb{R}$ and all $j = 1, \dots, 2m$ we have the convergence

$$H^\varepsilon_\mathbb{K}[U^\varepsilon_j(\tau, \cdot)] \overset{*}{\rightharpoonup} \mu_j(\tau; \cdot) \in \mathcal{M}(\mathbb{R}^d \times \mathbb{K}),$$

where μ_j satisfies the transport equation

$$\partial_\tau \mu_j(\tau) = \widetilde{\nabla_\theta} \omega_j(\kappa) \cdot \partial_y \mu_j(\tau) \text{ with } \mu_j(0) = \mu^0_j \tag{5.19}$$

in the sense of distributions, i.e., for all $\Psi \in \mathrm{C}^0_0(\mathbb{R}^d \times \mathbb{K})$ we have

$$\int_{\mathbb{R}^d \times \mathbb{K}} \Psi(y, \kappa) \mu_j(\tau; \mathrm{d}y, \mathrm{d}\kappa) = \int_{\mathbb{R}^d \times \mathbb{K}} \Psi(y - \tau \widetilde{\nabla_\theta} \omega_j(\kappa), \kappa) \mu^0_j(\mathrm{d}y, \mathrm{d}\kappa). \tag{5.20}$$

Remarks.

1. For eqn. (5.20) we do not need any differentiable structure for $\mathbb{K}$ as transport occurs only in the y direction but not in $\kappa \in \mathbb{K}$.

2. The assumptions about the concentration and about the Lipschitz continuity of $\nabla_\theta \omega_j$ can not be dispensed with as we show in Section 6.1.

Proof: The proof follows the same strategy as the one above. This time we use the Fourier transformed version of the Husimi transform and show convergence using suitable testfunctions and taking special care of the wave vectors near $\mathbb{S}$. In Step 1 we cut out the wave vectors near $\mathbb{S}$ by using the nonconcentration condition. Thus, it suffices to study a simplified measure $h^\varepsilon(\tau)$ instead of the full Husimi transform $H^\varepsilon_{\mathbb{K}}[U^\varepsilon_j(\tau)]$. In Step 2 we introduce the intermediate approximation $g^\varepsilon(\tau)$ solving (5.19) but having the initial condition $h^\varepsilon(0)$ and show its weak$*$ convergence to the solution $\mu_j(\tau)$ defined in (5.20). In Step 3 we estimate $h^\varepsilon(\tau) - g^\varepsilon(\tau)$ by using their explicit representations in Fourier space.

Step 1. Throughout the proof we fix $j \in \{1, ..., 2m\}$ and define the measures $\rho^\varepsilon_{\mathrm{W}}$ and $\rho^\varepsilon_{\mathrm{H}} = \rho^\varepsilon_{\mathrm{W}} * G^\varepsilon_\Gamma$ on $\mathcal{T}_{\Gamma_*}$ such that $\rho^\varepsilon_{\mathrm{W}}$ has the density $\theta \mapsto \frac{1}{(2\varepsilon\pi)^d}|\widehat{U}^\varepsilon_j(0;\theta/\varepsilon)|^2$ where $\widehat{U}^\varepsilon_j(\tau) = \mathcal{F}U^\varepsilon_j(\tau)$. By our assumption of nonconcentration on $\mathbb{S}$, there exists $R_\varepsilon > 0$ with $R_\varepsilon \to \infty$ for $\varepsilon \to 0$ such that

$$r_\varepsilon = \rho^\varepsilon_{\mathrm{W}}(\mathbb{S}_\varepsilon) \quad\longrightarrow\quad 0 \quad \text{for } \varepsilon \to 0, \text{ where } \mathbb{S}_\varepsilon = \{\, \theta \mid \mathrm{dist}(\theta, \mathbb{S}) < \varepsilon^{1/2} R_\varepsilon \,\}.$$

With Lemma 5.3 we may choose R_ε such that we also have $\rho^\varepsilon_{\mathrm{H}}(\mathbb{S}_\varepsilon) \to 0$ for $\varepsilon \to 0$.

Define the characteristic functions

$$p_\varepsilon = \mathcal{X}_{\mathbb{T}_\varepsilon} \colon \mathcal{T}_{\Gamma_*} \to \mathbb{R} \text{ with } \mathbb{T}_\varepsilon = \mathcal{T}_{\Gamma_*} \backslash \mathbb{S}_\varepsilon \;\text{ and }\; q_\varepsilon = \mathcal{X}_{\mathbb{B}_\varepsilon} \colon \mathbb{R}^d_* \to \mathbb{R} \text{ with } \mathbb{B}_\varepsilon = \tfrac{1}{\varepsilon}(B_{\Gamma_*} \backslash \mathbb{S}_\varepsilon)$$

and let $h^\varepsilon(\tau) = p_\varepsilon H^\varepsilon_\Gamma[U^\varepsilon_j(\tau)] \in \mathrm{L}^1(\mathbb{R}^d \times \mathcal{T}_{\Gamma_*})$. Then we have

$$\|h^\varepsilon(\tau) - H^\varepsilon_\Gamma[U^\varepsilon_j(\tau)]\|_{\mathrm{L}^1} = \rho^\varepsilon_H(\mathbb{S}_\varepsilon) \to 0.$$

Next we show that we may assume that $\widehat{U}^\varepsilon_j$ has support in $\mathbb{B}_\varepsilon$. Define $V^\varepsilon(\tau) \in \mathrm{L}^2(\mathbb{R}^d, \mathbb{C})$ via $\mathcal{F}V^\varepsilon(\tau, \zeta) = q_\varepsilon(\zeta)[\mathcal{F}U^\varepsilon_j(\tau)](\zeta)$, then we have

$$\|U^\varepsilon_j(\tau) - V^\varepsilon(\tau)\|^2_{\mathrm{L}^2} = \rho^\varepsilon_{\mathrm{W}}(\mathbb{S}_\varepsilon) = r_\varepsilon \to 0.$$

By (5.6) the corresponding Husimi transforms satisfy

$$\begin{aligned}
&\|h^\varepsilon(\tau) - p_\varepsilon H^\varepsilon_\Gamma[V^\varepsilon(\tau)]\|_{\mathrm{L}^1} \le \|H^\varepsilon_\Gamma[U^\varepsilon_j(\tau)] - H^\varepsilon_\Gamma[V^\varepsilon(\tau)]\|_{\mathrm{L}^1} \\
&\le \big(\|U^\varepsilon_j(\tau)\|_{\mathrm{L}^2} + \|V^\varepsilon(\tau)\|_{\mathrm{L}^2}\big)\|U^\varepsilon_j(\tau) - V^\varepsilon(\tau)\|_{\mathrm{L}^2} \le C r_\varepsilon^{1/2} \to 0.
\end{aligned}$$

Thus, the original family $(H^\varepsilon_\Gamma[U^\varepsilon_j])_\varepsilon$ and the two families $(h^\varepsilon)_\varepsilon$ and $(p_\varepsilon H^\varepsilon[V^\varepsilon])_\varepsilon$ generate the same Husimi measure. Hence, from now on it is sufficient to study the convergence of h^ε under the additional assumption that $U^\varepsilon_j = V^\varepsilon$ holds.

Step 2. To prove convergence to $\mu_j(\tau)$ we introduce an intermediate approximations $g^\varepsilon(\tau) \in \mathrm{L}^1(\mathbb{R}^d \times \mathcal{T}_{\Gamma_*})$ which is defined such that it solves the limit equation (5.20) with the ε-dependent initial datum $h^\varepsilon(0) \in \mathrm{L}^1(\mathbb{R}^d \times \mathcal{T}_{\Gamma_*})$. It is given by

$$g^\varepsilon(\tau; y, \theta) = h^\varepsilon(0; y + \tau \nabla_\theta \omega_j(\theta), \theta).$$

For this definition we do not need continuity of $\nabla_\theta \omega_j$. Now, the assumptions that the initial measures $\Phi h^\varepsilon(0)$ converge weak$*$ in $\mathcal{M}(\mathbb{R}^d \times \mathbb{K})$ to $\mu_j(0)$ immediately implies $\Phi g^\varepsilon(\tau) \overset{*}{\rightharpoonup} \mu_j(\tau)$ in $\mathcal{M}(\mathbb{R}^d \times \mathbb{K})$ by linearity and boundedness. Here, $\mu_j(\tau)$ is the solution defined via (5.20). This is the only step, where we need the convergence in the compactification and rely on the continuity of the extension $\widetilde{\nabla_\theta} \omega_j$.

The Fourier transform $\widehat{g^\varepsilon} = \mathcal{F}_{y \to \zeta} g^\varepsilon$ satisfies

$$\widehat{g}^\varepsilon(\tau; \zeta, \theta) = \mathrm{e}^{\mathrm{i}\zeta \cdot \nabla_\theta \omega_j(\theta)\tau} \widehat{h}^\varepsilon(0, \zeta, \theta).$$

Similarly, for $\widehat{h}^\varepsilon(\tau; \cdot, \theta) = \mathcal{F}_{y \to \zeta} h^\varepsilon(\tau; \cdot, \theta)$ we have the explicit formula

$$\widehat{h}^\varepsilon(\tau; \zeta, \theta) = \frac{\mathrm{e}^{-\varepsilon|\zeta|^2/4} p_\varepsilon(\theta)}{(2\varepsilon\pi)^d} \int_{\mathcal{T}_{\Gamma_*}} \widehat{U}_j^\varepsilon(0, \tfrac{\vartheta}{\varepsilon} + \tfrac{\zeta}{2}) \overline{\widehat{U}_j^\varepsilon}(0, \tfrac{\vartheta}{\varepsilon} - \tfrac{\zeta}{2})\, \mathrm{e}^{\mathrm{i}\Delta_\varepsilon(\zeta, \vartheta)\tau}\, G_\Gamma^\varepsilon(\vartheta - \theta)\, \mathrm{d}\vartheta,$$

where Δ_ε is defined in (5.16).

Step 3. Since $(g^\varepsilon)_\varepsilon$ and $(h^\varepsilon)_\varepsilon$ are bounded families in $\mathrm{L}^1(\mathbb{R}^d \times \mathcal{T}_{\Gamma_*})$, the desired convergence $\Phi g^\varepsilon(\tau) - \Phi h^\varepsilon(\tau) \overset{*}{\rightharpoonup} 0$ in $\mathcal{M}(\mathbb{R}^d \times \mathbb{K})$ follows, if we show

$$\forall\, \Psi \in \mathcal{C}:\ \int_{\mathbb{R}^d \times \mathcal{T}_{\Gamma_*}} \Psi(y, \theta)[g^\varepsilon(\tau; \mathrm{d}y, \mathrm{d}\theta) - h^\varepsilon(\tau; \mathrm{d}y, \mathrm{d}\theta)] \to 0 \quad \text{for } \varepsilon \to 0, \tag{5.21}$$

for a dense subset $\mathcal{C} \subset \mathrm{C}_0^0(\mathbb{R}^d, \mathrm{L}^\infty(\mathcal{T}_{\Gamma_*}))$. For this, note that using the embedding $\phi : \mathbb{T} = \mathcal{T}_{\Gamma_*} \backslash \mathbb{S} \to \mathbb{K}$ testfunctions $\Psi_\mathbb{K} \in \mathrm{C}_0^0(\mathbb{R}^d \times \mathbb{K})$ turn into $\Psi \in \mathrm{C}_0^0(\mathbb{R}^d, \mathrm{L}^\infty(\mathcal{T}_{\Gamma_*}))$ via $\Psi(y, \theta) = \Psi_\mathbb{K}(y, \phi(\theta))$. We choose $\mathcal{C}$ to be the set of those Ψ such that $\widehat{\Psi} = \mathcal{F}_{y \to \zeta} \Psi$ satisfies $\int_{\zeta \in \mathbb{R}^d_*} \|\widehat{\Psi}(\zeta, \cdot)\|_{\mathrm{L}^\infty(\mathcal{T}_{\Gamma_*})}\, \mathrm{d}\zeta < \infty$. E.g., all $\Psi \in \mathrm{W}^{d+1,1}(\mathbb{R}^d, \mathrm{L}^\infty(\mathcal{T}_{\Gamma_*}))$ satisfy this condition and, clearly, these functions are dense in $\mathrm{C}_0^0(\mathbb{R}^d \times \mathcal{T}_{\Gamma_*})$.

Using Fourier transform and the explicit representations of $\widehat{g}^\varepsilon$ and $\widehat{h}^\varepsilon$ the term to be estimated in (5.21) takes the form

$$\begin{aligned} F_\varepsilon = \frac{1}{(2\varepsilon\pi)^d} \int_{\theta \in \mathbb{T}_\varepsilon} \int_{(\zeta, \vartheta) \in \mathbb{M}_\varepsilon} & \widehat{\Psi}(\zeta, \theta) \mathrm{e}^{-\varepsilon|\zeta|^2/4} G_\Gamma^\varepsilon(\theta - \vartheta) \Big(\mathrm{e}^{\mathrm{i}\zeta \cdot \nabla_\theta \omega_j(\theta)\tau} - \mathrm{e}^{\mathrm{i}\Delta_\varepsilon(\zeta, \vartheta)\tau} \Big) \\ & \cdot \widehat{U}_j^\varepsilon(0, \tfrac{\vartheta}{\varepsilon} + \tfrac{\zeta}{2}) \overline{\widehat{U}_j^\varepsilon}(0, \tfrac{\vartheta}{\varepsilon} - \tfrac{\zeta}{2})\, \mathrm{d}\zeta\, \mathrm{d}\vartheta\, \mathrm{d}\theta, \end{aligned}$$

where $\mathbb{M}_\varepsilon = \{\, (\zeta, \vartheta) \in \mathbb{R}^d_* \times \mathcal{T}_{\Gamma_*} \mid \frac{\vartheta}{\varepsilon} - \frac{\zeta}{2} \in \mathbb{B}_\varepsilon \text{ and } \frac{\vartheta}{\varepsilon} + \frac{\zeta}{2} \in \mathbb{B}_\varepsilon \,\}$.

Using (5.4) we have for almost all $\zeta \in \mathbb{R}^d_*$ the estimate

$$\frac{1}{(2\varepsilon\pi)^d} \int_{\vartheta \in \mathcal{T}_{\Gamma_*}} |U_j^\varepsilon(0, \tfrac{\vartheta}{\varepsilon} + \tfrac{\zeta}{2}) \overline{\widehat{U}_j^\varepsilon}(0, \tfrac{\vartheta}{\varepsilon} - \tfrac{\zeta}{2})|\, \mathrm{d}\vartheta \le \|U_j^\varepsilon(0)\|^2_{\mathrm{L}^2(\mathbb{R}^d)}.$$

Hence, by Hölder's estimate in the $(\mathrm{L}^1, \mathrm{L}^\infty)$ version we find

$$|F_\varepsilon| \leq \int_{\zeta\in\mathbb{R}^d_*} \|\Upsilon_\varepsilon(\zeta,\cdot)\|_{\mathrm{L}^\infty(\mathcal{T}_{\Gamma_*})}\,\mathrm{d}\zeta\,\|U^\varepsilon_j(0)\|^2_{\mathrm{L}^2(\mathbb{R}^d)} \quad\text{with}$$
$$\Upsilon_\varepsilon(\zeta,\vartheta) = \int_{\theta\in\mathcal{T}_{\Gamma_*}} \widehat{\Psi}(\zeta,\theta)\mathrm{e}^{-\varepsilon|\zeta|^2/4}G^\varepsilon_\Gamma(\theta-\vartheta)\mathcal{X}_{\mathbb{T}_\varepsilon}(\theta)\mathcal{X}_{\mathbb{M}_\varepsilon}(\zeta,\vartheta)\big(\mathrm{e}^{\mathrm{i}\zeta\cdot\nabla_\theta\omega_j(\theta)\tau}-\mathrm{e}^{\mathrm{i}\Delta_\varepsilon(\zeta,\vartheta)\tau}\big)\,\mathrm{d}\theta,$$

where the characteristic functions $\mathcal{X}_{\mathbb{T}_\varepsilon}$ and $\mathcal{X}_{\mathbb{M}_\varepsilon}$ are due to the construction in Step 1. We now have

$$\|\Upsilon_\varepsilon(\zeta,\cdot)\|_{\mathrm{L}^\infty(\mathcal{T}_{\Gamma_*})} \leq \|\widehat{\Psi}(\zeta,\cdot)\|_{\mathrm{L}^\infty(\mathcal{T}_{\Gamma_*})}\|\|\upsilon_\varepsilon(\zeta,\cdot)\|_{\mathrm{L}^\infty(\mathcal{T}_{\Gamma_*})} \quad\text{with}$$
$$\upsilon_\varepsilon(\zeta,\vartheta) = \mathcal{X}_{\mathbb{M}_\varepsilon}(\zeta,\vartheta)\int_{\theta\in\mathcal{T}_{\Gamma_*}} G^\varepsilon_\Gamma(\theta-\vartheta)\mathcal{X}_{\mathbb{T}_\varepsilon}(\theta)\min\{2, |\zeta\cdot\nabla_\theta\omega_j(\theta)-\Delta_\varepsilon(\zeta,\vartheta)||\tau|\}\,\mathrm{d}\theta.$$

Because of $\|\upsilon_\varepsilon(\zeta)\|_\infty \leq C = 2\,\mathrm{vol}(\mathcal{T}_{\Gamma_*})$ we obtain the majorant $\|\Upsilon_\varepsilon(\zeta)\|_\infty \leq C\|\widehat{\Psi}(\zeta)\|_\infty$ which is independent of ε. Thus, it suffices to show the pointwise convergence $\|\upsilon_\varepsilon(\zeta)\|_\infty \to 0$ for $\varepsilon\to 0$ where $\zeta\in\mathbb{R}^d_*$ is fixed.

For fixed ζ and ε we only need to consider ϑ with $(\zeta,\vartheta)\in\mathbb{M}_\varepsilon$ because of the prefactor $\mathcal{X}_{\mathbb{M}_\varepsilon}$. For such ϑ we have $\mathrm{dist}(\vartheta+\varepsilon(\alpha-\frac12)\zeta,\mathbb{S}) \geq \varepsilon^{1/2}R_\varepsilon - \varepsilon|\zeta| \geq \frac12\varepsilon^{1/2}R_\varepsilon$ for sufficiently small ε. Hence, using the continuity (5.18) of $\nabla_\theta\omega_j$ outside of $\mathbb{S}$ we have for $\theta\notin\mathbb{S}_\varepsilon$

$$\begin{aligned}|\zeta\cdot\nabla_\theta\omega_j(\theta)-\Delta_\varepsilon(\zeta,\vartheta)| \;&\leq\; |\zeta|\int_{\alpha=0}^1 |\nabla_\theta\omega_j(\theta)-\nabla_\theta\omega_j(\vartheta+\varepsilon(\alpha-\tfrac12)\zeta)|\,\mathrm{d}\alpha\\ \leq\; |\zeta|\int_0^1 C_*\Big(\tfrac{2}{\varepsilon^{1/2}R_\varepsilon}&\mathrm{dist}(\theta,\vartheta+\varepsilon(\alpha-\tfrac12\zeta)\Big)^\sigma\,\mathrm{d}\alpha \;\leq\; \tfrac{2C_*|\zeta|}{\varepsilon^{\sigma/2}R^\sigma_\varepsilon}\big(\mathrm{dist}(\theta,\vartheta)^\sigma + (\varepsilon|\zeta|)^\sigma\big).\end{aligned}$$

This estimate can now be inserted into the definition of υ_ε. As for each $\sigma\geq 0$ there exists $C_\sigma >$ such that

$$\int_{\mathcal{T}_{\Gamma_*}} G^\varepsilon_\Gamma(\theta-\vartheta)\mathrm{dist}(\theta,\vartheta)^\sigma\,\mathrm{d}\theta \leq C_\sigma\varepsilon^{\sigma/2} \quad\text{for all } \varepsilon>0 \text{ and } \vartheta\in\mathcal{T}_{\Gamma_*}.$$

Hence, with $R_\varepsilon\to\infty$ we conclude the desired pointwise convergence from

$$\upsilon_\varepsilon(\zeta,\vartheta) \leq 2C_*|\zeta|\Big(\frac{C_\sigma}{R^\sigma_\varepsilon} + \big(\frac{\varepsilon^{1/2}|\zeta|}{R_\varepsilon}\big)^\sigma\Big) \;\longrightarrow 0.$$

Thus, $|F_\varepsilon| \leq C\int_{\mathbb{R}^d_*}\|\Upsilon_\varepsilon\|_\infty\,\mathrm{d}\zeta \to 0$ for $\varepsilon\to 0$ follows from Lebesgues dominated-convergence theorem.

Step 4. The above three steps conclude the proof. Step 2 gives $\Phi g^\varepsilon(t) \overset{*}{\rightharpoonup} \mu_j(\tau)$ and Step 3 gives $\Phi g^\varepsilon(\tau)-\Phi h^\varepsilon(\tau) \overset{*}{\rightharpoonup} 0$. According to Step 1 we have $\Phi h^\varepsilon(\tau)-\Phi H^\varepsilon_\Gamma[U^\varepsilon_j](\tau) \overset{*}{\rightharpoonup} 0$, which follows from $\|h^\varepsilon(\tau)-H^\varepsilon_\Gamma[U^\varepsilon_j](\tau)\|_{\mathrm{L}^1(\mathbb{R}^d\times\mathcal{T}_{\Gamma_*})} \to 0$. Thus, $H^\varepsilon_\mathbb{K}[U^\varepsilon_j](\tau) = \Phi H^\varepsilon_\Gamma[U^\varepsilon_j](\tau) \overset{*}{\rightharpoonup} \mu_j(\tau)$ in $\mathcal{M}(\mathbb{R}^d\times\mathbb{K})$ follows. ∎

It is to be expected that the above results can be sharpened by making specific assumptions on the singular set and by using suitable smooth coordinate changes near $\mathbb{S}$. Then, normal and tangential modes can be distinguished and suitable two-scale Wigner measures may be constructed, see [LT05, FL03]. Another way to compactify the measures near an isolated singularity like $\theta = 0$ in lattices is the H-measure introduced in [Tar90]. For this, one needs to introduce the extended vector V^ε as given in (5.14), whose Fourier transform $\widehat{V}^\varepsilon$ satisfies

$$\partial_\tau \widehat{V}^\varepsilon(\tau,\eta) = \tfrac{1}{\varepsilon}\mathbb{V}_\varepsilon(\varepsilon\eta)\widehat{V}^\varepsilon \quad \text{with } \mathbb{V}(\theta) = \begin{pmatrix} 0 & -M^{-1/2}\mathbb{L}(\theta)^* \\ \mathbb{L}(\theta)M^{-1/2} & 0 \end{pmatrix}.$$

As $\mathbb{V}(\cdot)$ is smooth in $\theta = 0$ this construction is more suitable to study energy concentrations there.

Remark 5.8 The above analysis was especially simple, since our problem is exactly periodic and hence does not allow for slow variations of the symbol matrix on the macroscopic spatial variable $y = \varepsilon\gamma$. According to [ST03] it is possible to generalize the theory to situations where such a macroscopic variation occurs. Assume that the mass matrix M as well as the interaction matrices A_β depend on y smoothly. Then we consider the infinite system

$$M(\varepsilon\gamma)\ddot{x}_\gamma = -\sum_{\beta\in\Gamma} A_\beta(\varepsilon\gamma)x_{\gamma+\beta} \quad \text{for } \gamma \in \Gamma.$$

Then we obtain the y–dependent symbol matrix $\mathbb{A}(y,\theta) = \sum_\beta \mathrm{e}^{\mathrm{i}\beta\cdot\theta}A_\beta(y)$ which again is assumed to be positive semi-definite and satisfying (3.6) in a uniform manner with constant kernel V. From $(\mathbb{A}(y,\theta) - \omega^2 M(y))\Phi = 0$ we then obtain dispersion relations $\omega = \omega_j(y,\theta)$ which also depend on y.

It is then possible to show that Wigner measures still exist and that they satisfy the generalized transport equation

$$\partial_\tau\mu_j(\tau,y,\theta) = \nabla_\theta\omega_j(y,\theta)\cdot\partial_y\mu_j(\tau,y,\theta) - \nabla_y\omega_j(y,\theta)\cdot\partial_\theta\mu_j(\tau,y,\theta), \tag{5.22}$$

where now also transport in the direction of θ occurs. In such situations it is not possible to resolve the singularities of the dispersion relation by the compactification given above. The compactification destroys the differentiable structure and thus can no longer be used. In fact, it is well-known that new phenomena occur in such energy crossings, since energy can be transfered from one branch to another, cf. [FL03, LT05, ST03].

6 Some examples

6.1 A counterexamples for the transport equation

In this section we want to discuss a few postive and negative results concerning the derivation of the energy-transport equations in Theorems 5.6 and 5.7. For this, we consider the nonsmooth dispersion relation $\omega(\theta) = 2|\sin(\theta/2)|$ on $\mathcal{T}_{\Gamma_*} = S^1 = \mathbb{R}_{/(2\pi\mathbb{Z})}$. The singular set is $\mathbb{S} = \{0\}$ and we may use the compactification $[0, 2\pi]$ with the smooth extension $\widetilde{\nabla}\omega = \cos(\kappa/2)$. However, to avoid confusion with the neighborhood of $\mathbb{S}$, we use $\mathbb{K} = ([-\pi, 0^-] \cup [0^+, \pi])_\sim$, where $\sim$ denotes the identification of $-\pi$ with π. The "continuous" extension of ω' is given via

$$\widetilde{\nabla}\omega(\kappa) = \begin{cases} \cos(\kappa/2) & \text{for } \kappa \in [0^+, \pi], \\ -\cos(\kappa/2) & \text{for } \kappa \in [-\pi, 0^-]. \end{cases}$$

Thus, the generalized energy-transport equation we have derived in Theorem 5.7 tasks the form

$$\partial_\tau \mu(\tau, \mathrm{d}y, \mathrm{d}\kappa) = \widetilde{\nabla}\omega(\kappa)\partial_y \mu(\tau, \mathrm{d}y, \mathrm{d}\kappa) \quad \text{on } \mathbb{R}\times\mathbb{K}. \tag{6.1}$$

We consider the solutions of $\partial_\tau \widehat{U}^\varepsilon = \frac{\mathrm{i}}{\varepsilon}\omega(\varepsilon\eta)\widehat{U}^\varepsilon$ with the initial conditions

$$\widehat{U}_0^\varepsilon(\eta) = \varepsilon^{(1-\beta)/2}\big(a_+\mathcal{X}_{B_\varepsilon}(\varepsilon\eta) + a_-\mathcal{X}_{-B_\varepsilon}(\varepsilon\eta)\big) \quad \text{where } B_\varepsilon = [\varepsilon^\beta, 2\varepsilon^\beta],$$

where we assume $0 < \beta$. Clearly, the Wigner and the Husimi transforms concentrate on $\mathbb{S} = \{0\}$ in the order ε^β. From solving the linear system we expect that the waves associated with $\pm B_\varepsilon$ travel with speed $c_\pm = \nabla_\theta \omega(0^\pm) = \pm 1$. Thus, the expected limit measure is

$$\mu(\tau) = |a_+|^2\delta_{0^+}(\mathrm{d}\kappa)\delta_{-c_+\tau}(\mathrm{d}y) + |a_-|^2\delta_{0^-}(\mathrm{d}\kappa)\delta_{-c_-\tau}(\mathrm{d}y). \tag{6.2}$$

We now discuss under which conditions we obtain this result for the Wigner and for the Husimi measure.

In this specific simple example we may study the distributional limit of the Wigner measures on $\mathbb{R}\times\mathbb{K}$ and retrieve the classical Wigner limit a subsequent identification of 0^+ and 0^-. For the computations we replace the space $\mathbb{K}$ simply by $\mathcal{T}_{\Gamma_*}$ and realize the compactification by chosing the set of testfunction ψ such that $\psi(\zeta, \cdot)$ is continuous on all of $\mathcal{T}_{\Gamma_*}\backslash\{0\}$, where we assume that the limits $\psi(\zeta, 0^+)$ and $\psi(\zeta, 0^-)$ exists. After applying a testfunction $\widehat{\psi} \in C_0^0(\mathbb{R}_*\times\mathbb{K})$ to $\widehat{w}^\varepsilon$ we have to study the limit of

$$\frac{1}{2\varepsilon\pi}\int\limits_{\mathbb{R}\times\mathbb{K}} \widehat{\psi}(\zeta, \kappa)\mathrm{e}^{\mathrm{i}\Delta_\varepsilon(\zeta,\kappa)\tau} \sum_{\sigma_1,\sigma_2\in\{+,-\}} \frac{a_{\sigma_1}\overline{a}_{\sigma_2}}{\varepsilon^{\beta-1}}\mathcal{X}_{\sigma_1 B_\varepsilon}(\kappa+\varepsilon\tfrac{\zeta}{2})\mathcal{X}_{\sigma_2 B_\varepsilon}(\kappa-\varepsilon\tfrac{\zeta}{2})\,\mathrm{d}\zeta\,\mathrm{d}\kappa. \tag{6.3}$$

Using the transformation $\kappa+\varepsilon\zeta/2 = \varepsilon^\beta\theta_1$ and $\kappa-\varepsilon\zeta/2 = \varepsilon^\beta\theta_2$, each of the four terms takes the form

$$\varepsilon^{\beta-1}\int\limits_{|\theta_1|,|\theta_2|\leq 2} \widehat{\psi}(\varepsilon^{\beta-1}(\theta_1-\theta_2), \varepsilon^\beta(\theta_1+\theta_2)/2)\mathrm{e}^{\mathrm{i}(\omega(\varepsilon^\beta\theta_1)-\omega(\varepsilon^\beta\theta_2))\tau/\varepsilon}\mathcal{X}_{\sigma_1[1,2]}(\theta_1)\mathcal{X}_{\sigma_2[1,2]}(\theta_2)\,\mathrm{d}\theta$$

For $\beta > 1$ we now see that the integrals tend to 0, which means $w^\varepsilon(\tau) = W^\varepsilon[U^\varepsilon(\tau)] \to 0$ in the sense of distributions. This is due to the effect that the corresponing initial conditions U^ε are not tight, they are spreading out too fast in physical space.

For $\beta = 1$ we can pass to the limit easily, when taking care of the possibly different values $\widehat{\psi}(\zeta, 0^+)$ and $\widehat{\psi}(\zeta, 0^-)$:

$$\begin{aligned} &\tfrac{1}{2\pi}\int_{\theta_1+\theta_2>0} \widehat{\psi}(\theta_1-\theta_2, 0^+)\mathrm{e}^{\mathrm{i}(|\theta_1|-|\theta_2|)\tau}\mathcal{X}_{\sigma_1[1,2]}(\theta_1)\mathcal{X}_{\sigma_2[1,2]}(\theta_2)\,\mathrm{d}\theta \\ &+\tfrac{1}{2\pi}\int_{\theta_1+\theta_2<0} \widehat{\psi}(\theta_1-\theta_2, 0^-)\mathrm{e}^{\mathrm{i}(|\theta_1|-|\theta_2|)\tau}\mathcal{X}_{\sigma_1[1,2]}(\theta_1)\mathcal{X}_{\sigma_2[1,2]}(\theta_2)\,\mathrm{d}\theta. \end{aligned}$$

For $\sigma_1 = \sigma_2$ we arrive at

$$\tfrac{1}{2\pi} \int \widehat{\psi}(\theta_1{-}\theta_2, 0^{\sigma_1}) \mathrm{e}^{\mathrm{i}\sigma_1(\theta_1-\theta_2)\tau} \mathcal{X}_{\sigma_1[1,2]}(\theta_1)\mathcal{X}_{\sigma_1[1,2]}(\theta_2)\,\mathrm{d}\theta = \int_{-1}^{1} \widehat{\psi}(s, 0^{\sigma_1})\mathrm{e}^{\mathrm{i}\sigma_1 s\tau}\tfrac{1}{\pi}(1{-}|s|)\,\mathrm{d}s,$$

which tells us that the energy located at 0^{σ_1}, which is proportional to $|a_{\sigma_1}|^2$, is transported with the group velocity $c = \sigma_1 1$. Inverse Fourier transform leads to the first two terms in the following expression for the limiting Wigner measure:

$$\begin{aligned} \mu^{\mathrm{W}}(\tau) \;=\; \lim W^\varepsilon[U^\varepsilon(\tau)] \;&=\; |a_+|^2 S(y{-}\tau)\delta_{0^+}(\mathrm{d}\kappa) + |a_-|^2 S(y{+}\tau)\delta_{0^-}(\mathrm{d}\kappa) \\ &\qquad + \mathrm{Re}\,\big(a_+\overline{a}_-\big[(R_+(\tau,y)\delta_{0^+}{+}(R_-(\tau,y)\delta_{0^-}\big]\big), \end{aligned}$$

where $S(x) = \frac{1}{x^2}(\sin(x/2))^2$. The third term arises from the two cases with $\sigma_1 \neq \sigma_2$. Now, time dependence occurs through $\sigma_1(\theta_1{+}\theta_2)\tau$, while $\widehat{\psi}(\cdot, 0^\pm)$ still depends on $\theta_1{-}\theta_2$. Thus, all energy is concentrated in the two wave number 0^+ and 0^-, but all wave speeds $c \in [-1, 1]$ are realized. Hence, the measure $\mu^{\mathrm{H}}(\tau)$ doesn't satisfy the transport equation (6.1).

The case $\beta \in (0, 1)$ is better behaved. To study the limit in (6.3) we keep ζ and substitute $\kappa = \varepsilon^\beta \vartheta$. Because of $\beta \in (0, 1)$ we have $\Delta_\varepsilon(\zeta, \varepsilon^\beta\vartheta) \to \mathrm{sign}(\vartheta)\zeta$ and find the limit

$$\int_{\mathbb{R}} \big(\widehat{\psi}(\zeta, 0^+)\mathrm{e}^{\mathrm{i}\zeta\tau}|a_+|^2 + \widehat{\psi}(\zeta, 0^-)\mathrm{e}^{-\mathrm{i}\zeta\tau}|a_-|^2\big)\,\mathrm{d}\zeta,$$

which corresponds to the desired resulting Wigner measure $\mu^{\mathrm{W}}(\tau) = \mu(\tau)$ as given in (6.2).

We also want to study the same convergence question for the Husimi transform for the problem above. The action of $H^\varepsilon[U^\varepsilon(\tau)]$ on a testfunction ψ is again studied in terms of the Fourier transform, which leads to four terms of the form

$$\tfrac{1}{2\varepsilon^\beta\pi} \int_{\mathbb{R}\times\mathcal{T}_{\Gamma_*}\times\mathcal{T}_{\Gamma_*}} \widehat{\psi}(\zeta, \vartheta) G^\varepsilon_\Gamma(\vartheta{-}\kappa)\mathrm{e}^{-\varepsilon|\zeta|^2/4}\mathrm{e}^{\mathrm{i}\Delta_\varepsilon(\zeta,\kappa)\tau}\mathcal{X}_{\sigma_1 B_\varepsilon}(\kappa{+}\varepsilon\tfrac{\zeta}{2})\mathcal{X}_{\sigma_2 B_\varepsilon}(\kappa{-}\varepsilon\tfrac{\zeta}{2})\,\mathrm{d}\vartheta\,\mathrm{d}\zeta\,\mathrm{d}\kappa.$$

Introducing the scalings $\kappa = \varepsilon^\beta\theta$ and $\vartheta = \varepsilon^{1/2}\eta$ and proceeding as above, we derive, for $\beta \in (0, 1)$, the limit measure

$$\mu^{\mathrm{H}}(\tau) = \rho_+\delta_{0^+}(\mathrm{d}\kappa)\delta_{-\tau}(\,\mathrm{d}y) + \rho_-\delta_{0^-}(\mathrm{d}\kappa)\delta_{+\tau}(\,\mathrm{d}y) \quad \text{with } \rho_\pm = (1{-}\alpha_\beta)|a_\pm|^2 + \alpha_\beta|a_\mp|^2,$$

where $\alpha_\beta = 0$ for $\beta \in (0, 1/2)$, $\alpha_{1/2} = \int_{\eta\in\mathbb{R}}\int_{\theta=-2}^{-1} G^1(\eta{-}\theta)\,\mathrm{d}\theta\,\mathrm{d}\eta \approx 0.02464$, and $\alpha_\beta = 1/2$ for $\beta \in (1/2, 1)$.

Thus, we make the following observations. Theorem 5.7 is applicable to the case $\beta \in (0, 1/2)$ where we obtain the correct limiting measure, $\mu^{\mathrm{H}}(\tau) = \mu(\tau)$ as given in (6.2). For the critical case $\beta = 1/2$ we still obtain a solution of the transport equation (6.1), but it is not the desired one, since the smearing out of the energy via the Gaussian kernel led to a wrong partition of the energy. The same happens for $\beta \in (1/2, 1)$, where the faster concentration rate leads even to equals contributions on both sides. A similar effect can be established in the case $\beta = 1$, where $\mu^{\mathrm{H}}(\tau)$ is again a symmetrized version of $\mu^{\mathrm{W}}(\tau)$.

It is also interesting to observe that due to the compactification, the Wigner measure μ^{W} and the Husimi measure μ^{H} do no longer need to be the same, as is seen for $\beta \geq 1/2$.

6.2 The harmonic chain

The simplest example is the harmonic chain with nearest-neighbor interaction. After normalizing all constants it takes the form

$$\ddot{x}_j = x_{j+1} - 2x_j + x_{j-1} \quad \text{for } j \in \mathbb{Z}. \tag{6.4}$$

The lattice is $\Gamma = \mathbb{Z}$ and the dual lattice is $\Gamma_* = 2\pi\mathbb{Z}$ with the Brillouin zone $B_{\Gamma_*} = (-\pi, \pi)$, cf. [Bri46].

The dispersion relation reads $\omega^2 = 2(1-\cos\theta) = 4(\sin(\theta/2))^2$. This gives $\omega_{1,2}(\theta) = \pm\omega(\theta)$ with $\omega(\theta) = 2|\sin(\theta/2)|$ and non-smoothness occurs only at $\theta = 0$. The compactification $\mathbb{K}$ of $\mathbb{S}^1 \setminus \{0\}$ is simply a closed interval $[0, 2\pi]$ where $\theta > \pi$ should be identified with $\theta - 2\pi \in (-\pi, 0]$.

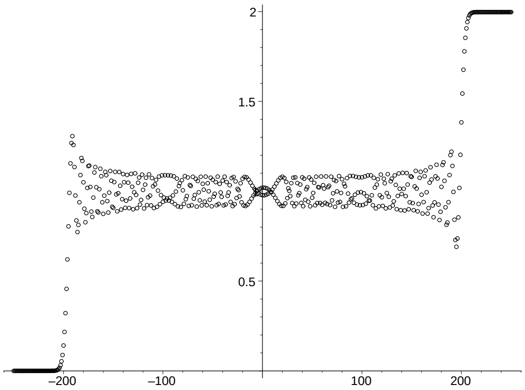
Because of $\omega(k)^2 = k^2 + O(k^4)_{k\to 0}$, the macroscopic wave equation takes the form $Z_{\tau\tau} = Z_{yy}$. The energy transport is governed by the two equations

$$\partial_\tau \mu_1 = \omega'(k)\partial_y \mu_1, \quad \partial_\tau \mu_2 = -\omega'(k)\partial_y \mu_2 \quad \text{for } (\tau, y, k) \in \mathbb{R}^2 \times \mathbb{K}. \tag{6.5}$$

Since we are mainly interested in the total energy $e(\tau, y) = \int_{\mathbb{K}} \mu_1 + \mu_2 \, \mathrm{d}\theta$, it suffices to consider $\widehat{\mu} = \operatorname{tr}\mu = \mu_1 + \mu_2 \in \mathcal{M}(\mathbb{R}^2 \times \mathbb{K})$ which now satisfies

$$\partial_\tau^2 \widehat{\mu} = (\omega'(\theta))^2 \partial_y^2 \widehat{\mu}.$$

This is a second order equation in τ and y, containing θ as a parameter.



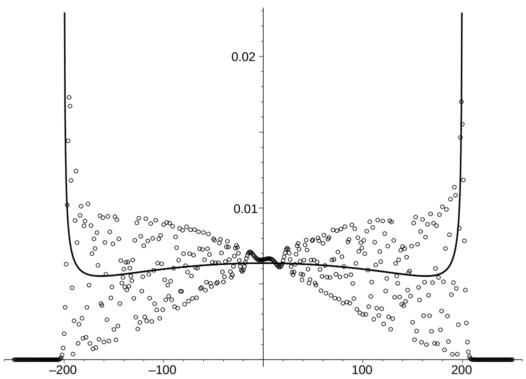


Figure 6.1: Displacement (left) and energy distribution (right) for the harmonic chain. The full line (right) gives $e(\tau, y)$ for $\tau = 200$.

We illustrate the results with some simulations. In Figure 6.1 we display the solution of (6.4) with initial data

$$x_j(0) = 2 \text{ for } j > 0, \quad x_j(0) = 0 \text{ for } j \le 0, \quad \text{and } \dot{x}_j(0) = 0,$$

at time $t = 200$. We clearly see that the propagation speeds are ± 1, since the fronts have reached the atoms at $j = \pm 200$. Moreover, in the sense of weak convergence the function

Figure 6.2: The dipole solution at $t = 200$: displacement (left) and energy distribution (right).

is close to the step function

$$Z(\tau, y) = \begin{cases} 2 & \text{for } y > \tau, \\ 1 & \text{for } |y| < \tau, \\ 0 & \text{for } y < -\tau, \end{cases}$$

which is the unique solution of $Z_{\tau\tau} = Z_{yy}$ with initial data $Z(0, y) = 1 + \operatorname{sign}(y)$ and $\partial_\tau Z(0, y) = 0$. The convergence is rather slow and near the fronts there is a overshooting of about 40 %, which can be explained by the help of the Airy function.

Here, we want to explain the energy distribution given in the right of Figure 6.1. The circles indicate the energies in the atoms and the full line gives the function $e(\tau, \cdot)$ calculated via Wigner measures. We obtain $e(\tau, y) = \frac{1+(y/\tau)^2}{\pi\tau\sqrt{1-(y/\tau)^2}}$. In Figure 1.1 we show the Green's function obtained from the initial data $x_j(0) = \delta_j$ and $\dot{x}_j(0) = 0$. The Wigner measure for the energy distribution satisfies a semicircle law, namely $e(\tau, y) = \frac{1}{\tau\pi}\sqrt{1-(y/\tau)^2}$. In Figure 6.2 we displayed the so-called dipole solution obtained as a difference of two Green's functions, i.e., $x_j(0) = \delta_j - \delta_{j-1}$ and $\dot{x}_j(0) = 0$. For the method to calculate the functions $e(\tau, cdot)$ explicitly, we refer to Section 6.4.

It is interesting to note that the convergence against the Wigner measure is again a real weak limit. In fact, it can be shown that the family of energy distribution $(E^\varepsilon(\tau))_\varepsilon$ generates a Young measure $Y(\tau) \in \mathrm{YM}(\mathbb{R}, [0, \infty))$ which is, for each τ and y, an "arcsin" distribution with the mean value $e(\tau, y)$ (from the Wigner measure) and a width $C_*(y/\tau)^2 e(\tau, y)$. The constant C_* however, depends of the kind of definition of local energy (see e_γ, E^ε and $\widetilde{E}^\varepsilon$ in Section 5.4). If we average over several particles, then C_* decreases like the inverse of the particle size.

We also refer to [Fri03] for a very detailed study of the solution of (6.4) using a careful analysis of the explicit form of the solution in terms of oscillatory integrals. There, the region near $y = 0$ is studied where the presence of the wave number $\theta = \pm\pi$ leads to so-called binary oscillations which form a rather rigid, synchronized structure.

6.3 The bi-atomic chain

We consider two types of atoms having weights m and $\widetilde{m}$ respectively. Their equilibrium positions are $j \in \mathbb{Z}$ and they are placed alternatingly such that $m_{2j} = m$ and $m_{2j+1} = \widetilde{m}$. Between adjacent masses there are linear springs with constant k (nearest neighbor interaction). Additionally, we consider forces between next-nearest neighbors with Hooke's constants κ and $\widetilde{\kappa}$ between mass point with mass m and $\widetilde{m}$, respectively. Thus, the equations for the displacements y_j are

$$m_j \ddot{y}_j = k(y_{j-1}-2y_j+y_{j+1}) + \kappa_j(y_{j-2}-2y_j+y_{j+2})$$

with $\kappa_{2\gamma} = \kappa$ and $\kappa_{2\gamma+1} = \widetilde{\kappa}$. We define $x_\gamma = (y_{2\gamma}, y_{2\gamma+1})$ for $\gamma \in \mathbb{Z}$ and obtain

$$M\ddot{x}_\gamma + A_{-1}x_{\gamma-1} + A_0 x_\gamma + A_1 x_{\gamma+1} = 0 \quad \text{for } \gamma \in \mathbb{Z} \quad \text{with}$$

$$M = \begin{pmatrix} m & 0 \\ 0 & \widetilde{m} \end{pmatrix}, \; A_{-1} = \begin{pmatrix} -\kappa & -k \\ 0 & -\widetilde{\kappa} \end{pmatrix}, \; A_0 = \begin{pmatrix} 2k+2\kappa & -k \\ -k & 2k+2\widetilde{\kappa} \end{pmatrix}, \; A_1 = \begin{pmatrix} -\kappa_m & 0 \\ -k & -\widetilde{\kappa} \end{pmatrix}.$$

The symbol matrix reads

$$\mathbb{A}(\theta) = \begin{pmatrix} 2k + 2\kappa(1-\cos\theta) & -k(1+\mathrm{e}^{-\mathrm{i}\theta}) \\ -k(1+\mathrm{e}^{\mathrm{i}\theta}) & 2k + 2\widetilde{\kappa}(1-\cos\theta) \end{pmatrix}.$$

Hence, assumption (3.4) is satisfied with $1 = d = \dim V$ if $k, k{+}2\kappa, k{+}2\widetilde{\kappa} > 0$, where $V = \ker \mathbb{A}(0) = \operatorname{span}\binom{1}{1}$. The dispersion relation reads

$$[m\omega^2 - 2(k+\kappa(1-\cos\theta))][\widetilde{m}\omega^2 - 2(k+\widetilde{\kappa}(1-\cos\theta))] = 2k^2(1+\cos\theta).$$

For $\theta \approx 0$ we find the frequencies $\omega_1^2 = \frac{k+\kappa+\widetilde{\kappa}}{m+\widetilde{m}}\theta^2 + O(\theta^4)$ and $\omega_2^2 = \frac{2k(m+\widetilde{m})}{m\widetilde{m}} + O(\theta^2)$. This provieds the macroscopic wave speed $c^{\mathrm{macro}} = [(k+\kappa+\widetilde{\kappa})/(m+\widetilde{m})]^{1/2}$ and the macroscopic wave equation

$$\tfrac{m+\widetilde{m}}{2}\,\partial_\tau^2 Z = \tfrac{k+\kappa+\widetilde{\kappa}}{2}\,\partial_y^2 Z.$$

For $\theta = \pm\pi$ we have $1+\cos\theta = 0$ and the frequencies ω_j are given via $\omega^2 = (2k+4\kappa)/m$ and $\omega = (2k+4\widetilde{\kappa})/\widetilde{m}$. Hence, eigenvalue crossings at $\theta = \pm\pi$ are easily constructed, see Figure 6.3 (right), where the parameters $m = 6$, $\widetilde{m} = 10$, $k = \kappa = 1$, and $\widetilde{\kappa} = 2$ have been used.

Figure 6.3: Two typical dispersion relations for the bi-atomic chain.

6.4 Energy distribution in scalar models

For simplicity we restrict in this section to scalar models, but in arbitrary space dimensions. Assume that we have

$$\ddot{x}_\gamma = -\sum_{|\beta|\leq R} a_\beta x_{\gamma+\beta} \qquad \text{for } \gamma \in \Gamma, \tag{6.6}$$

with a_β such that $\omega(\theta)^2 = \sum_\beta a_\beta \mathrm{e}^{\mathrm{i}\beta\cdot\theta}$ is real and nonnegative. The Green's function associated with (6.6) is the unique solution associated with the initial conditions $x_\gamma(0) = \delta_\gamma$ and $\dot{x}_\gamma(0) = 0$. We want to study the energy distribution for this system, the total energy being just a_0.

In Fourier space the system has the initial conditions $\widetilde{X}(0) \equiv c_{\Gamma_*}$ and $\partial_\tau \widetilde{X}(0) = 0$ and transforming it into the normal form (5.12) we find

$$\partial_\tau \widehat{U}^\varepsilon(\tau,\eta) = \tfrac{\mathrm{i}}{\varepsilon}\begin{pmatrix} \omega(\varepsilon\eta) & 0 \\ 0 & -\omega(\varepsilon\eta)\end{pmatrix}\widehat{U}^\varepsilon(\tau,\eta) \quad \text{with } \widehat{U}^\varepsilon(0,\eta) = \tfrac{\varepsilon^{d/2}}{2\mathrm{vol}(\mathcal{T}_{\Gamma_*})^{1/2}}\begin{pmatrix}\omega(\varepsilon\eta) \\ \omega(\varepsilon\eta)\end{pmatrix}. \tag{6.7}$$

These initial conditions immediately define the initial Wigner-Husimi measures $\mu_j(0) = \frac{1}{4\mathrm{vol}(\mathcal{T}_{\Gamma_*})}\omega(\theta)^2 \mathrm{d}\theta \delta_0(\mathrm{d}y)$ as $\omega(\theta+\frac{\varepsilon}{2}\zeta)\omega(\theta-\frac{\varepsilon}{2}\zeta) \to \omega(\theta)^2$. There is no concentration on any singular set, we rather have a smooth density on $\mathcal{T}_{\Gamma_*}$. According to Theorem 5.6, the evolution of the energy is given via $\mu(\tau)$ defined via

$$\int_{\mathbb{R}^d\times\mathcal{T}_{\Gamma_*}} \Psi(y,\theta)\sum_1^2 \mu_j(\tau;\mathrm{d}y,\mathrm{d}\theta) = \frac{1}{2\mathrm{vol}(\mathcal{T}_{\Gamma_*})}\int_{\mathcal{T}_{\Gamma_*}} \Psi(-\tau\nabla_\theta\omega(\theta),\theta)\omega^2(\theta)\,\mathrm{d}\theta,$$

where we used $\omega(-\theta) = \omega(\theta)$. Under the assumption that the mapping $\theta \mapsto c = \nabla_\theta \omega(\theta)$ from $\mathcal{T}_{\Gamma_*} \to C \subset \mathbb{R}^d$ has the inverse $\theta = \Theta(c)$, we obtain by the transformation rule, that $\mu(\tau)$ can be represented by the density

$$m(\tau,y) = \begin{cases} \frac{1}{\tau^d} g(y/\tau) & \text{for } y \in \tau Y, \\ 0 & \text{else,}\end{cases} \qquad \text{where } g(c) = \frac{\omega(\Theta(c))^2}{2\mathrm{vol}(\mathcal{T}_{\Gamma_*})|\det \mathrm{D}^2\omega(\Theta(c))|}.$$

In the case of multivaluedness of $c = \nabla_\theta \omega(\theta)$ this is easily generalized by adding up the contribution of each preimage of c. However, the zeros of $\det \mathrm{D}^2\omega(\Theta(c))$ will generate singularities

One special case was already discussed in Section (6.2). There the mapping $\nabla_\theta\omega(\theta) = \mathrm{sign}(\theta)\cos(\theta/2)$ is indeed invertible and we obtain

$$g(c) = \tfrac{\omega(\theta)^2}{4\pi|\omega''(\theta)|} = \tfrac{2(1-\cos\theta)}{2\pi|\sin\theta/2|} = \tfrac{2}{\pi}|\sin(\theta/2)| = \tfrac{2}{\pi}\sqrt{1-c^2}$$

We now illustrate that in the general case the invertiblity breaks down, which leads to densities $g \in \mathrm{L}^1(Y)$ which have singularities arising from the caustics associated with the multivaluedness of $\nabla_\theta\omega(\theta)$.

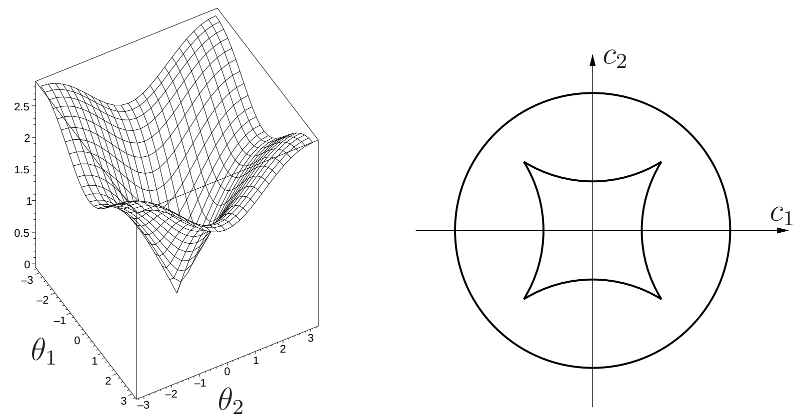


Figure 6.4: Dispersion relation (left) and the wave-vector domain $Y = \mathrm{sppt}(g)$ (right) with the singular set of g.

As an example consider the square lattice with nearest-neighbor interaction:

$$\ddot{x}_\gamma = -4x_\gamma + x_{\gamma+\beta_1} + x_{\gamma-\beta_1} + x_{\gamma+\beta_2} + x_{\gamma-\beta_2},$$

where $\beta_1 = (1,0)$ and $\beta_2 = (0,1)$. This equation arises as a numerical approximation of the linear wave equation $\partial_\tau^2 u = \Delta_y u$, which is the macroscopic limit in the sense of Section 4. Note that the macroscopic equation is isotropic while the microscopic system is anisotropic. This will be reflected in the properties of the density g.

The dispersion relation is given as

$$\omega(\theta)^2 = 4 - 2\cos\theta_1 - 2\cos\theta_2 \quad \text{for } \theta \in \mathcal{T}_{\Gamma_*} = \mathbb{R}^2/_{(2\pi\mathbb{Z})^2}.$$

We find $C = \{\, c \in \mathbb{R}^2 \mid |c| < 1 \,\}$ where the boundary corresponds to the macroscopic wave speeds associated with the limit $\theta \to 0$. The mapping $\nabla_\theta \omega$ is not 1-1, as $\mathrm{D}^2\omega(\theta)$ vanishes on a closed smooth curve $\mathcal{C}$. Thus, almost all points have either 1 or 3 preimages, see Figure 6.4. The image of $\mathcal{C}$ under the mapping $\nabla_\theta \omega$ forms the cusp-like figure inside C. Along this curve the density has a singularity which is also seen in the numerical approximation displayed in Figure 6.5. The cusps occur exactly in the points with $|c_1| = |c_2| = 1/2$. In these points the strongest singularities in g occurs and, thus, lead to dominant patterns with microscopic wave vectors with $|\theta_1| = |\theta_2| = \pi/2$.

With the same idea we are able to find the asymptotic behavior of the energy for any fixed initial distribution, like the dipole solution considered in Section 6.2. Any solution $x(t)$ of (6.6) with initial fixed initial condition $(x(0), \dot{x}(0)) = (x^{(0)}, x^{(1)}) \in \ell^2 \times \ell^2$ can be considered as a sequence of solutions, since letting $\tau = \varepsilon t$ and $y = \varepsilon\gamma$ just leads to a rescaling of space and time. We may fix $\tau = \tau_*$ and then set $\varepsilon = \tau_*/t$ which leads to $y = \tau_*\gamma/t$. For $t \to \infty$ we obtain the desired macroscopic limit. In (6.7) we obtain the initial data

$$\widehat{U}(0, \theta/\varepsilon) = \varepsilon^{d/2}\binom{f_1(\theta)}{f_2(\theta)} \text{ with } \binom{f_1(\theta)}{f_2(\theta)} = \frac{1}{2\mathrm{vol}(\mathcal{T}_{\Gamma_*})}\binom{\omega(\theta)\widetilde{X}^{(0)}(\theta) - \mathrm{i}\widetilde{X}^{(1)}(\theta)}{\omega(\theta)\widetilde{X}^{(0)}(\theta) + \mathrm{i}\widetilde{X}^{(1)}(\theta)},$$

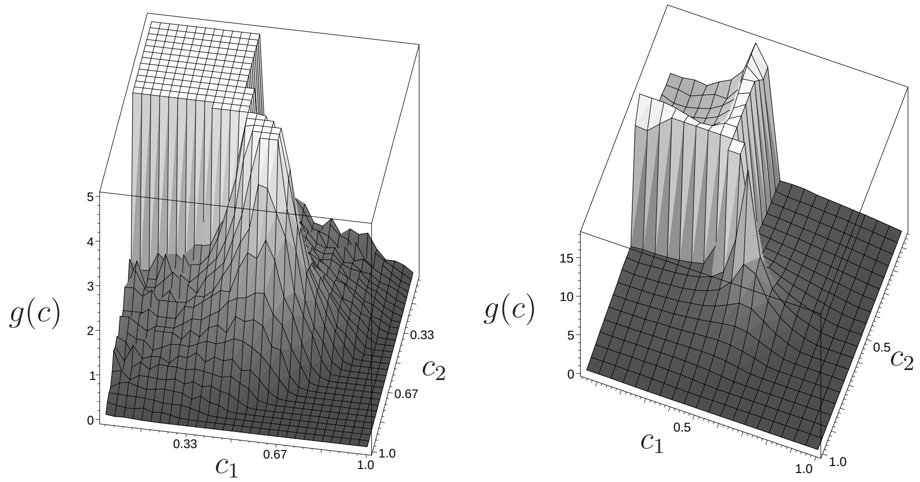


Figure 6.5: The energy density g (one quarter): the support can be seen on the left and the singular behavior is displaced to the right.

where $\widetilde{X}^{(j)}(\theta) = \sum_\gamma x_\gamma^{(j)} \mathrm{e}^{-\mathrm{i}\gamma\cdot\theta}$ for $j = 1, 2$. Thus, the initial Wigner measures are given by $\mu_j(0) = f_j(\theta)^2 \mathrm{d}\theta \delta_0(\mathrm{d}y)$ and the macroscopic density distribution has again the self-similar structure $e(\tau, y) = \frac{1}{\tau^d} g^*(y/\tau)$ where g^* is given implicitly by

$$\int_{\mathbb{R}^d} \psi(c) g^*(c)\,\mathrm{d}c = \int_{\mathcal{T}_{\Gamma_*}} \big(\psi(-\nabla_\theta \omega(\theta)) f_1(\theta)^2 + \psi(\nabla_\theta \omega(\theta)) f_2(\theta)^2\big)\,\mathrm{d}\theta$$

for all testfunctions $\psi \in \mathrm{C}^0_0(\mathbb{R}^d)$.

6.5 Square lattice

We consider equal atoms placed at $\mathbb{Z}^2$. The masses are 1 and the nearest-neighbor forces have constant 1. Additionally, we have next-nearest neighbor interaction (along the diagonals of squares) with constant k.

With $e_1 = \binom{1}{0}$, $e_2 = \binom{0}{1}$, $e_+ = \binom{1}{1}$, $e_- = \binom{1}{-1}$ we find for the displacements $x_\gamma \in \mathbb{R}^2$, $\gamma \in \Gamma = \mathbb{Z}^2$ the coupled system

$$\begin{aligned} \ddot{x}_\gamma &= \langle e_1, x_{\gamma-e_1} - 2x_\gamma + x_{\gamma+e_1}\rangle e_1 + \langle e_2, x_{\gamma-e_2} - 2x_\gamma + x_{\gamma+e_2}\rangle e_2 \\ &\quad + \tfrac{k}{2}\langle e_+, x_{\gamma-e_+} - 2x_\gamma + x_{\gamma+e_+}\rangle e_+ + \tfrac{k}{2}\langle e_-, x_{\gamma-e_-} - 2x_\gamma + x_{\gamma+e_-}\rangle e_- \\ &= -\textstyle\sum_{|\alpha|\le\sqrt{2}} A_\alpha x_{\gamma+\alpha} \end{aligned}$$

where the interaction matrices are given by

$$A_0 = \begin{pmatrix} 2+2k & 0 \\ 0 & 2+2k \end{pmatrix}, \quad A_{\pm e_1} = \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}, \quad A_{\pm e_2} = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix},$$

$$A_{\pm e_+} = -\frac{k}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad A_{\pm e_-} = -\frac{k}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

The dispersion matrix $\mathbb{A}(\theta)$ takes the form

$$\mathbb{A}(\theta) = 2\begin{pmatrix} 1-\cos\theta_1 + k(1-\cos\theta_1\cos\theta_2) & k\sin\theta_1\sin\theta_2 \\ k\sin\theta_1\sin\theta_2 & 1-\cos\theta_2 + k(1-\cos\theta_1\cos\theta_2). \end{pmatrix}$$

This leads to the quadratic part $\mathbb{Q}^{(2)}(\eta,\eta) = \begin{pmatrix} \eta_1^2 + k(\eta_1^2+\eta_2^2) & 2k\eta_1\eta_2 \\ 2k\eta_1\eta_2 & \eta_2^2 + k(\eta_1^2+\eta_2^2) \end{pmatrix}$ and the

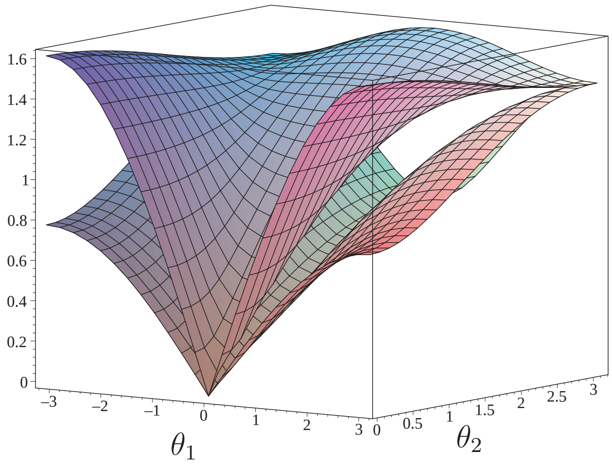


Figure 6.6: The two dispersion relations for the two-dimensional lattice (one half of $\mathcal{T}_{\Gamma_*}$ is displayed only).

macroscopic wave equation

$$Z'' = \mathrm{div}\left(k(\nabla\cdot Z)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + k(\mathrm{D}Z+\mathrm{D}Z^{\mathsf{T}}) + (1-2k)\begin{pmatrix} \partial_{y_1}Z & 0 \\ 0 & \partial_{y_2}Z \end{pmatrix}\right).$$

For $k = 1/2$ this gives exactly linearized, isotropic elasticity with Lamé constants $\mu = 1/2$ and $\lambda = 1/2$. For $k \neq 1/2$ the wave equation is anisotropic.

6.6 Comparison with Whitham's modulation equation

In Whitham's theory of modulated waves, one assumes that the solution behaves locally as a periodic wave which is modulated on a macroscopic scale. For each macroscopic point the wave pattern is taken from a family of waves which is described by a finite-dimensional set of parameters. The question is then, how these parameters evolve on the macroscopic scale.

The strength of Whitham's theory is that it is applicable also in nonlinear problems, see [HLM94, FV99, DHM04]. Here we want to compare its impact in the linear setting with the corresponding result obtained from the energy-transport equation for the Wigner measure.

The modulated wave train is constructed from the explicit periodic solutions

$$x_\gamma(t) = F\gamma + vt + a\,\mathrm{e}^{\mathrm{i}(\theta\cdot\gamma+\omega t)}\Phi, \tag{6.8}$$

where $F \in \mathrm{Lin}(\mathbb{R}^d, V)$ denotes the macroscopic strain, $v \in V$ is the macroscopic speed, $a > 0$ is the amplitude, $\theta \in B_{\Gamma_*}$ is the wave vector and $\omega \in \mathbb{R}$ is the frequency.

A modulated wave train is now given in the form

$$x_\gamma(t) = \frac{1}{\varepsilon}\mathcal{U}(\tau, y) + a(\tau, y)\,\mathrm{e}^{\mathrm{i}\Psi(\tau,y)/\varepsilon}\Phi(\tau, y),$$

where $\tau = \varepsilon t$, $y = \varepsilon\gamma$ and the deformation $\mathcal{U}$ and the microscopic phase Ψ are given such that $\mathcal{U}(0, 0) = 0$, $\Phi(0, 0) = 0$, and

$$\partial_\tau\mathcal{U}(\tau, y) = v(\tau, y),\ \partial_y\mathcal{U}(\tau, y) = F(\tau, y),\ \partial_\tau\Phi(\tau, y) = \omega(\tau, y),\ \partial_y\Phi(\tau, y) = \theta(\tau, y).$$

Moreover, at each macroscopic point (τ, y) it is assumed that θ, ω and Φ are related by the y–dependent microscopic eigenvalue problem $\mathbb{A}(y, \theta)\Phi - \omega^2 M\Phi = 0 \in \mathbb{C}^m$. From now on, we fix a smooth branch $\omega = \Omega(y, \theta)$ of the dispersion relation and assume that $\Phi = \widetilde{\Phi}(y, \theta)$ with the normalization $\langle M(y)\Phi, \Phi\rangle = 1$. Note, however, that the formal derivation of Whitham's equation will need ω to be an independent parameter. We will always write Ω if we relate to a particular branch.

Since the analysis in this section is purely formal, we treat a harmonic lattice system whose material parameter may be modulated on the macroscopic scale as well:

$$M(\varepsilon\gamma)\ddot{x}_\gamma = -\sum_{\beta\in\mathbb{Z}^d} A_\beta(\varepsilon\gamma)x_{\gamma+\beta}; \qquad \mathbb{A}(y, \theta) \stackrel{\text{def}}{=} \sum_\beta \mathrm{e}^{\mathrm{i}\theta\cdot\beta}A_\beta(y). \tag{6.9}$$

The aim is to find an evolution equation for the function F, v, θ, ω and a.

First we provide the easiest method for deriving Whitham's modulation equation formally and refer to [DHM04] for further information. Since the lattice dynamics is given via a Hamiltonian, the equation can be obtained by making the Lagrangian $\mathcal{L}_\varepsilon$ with

$$\mathcal{L}_\varepsilon(\gamma, x, \dot{x}) = \tfrac{1}{2}\langle M(\varepsilon\gamma)\dot{x}_\gamma, \dot{x}_\gamma\rangle - \textstyle\sum_{|\beta|\le R}\tfrac{1}{2}\langle A_\beta(\varepsilon\gamma)x_\gamma, x_{\gamma+\beta}\rangle$$

stationary, i.e., a function $t \mapsto x(t) \in \ell_2(\Gamma)$ is a solution of (6.9) if and only if it is a critical point of $\int_{t_1}^{t_2}\sum_{\gamma\in\Gamma}\mathcal{L}_\varepsilon(\gamma, x(t), \dot{x}(t))\,\mathrm{d}t$. We now insert the ansatz

$$x_\gamma(t) = \mathbb{X}(y, F, v, a; \theta\gamma{+}\omega t) \quad \text{with } \mathbb{X}(F, v, \theta, \omega, a; \psi) = F\gamma + vt + a\mathrm{e}^{\mathrm{i}\psi}\Phi(y, \theta, \omega)$$

into $\int_{\tau_1/\varepsilon}^{\tau_2/\varepsilon}\sum_\Gamma\mathcal{L}_\varepsilon(\gamma, x(t), \dot{x}(t))\,\mathrm{d}t$, where F, v, a, θ and ω are assumed to depend on the slow variables. We now use the clear separation of the microscopic and macroscopic scales, due to $\varepsilon \ll 1$. In $\int_{t_1}^{t_2}\sum_\Gamma\mathcal{L}(\gamma, x(t), \dot{x}(t))\ \mathrm{d}t$ integration over the fast phase variable $\psi \in \mathbb{S}^1$ can be done explicitly. Moreover, the discrete sum over $\varepsilon\gamma \in \varepsilon\mathbb{Z}^d \subset \mathbb{R}^d$ is a Riemann approximation for an integral over $\mathbb{R}^d$.

This motivates the usage of the averaged Lagrangian

$$\mathbb{L}(y,F,v,\theta,\omega,a)=\tfrac{1}{2\pi}\int_{\psi\in\mathbb{S}^1}\langle M(y)(\partial_v\mathbb{X}+\omega\partial_\phi\mathbb{X}),(\partial_v\mathbb{X}+\omega\partial_\phi\mathbb{X})\rangle \\ -\textstyle\sum_{|\beta|\le R}\langle A_\beta(y)\mathbb{X},\mathbb{X}(\theta\cdot\beta+\cdot)\rangle\,\mathrm{d}\psi$$

An explicit calculation leads to the following simple formula

$$ts\mathbb{L}(y,F,v,\theta,\omega,a)=\frac{1}{2}\big[\langle M(y)v,v\rangle+\omega^2|a|^2-(\mathbb{E}(y)F){:}F-\Omega(y,\theta)^2|a|^2\big], \tag{6.10}$$

where $\mathbb{E}$ is the tensor defined in (4.4). The Whitham equation is now obtained by making the functional

$$(\mathcal{U},\Psi,a)\mapsto\textstyle\int_{\tau_1}^{\tau_2}\int_{y\in\mathbb{R}^d}\mathbb{L}(y,\nabla_y\mathcal{U},\partial_\tau\mathcal{U},\nabla_y\Psi,\partial_\tau\Psi,a)\,\mathrm{d}y\,\mathrm{d}\tau$$

stationary. This leads to the equations

$$\partial_\tau\big(\partial_v\mathbb{L}\big)+\mathrm{div}\,\big(\partial_F\mathbb{L}\big)=0,\quad \partial_\tau\big(\partial_\omega\mathbb{L}\big)+\mathrm{div}\,\big(\partial_\theta\mathbb{L}\big)=0,\quad \partial_a\mathbb{L}=0.$$

Inserting the special form of $\mathbb{L}$ given in (6.10) we immediately see that the first equation is exactly the equation for linear elastodynamics derived in Section 4:

$$M(y)\partial_\tau^2\mathcal{U}=\mathrm{div}\,\big[\mathbb{E}(y)\nabla_y\mathcal{U}\big].$$

The third equation reads simply $(\omega^2-\Omega(y,\theta)^2)\overline{a}=0$ and thus provides the dispersion relation.

The most interesting part of Whitham's theory is obtained from the second equation. Using the variables θ and ω instead of the phase Ψ it takes the form

$$\partial_\tau\theta=\nabla_y\omega,\quad \partial_\tau(\omega|a|^2)=\mathrm{div}(-\partial_\theta\mathbb{L})=\mathrm{div}\,\Big(\Omega|a|^2\nabla_\theta\Omega\Big). \tag{6.11}$$

Defining the new variable $e_*=\omega|a|^2$ and using the dispersion relation we obtain the two conservation laws

$$\partial_\tau\theta(\tau,y)=\nabla_y[\Omega(y,\theta(\tau,y))],\quad \partial_\tau e_*(\tau,y)=\mathrm{div}\,[e_*(\tau,y)\,\nabla_\theta\Omega(y,\theta(\tau,y))], \tag{6.12}$$

which express the fact that the energy as well as the wave vector is transported with the group velocity.

We want to compare this result with the energy-transport equation for the Wigner measure. To this end we restrict to Wigner measures which arise from modulated waves of the type considered in Whitham's theory. To simplify the presentation we subtract of the macroscopic deformation $\mathcal{U}$ and restrict to the oscillating wave train defined via $\widetilde{a}$ and $\widetilde{\theta}$ as given functions of (τ,y). It is easy to see that such a modulated pattern generates the Wigner measure

$$\mu(\tau,y,\theta)=e_*(\tau,y)\delta_{\theta_*(\tau,y)}(\mathrm{d}\theta),$$

where δ_b denotes the Dirac measure with mass 1 in the point b.

This measure has to solve the energy-transport equation of Section 5.4, namely (5.22). This is equivalent that for all test function $\phi \in \mathrm{C}^1_\mathrm{c}(\mathbb{R}\times\mathbb{R}^d\times\mathcal{T}_{\Gamma_*})$ the following identities hold (all integrals $\iiint$ extend over $\mathbb{R}\times\mathbb{R}^d\times\mathcal{T}_{\Gamma_*}$):

$$\begin{aligned} 0 &= \iiint \phi(\partial_\tau\mu - \nabla_\theta\Omega\cdot\partial_y\mu + \nabla_y\Omega\cdot\partial_\theta\mu)\,\mathrm{d}(\tau,y,\theta) \\ &= \iiint [-\mu\partial_\tau\phi - \mu\mathrm{div}_y(\phi\nabla_\theta\Omega) - \nabla_\theta\phi\cdot\nabla_y\Omega\mu]\,\mathrm{d}(\tau,y,\theta) \\ &= \iiint [-\partial_\tau\phi - \nabla_y\Omega\cdot\nabla_\theta\phi + \nabla_y\phi\cdot\nabla_\theta\Omega]\mu\,\mathrm{d}(\tau,y,\theta) \\ &= \iint_{\mathbb{R}\times\mathbb{R}^d} [-\partial_\tau\phi(\tau,y,\theta_*) - \nabla_y\Omega(y,\theta_*)\cdot\nabla_\theta\phi(\tau,y,\theta_*) \\ &\qquad\qquad + \nabla_y\phi(\tau,y,\theta_*)\cdot\nabla_\theta\Omega(y,\theta_*)]e_*(\tau,y)\,\mathrm{d}(\tau,y). \end{aligned}$$

Since ϕ is a free testfunction, it is possible for each pair $\widetilde{\phi}_1,\widetilde{\phi}_2 \in \mathrm{C}^1_\mathrm{c}(\mathbb{R}\times\mathbb{R}^d)$ to find a function ϕ such that

$$\widetilde{\phi}_1(\tau,y) = \phi(\tau,y,\theta_*(\tau,y)) \quad \text{and} \quad \widetilde{\phi}_2(\tau,y) = \nabla_\theta\phi(\tau,y,\theta_*(\tau,y)) \in \mathbb{R}^d_*.$$

This implies $\nabla_y\phi|_{\theta=\theta_*} = \nabla_y\widetilde{\phi}_1 - \widetilde{\phi}_2\cdot\nabla_y\theta_*$ and $\partial_\tau\phi|_{\theta=\theta_*} = \partial_\tau\widetilde{\phi}_1 - \widetilde{\phi}_2\cdot\partial_\tau\theta_*$, and hence

$$0 = \iint_{\mathbb{R}\times\mathbb{R}^d} [-\widetilde{\phi}_2\cdot\nabla_y\Omega - (\partial_\tau\widetilde{\phi}_1 - \widetilde{\phi}_2\cdot\partial_\tau\theta_*) + (\nabla_y\widetilde{\phi}_1 - \widetilde{\phi}_2\cdot\nabla\theta_*)\cdot\nabla_\theta\Omega]e_*\,\mathrm{d}(\tau,y)$$

Since $\widetilde{\phi}_1$ and $\widetilde{\phi}_2$ are free, we arrive at the same two conservation laws as in (6.12):

$$\begin{aligned} &\partial_\tau\theta_*(\tau,y) = \nabla_y\Omega + \nabla_y\theta_*\nabla_\theta\Omega = \nabla_y\Big(\Omega(y,\theta_*(\tau,y))\Big), \\ &\partial_\tau e_*(\tau,y) = \mathrm{div}\Big(e_*(\tau,y)\nabla_\theta\Omega(y,\theta_*)\Big). \end{aligned}$$

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References

[AMM00] J. Archilla, R. MacKay, and J. Marin. Discrete breathers and Anderson modes: two faces of the same phenomenon. *Physica D*, 2000. submitted.

[BB04] M. Berezhnyy and L. Berlyand. Continuum limit three-dimensional mass-spring networks and discrete korn's inequality. *Preprint Penn State Univ.*, July 2004.

[BCS01] A. M. Balk, A. V. Cherkaev, and L. I. Slepyan. Dynamics of chains with non-monotone stress-strain relations. I. Model and numerical experiments. II. Nonlinear waves and waves of phase transition. *J. Mech. Phys. Solids*, 49(1), 131–148, 149–171, 2001.

[Bla01] X. Blanc. Geometry optimization for crystals in Thomas-Fermi type theories of solids. *Comm. Partial Differential Equations*, 26(3-4), 651–696, 2001.

[Bri46] L. Brillouin. *Wave Propagation in Periodic Structures. Electric Filters and Crystal Lattices.* McGraw-Hill Book Company, Inc., New York, 1946.

[Bri60] L. Brillouin. *Wave propagation and group velocity.* Academic Press, New York, 1960.

[CF78] A. Córdoba and C. Fefferman. Wave packets and Fourier integral operators. *Comm. Partial Differential Equations*, 3, 979–1005, 1978.

[DHM04] W. Dreyer, M. Herrmann, and A. Mielke. Micro–macro transition for the atomic chain via Whitham's modulation equation. 2004. Preprint AMS MSP no. 119.

[DK00] W. Dreyer and M. Kunik. Cold, thermal and oscillator closure of the atomic chain. *J. Phys. A*, 33(10), 2097–2129, 2000. (Corrigendum: J. Phys. A 33 (2000) 2458).

[DKKZ96] P. Deift, S. Kamvissis, T. Kriecherbauer, and X. Zhou. The Toda rarefaction problem. *Comm. Pure Appl. Math.*, 49(1), 35–83, 1996.

[DKV95] P. Deift, T. Kriecherbauer, and S. Venakides. Forced lattice vibrations. I, II. *Comm. Pure Appl. Math.*, 48, 1187–1249, 1251–1298, 1995.

[DPS90] R. L. Dobrushin, A. Pellegrinotti, and Y. M. Suhov. One-dimensional harmonic lattice caricature of hydrodynamics: a higher correction. *J. Statist. Phys.*, 61(1-2), 387–402, 1990.

[DPST86] R. L. Dobrushin, A. Pellegrinotti, Y. M. Suhov, and L. Triolo. One-dimensional harmonic lattice caricature of hydrodynamics. *J. Statist. Phys.*, 43(3-4), 571–607, 1986.

[DPST88] R. L. Dobrushin, A. Pellegrinotti, Y. M. Suhov, and L. Triolo. One-dimensional harmonic lattice caricature of hydrodynamics: second approximation. *J. Statist. Phys.*, 52(1-2), 423–439, 1988.

[FJ00] G. Friesecke and R. D. James. A scheme for the passage from atomic to continuum theory for thin films, nanotubes and nanorods. *J. Mech. Phys. Solids*, 48(6-7), 1519–1540, 2000.

[FL03] C. Fermanian Kammerer and C. Lasser. Wigner measures and codimension two crossings. *J. Math. Phys.*, 44, 507–527, 2003.

[FP99] G. Friesecke and R. L. Pego. Solitary waves on FPU lattices: I. Qualitative properties, renormalization and continuum limit. *Nonlinearity*, 12, 1601–1627, 1999.

[Fri03] G. Friesecke. Dynamics of the infinite harmonic chain: conversion of coherent initial data into synchronized oscillations. *Preprint, Univ. Warwick*, July 2003.

[FT02] G. Friesecke and F. Theil. Validity and failure of the Cauchy–Born hypothesis in a two–dimensional mass–spring lattice. *J. Nonlin. Science*, 12, 445–478, 2002.

[FV99] A.-M. Filip and S. Venakides. Existence and modulation of traveling waves in particle chains. *Comm. Pure Appl. Math.*, 52(6), 693–735, 1999.

[FW94] G. Friesecke and J. A. D. Wattis. Existence theorem for solitary waves on lattices. *Comm. Math. Phys.*, 161(2), 391–418, 1994.

[GL93] P. Gérard and É. Leichtnam. Ergodic properties of eigenfunctions for the Dirichlet problem. *Duke Math. J.*, 71, 559–607, 1993.

[GM04a] J. Giannoulis and A. Mielke. Macroscopic dynamics of an oscillator chain described by the nonlinear Schrödinger equation. 2004. Preprint AMS MSP no. 117.

[GM04b] J. Giannoulis and A. Mielke. The nonlinear Schrödinger equation as a macroscopic limit for an oscillator chain with cubic nonlinearities. *Nonlinearity*, 17, 551–565, 2004.

[GMMP97] P. Gérard, P. A. Markowich, N. J. Mauser, and F. Poupaud. Homogenization limits and Wigner transforms. *Comm. Pure Appl. Math.*, 50, 323–379, 1997. Erratum: Comm. Pure Appl. Math. 53 (2000) 280–281.

[Hag98] G. A. Hagedorn. Classification and normal forms for avoided crossings of quantum-mechanical energy levels. *J. Phys. A*, 31, 369–383, 1998.

[HLM94] M. H. Hays, C. D. Levermore, and P. D. Miller. Macroscopic lattice dynamics. *Physica D*, 79(1), 1–15, 1994.

[IK00] G. Iooss and K. Kirchgässner. Travelling waves in a chain of coupled nonlinear oscillators. *Comm. Math. Phys.*, 211(2), 439–464, 2000.

[Ioo00] G. Iooss. Travelling waves in the Fermi-Pasta-Ulam lattice. *Nonlinearity*, 13(3), 849–866, 2000.

[Jam01] G. James. Existence of breathers on FPU lattices. *C. R. Acad. Sci. Paris Sér. I Math.*, 332(6), 581–586, 2001.

[Jam02] G. James. Centre manifold reduction for quasilinear discrete systems. Preprint, August, 2002.

[LT05] C. Lasser and S. Teufel. Propagation through conical crossings: an asymptotic semigroup. *Comm. Pure Appl. Math.*, 114, 2005. To appear (AMSMSP Preprint no. 114, 2004).

[MA94] R. S. MacKay and S. Aubry. Proof of existence of breathers for time-reversible or Hamiltonian networks of weakly coupled oscillators. *Nonlinearity*, 7(6), 1623–1643, 1994.

[Mac02] F. Macià. *Propagación y control de vibraciones en medios discretos y continuos*. PhD thesis, Universidad Complutense de Madrid, Dept. de Matem. Aplicada, 2002.

[Mac04] F. Macià. Wigner measures in the discrete setting: high-frequency analysis of sampling and reconstruction operators. *SIAM J. Math. Anal.*, 36(2), 347–383 (electronic), 2004.

[MMP94] P. A. Markowich, N. J. Mauser, and F. Poupaud. A Wigner-function approach to (semi)classical limits: electrons in a periodic potential. *J. Math. Phys.*, 35, 1066–1094, 1994.

[RPK96] L. Ryzhik, G. Papanicolaou, and J. B. Keller. Transport equations for elastic and other waves in random media. *Wave Motion*, 24, 327–370, 1996.

[SL03] H. Spohn and J. Lukkarinen. The phonon Boltzmann equation for waves in weakly disordered harmonic lattices. Talk in WIAS Berlin, Dec., 2003.

[ST03] H. Spohn and S. Teufel. Personal communication. 2003.

[SW00] G. Schneider and C. E. Wayne. Counter-propagating waves on fluid surfaces and the continuum limit of the Fermi-Pasta-Ulam model. In B. Fiedler, K. Gröger, and J. Sprekels, editors, *International Conference on Differential Equations*, volume 1, pages 390–404. World Scientific, 2000.

[Tar90] L. Tartar. *H*-measures, a new approach for studying homogenisation, oscillations and concentration effects in partial differential equations. *Proc. Roy. Soc. Edinburgh Sect. A*, 115(3-4), 193–230, 1990.

[TP04] S. Teufel and G. Panati. Propagation of Wigner functions for the Schrödinger equation with a perturbed periodic potential. In *Multiscale methods in quantum mechanics*, Trends Math., pages 207–220. Birkhäuser Boston, 2004.