

Energy transport in harmonic lattices

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Abstract.

We study the large scale evolution induced by a discrete scalar wave-equation in three dimensions $\ddot{u}_t(\gamma) = \sum_{\gamma'} \alpha(\gamma - \gamma') u_t(\gamma')$, where $\gamma, \gamma' \in \mathbb{Z}^3$ are lattice sites, and $\alpha(\gamma - \gamma')$ is the coupling constant between site γ and γ' . The evolution preserves a Hamiltonian which is the sum of kinetic energy and potential energy. To derive equations that describe the macroscopic energy transport we introduce the Wigner transform and change variables so that the spatial and temporal scales are of the order of ε . In the limit, where the parameter ε is taken to 0 the Wigner transform disintegrates into three different limit objects: the transform of the weak limit, the H-measure and the Wigner-measure. We demonstrate that these three limit objects satisfy a set of decoupled transport equations: a wave-equation for the weak limit of the rescaled initial data, a dispersive transport equation for the regular limiting Wigner measure, and a geometric optics transport equation for the H-measure limit of the initial data concentrating to $k = 0$.

A simple consequence of our result is the complete characterization of energy transport in harmonic lattices with acoustic dispersion relation.

Keywords: Semiclassical analysis, discrete systems

1. Introduction.

The energy transport by atomistic oscillations in crystalline solids is a central question in solid state physics. To the first order approximation, the oscillations can be described by a discrete wave equation

$$\ddot{u}_t(\gamma) = - \sum_{\gamma'} \alpha(\gamma - \gamma') u_t(\gamma')$$

where $u(\gamma) \in \mathbb{R}$ is composed out of the displacements of the crystal atoms from their equilibrium position. Solutions of the discrete wave equation preserve the Hamiltonian $H(u, \dot{u})$ which is defined in equation (2). To analyze physically relevant properties of the crystal, such as its thermal conductivity, we first need to understand how energy is

transported within the crystal via purely harmonic vibrations. Such transport properties are determined by the dispersion relation ω of the crystal, here $\omega(k) = \sqrt{\hat{\alpha}(k)}$, the “hat” denotes a discrete Fourier transform. If ω is not smooth, then depending on the wavelength different types of continuum energy transport equations can arise.

Our main interest is to characterize the macroscopic evolution of the energy density. The starting point of our mathematical analysis is the *Wigner transform* which can be interpreted as a “wavenumber resolved” energy density. The Wigner transform $W^\varepsilon = W^\varepsilon[\psi]$ of the field $\psi \in \ell_2(\mathbb{Z}^3)$ corresponding to a given normal mode allows defining the corresponding energy density, $e^\varepsilon = e^\varepsilon[\psi]$, by the formula

$$(1) \quad e^\varepsilon(x) = \int_{\mathbb{T}^3} dk W^\varepsilon(x, k),$$

where $\varepsilon > 0$ denotes the “lattice spacing” and $x \in \mathbb{R}^3$ is a variable which interpolates between the points on the scaled lattice $\varepsilon\mathbb{Z}^3$. Here \mathbb{T}^3 denotes the 3-torus, and we identify $\mathbb{T}^3 = \mathbb{R}^3/\mathbb{Z}^3$. Thanks to the equality $\int_{\mathbb{R}^3} dq \int_{\mathbb{T}^3} dk W^\varepsilon(x, k) = H(u_{t=0}, \dot{u}_{t=0})$ we are able to identify $e^\varepsilon(x)$ as the energy density at position $x \in \mathbb{R}^d$.

A limit of a sequence $(W^\varepsilon[\psi^\varepsilon])$, where ε tends to 0, is in general given by a non-negative Radon-measure $\mu \in M_+$. Such limit measures μ_t can only satisfy an autonomous evolution equation if the initial measure doesn’t concentrate on the singular set of ω , i.e., at the points where ω is not smooth. Here we will augment the above Wigner transform scheme to encompass the most common type of singularity encountered in solid state physics: the case when ω behaves like $|k|$ near $k = 0$. Such modes will occur in general within crystal models with short range interactions, and they are particularly important as they are responsible for sound propagation in the crystal.

If the dispersion relation is not almost everywhere C^1 (with respect to the initial Wigner-measure), we have to resolve finer details of the asymptotic behavior of the sequence of initial conditions. More precisely, we show that if the sequence of initial excitations is bounded and tight in $\ell_2(\varepsilon\mathbb{Z}^3)$ then for all $t \in \mathbb{R}$ there are two measures, a Wigner-measure μ_t on $\mathbb{R}^3 \times \mathbb{T}_*^3$ and an H-measure μ_t^H on $\mathbb{R}^3 \times S^2$, and an L^2 -function ϕ_t such that $W^\varepsilon[\psi^\varepsilon(t/\varepsilon)]$ converges along a subsequence to (μ_t, μ_t^H, ϕ_t) in a certain weak sense (Theorem 3.2). The subsequence can be chosen independently of t , and it will only be relevant for determining the limit of the initial data, that is, (μ_0, μ_0^H, ϕ_0) . For all other times $t \in \mathbb{R}$, the measures μ_t, μ_t^H and the L^2 -function ϕ_t can be determined using the transport equations

$$(2) \quad \partial_t \mu_t(x, k) + \frac{1}{2\pi} \nabla \omega(k) \cdot \nabla_x \mu_t(x, k) = 0, \quad k \in \mathbb{T}_*^3,$$

$$(3) \quad \partial_t \mu_t^H(x, q) + \frac{1}{2\pi} \nabla \omega_0(q) \cdot \nabla_x \mu_t^H(x, q) = 0, \quad q \in S^2,$$

$$(4) \quad \partial_t^2 \phi = \operatorname{div}\left(\frac{1}{(2\pi)^2} A_0 \nabla \phi\right),$$

together with the initial conditions

$$(5) \quad \mu|_{t=0} = \mu_0, \quad \mu^H|_{t=0} = \mu_0^H, \quad \phi|_{t=0} = \phi_0, \quad \partial_t \hat{\phi}(t, q)|_{t=0} = -i\omega_0(q) \hat{\phi}_0(q).$$

Here the constant matrix A_0 and the function ω_0 are determined by the Hessian of the square of the dispersion relation ω at $k = 0$, explicitly

$$(6) \quad A_0 = \frac{1}{2} D^2 \omega^2(0), \quad \omega_0(q) = \sqrt{q \cdot A_0 q}.$$

Equation (2) describes the propagation of energy along the harmonic lattice with the group velocity $\nabla\omega(k)/(2\pi)$. Equation (4) is the wave equation which describes the evolution of macroscopic fluctuations. Equation (3) is usually known under the name “geometric optics” and it describes the evolution of macroscopic fluctuations whose wavelength is much longer than the lattice spacing ε and much smaller than 1, the wavelength of the fluctuations resolved by ϕ .

It follows easily from our analysis that the sum of the energies of μ , μ^H and ϕ is a constant of motion and equals the limiting value of the total energy of the initial excitations.

Our result can be seen as a generalization of the analysis in⁵ where it is shown that μ_t can be computed from μ_0 by solving a dispersive linear transport equation provided that μ has no concentrations at wavenumbers k where the dispersion relation ω is not C^1 .

The measure μ^H is closely related to the H-measure which was introduced by L. Tartar in⁷ and P. Gérard in,¹ but in general it differs from the H-measure.

The Wigner transform, or the Wigner function, was originally introduced to study semi-classical behavior in quantum mechanics but it has been proven to be a useful tool in studying large scale behavior of wave equations, as well.^{3,6}

2. The microscopic model

We assume that the excitation $u_t(\gamma) \in \mathbb{R}$, $\gamma \in \mathbb{Z}^3$ satisfies the discrete wave equation

$$(1) \quad \frac{\partial^2}{\partial t^2} u_t(\gamma) = - \sum_{\gamma' \in \mathbb{Z}^3} \alpha(\gamma - \gamma') u_t(\gamma')$$

with initial data $(u|_{t=0}, \partial_t u|_{t=0}) \in X = \ell_2 \times \ell_2$. The numbers $\alpha(\gamma - \gamma') \in \mathbb{R}$ are the elastic coupling constants between site γ and γ' . We assume that α is symmetric, i.e. $\alpha(\gamma) = \alpha(-\gamma)$. Clearly system (1) is Hamiltonian, and the energy

$$(2) \quad E(u) = H(u, \dot{u}) = \frac{1}{2} \left(\sum_{\gamma \in \mathbb{Z}^3} |\dot{u}(\gamma)|^2 + \sum_{\gamma \in \mathbb{Z}^3} \left[\sum_{\gamma' \in \mathbb{Z}^3} u(\gamma) \alpha(\gamma - \gamma') u(\gamma') \right] \right)$$

is constant along solutions. Depending on the initial conditions the solutions of system (1) may develop lattice scale oscillations which carry a finite amount of energy, cf. fig 1, where snapshots of u at several times are plotted. Since system (1) is linear and invariant

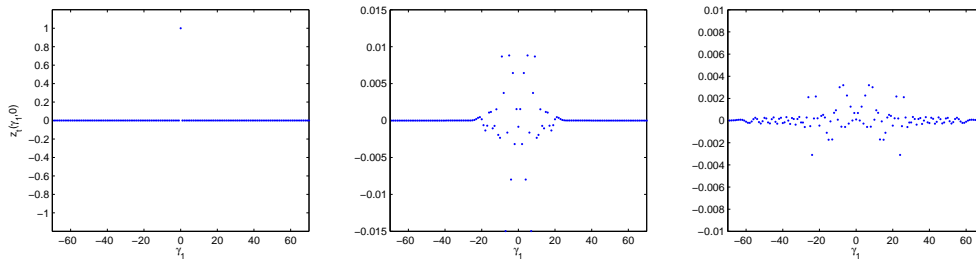


Fig. 1. Values of $u(\gamma, t)$ along the axis $\gamma_2 = \gamma_3 = 0$ for $t = 0$, $t = 0.1/\varepsilon$, $t = 0.9/\varepsilon$ with $\varepsilon = \frac{1}{7} * 10^{-1}$. The evolution is given by (1) with the nearest neighbor elastic couplings, and the initial conditions are $u_{t=0}(0) = 1$, $u_{t=0}(\gamma) = 0$ for all $\gamma \neq 0$ and $\dot{u}_{t=0} \equiv 0$.

under discrete translations we can construct explicit solutions using the discrete Fourier transform. However, to trace the evolution of energy densities it is necessary to arrange

the explicitly computed solution in a specific way so that the motion of the waves with different wavelengths can be analyzed individually. The details of the necessary steps are explained in the following.

We will see later that the dynamics is completely determined by the *dispersion relation* $\omega : \mathbb{T}^3 \rightarrow \mathbb{R}$ which is defined by

$$\omega(k) = \sqrt{2 \sum_{\gamma \in \mathbb{Z}^3 \setminus \{0\}} \alpha(\gamma)(1 - \cos(2\pi k \cdot \gamma))}.$$

Since we assumed that α is real and satisfies the symmetry property $\alpha(\gamma) = \alpha(-\gamma)$, we find that ω is also real and symmetric, i.e. $\omega(-k) = \omega(k)$.

Definition 2.1. A dispersion relation $\omega \in C(\mathbb{T}^3, [0, \infty))$ is called *acoustic* if $\lambda = \omega^2$ satisfies:

1. $\lambda \in C^{(3)}(\mathbb{T}^3, [0, \infty))$.
2. $\lambda(0) = 0$, and the Hessian of λ is invertible at 0.

A dispersion relation is called *regular acoustic*, if it is acoustic and $\lambda(k) > 0$ for $k \neq 0$. The 3×3 -matrix A_0 is the Hessian of $\frac{1}{2}\lambda$ at $k = 0$ and $\omega_0(q) = \sqrt{q \cdot A_0 q}$.

These assumptions are fairly general: as discussed in the introduction, all stable harmonic interactions have non-negative eigenvalue functions λ , and for interactions of the type discussed in⁵ $\omega = \sqrt{\lambda}$ is Lipschitz continuous.

As a means of solving (1), we rewrite the equation using the Fourier transform. This yields

$$(3) \quad \frac{\partial}{\partial t} \begin{pmatrix} \hat{u}(k, t) \\ \hat{v}(k, t) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\omega^2(k) & 0 \end{pmatrix} \begin{pmatrix} \hat{u}(k, t) \\ \hat{v}(k, t) \end{pmatrix},$$

where $\hat{u}, \hat{v} : \mathbb{T}^3 \rightarrow \mathbb{C}$ are the discrete Fourier transforms of u and v . Now diagonalizing the matrix on the right hand side motivates combining the real scalar fields u, v into the two complex fields $\psi_{\pm} = \psi_{\pm}[u, v] \in \ell_2(\mathbb{Z}^3, \mathbb{C})$ defined by the formula

$$(4) \quad \hat{\psi}_{\sigma}(k) = \frac{1}{\sqrt{2}} (\omega(k)\hat{u}(k) + i\sigma\hat{v}(k))$$

where $\sigma = \pm 1$. For all $(u, v) \in X$, we clearly have $\hat{\psi}_{\sigma} \in L^2(\mathbb{T}^3)$, and thus $\psi_{\sigma} \in \ell_2(\mathbb{Z}^3)$. In addition, since we assumed $\omega(-k) = \omega(k)$, we also have $\psi_{-}(\gamma) = \overline{\psi_{+}(\gamma)}$ for all γ . The transformation can always be inverted by applying

$$(5) \quad \hat{v} = -\frac{i}{\sqrt{2}}(\hat{\psi}_{+} - \hat{\psi}_{-}), \quad \hat{u} = \frac{1}{\omega\sqrt{2}}(\hat{\psi}_{+} + \hat{\psi}_{-}).$$

These fields are normal modes of the harmonic system, since (3) implies that $\psi_{\pm}(\gamma, t) = \psi_{\pm}[u(t), v(t)](\gamma)$ satisfy the evolution equations

$$(6) \quad \frac{\partial}{\partial t} \begin{pmatrix} \hat{\psi}_{+}(k, t) \\ \hat{\psi}_{-}(k, t) \end{pmatrix} = -i \begin{pmatrix} \omega(k) & 0 \\ 0 & -\omega(k) \end{pmatrix} \begin{pmatrix} \hat{\psi}_{+}(k, t) \\ \hat{\psi}_{-}(k, t) \end{pmatrix},$$

which are readily solved to yield for all $t \in \mathbb{R}, k \in \mathbb{R}$

$$(7) \quad \hat{\psi}_{\pm}(k, t) = e^{\mp i\omega(k)t} \hat{\psi}_{\pm}(k, 0).$$

These are exactly the two evolution equations corresponding to a mode with a dispersion relation ω .

To allow the creation of macroscopic oscillations we work with sequences of initial conditions that depend on the scaling-parameter $\varepsilon > 0$ and consider the asymptotic behavior of the solutions as ε tends to 0.

2.1. Energy density and the lattice Wigner transform

As is carefully discussed in,⁵ generalizing the definitions of the energy density and of the Wigner transform to the discrete setting is not completely obvious. In an attempt to minimize unnecessary repetition of certain basic results related to Wigner transforms, we will resort here to the definitions used in⁴ which will allow us to rely on the properties proven in Appendix B of that reference.

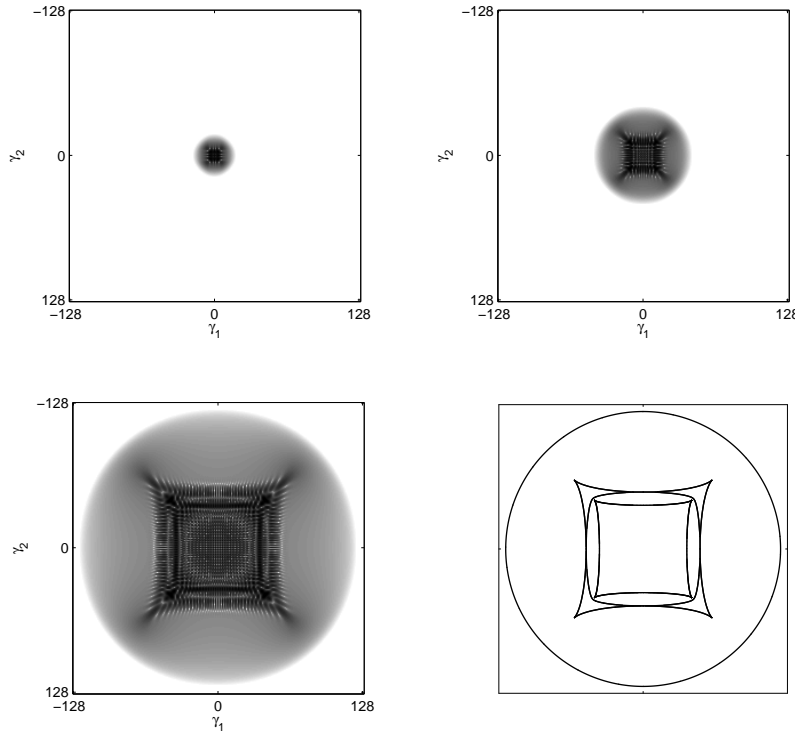


Fig. 2. Snapshots of the energy density $|\psi_+(\gamma, t)|^2$ in the plane $\gamma_3 = 0$ at $t = 0.1/\varepsilon$, $t = 0.3/\varepsilon$ and $t = 0.9/\varepsilon$ with ε , initial data and elastic constants as in Fig. 1.

We employ here the definition that for any state (u, v) , its energy density, $e^\varepsilon = e^\varepsilon[u, v]$, scaled to a lattice spacing $\varepsilon > 0$, is the tempered distribution defined via the complex fields $\psi_\sigma = \psi_\sigma[u, v]$ in (4):

$$(8) \quad e^\varepsilon(x) = \sum_{\gamma \in \mathbb{Z}^3} \delta(x - \varepsilon\gamma) \frac{1}{2} \sum_{\sigma=\pm 1} |\psi_\sigma(\gamma)|^2$$

where δ denotes the Dirac delta-distribution. This is a manifestly positive distribution,

and identifiable with a measure whose total mass equals the total energy:

$$(9) \quad \begin{aligned} \int dx e^\varepsilon(x) &= \sum_{\gamma \in \mathbb{Z}^3} \frac{1}{2} \sum_{\sigma=\pm 1} |\psi_\sigma(\gamma)|^2 = \frac{1}{2} \sum_{\sigma=\pm 1} \|\psi_\sigma\|^2 \\ &= \frac{1}{4} \sum_{\sigma=\pm 1} \int dk |\omega(k)\hat{u}(k) + i\sigma\hat{v}(k)|^2 = H(u, v) < \infty. \end{aligned}$$

This justifies calling e^ε an energy density: it defines a distribution of the positive total energy between the lattice sites. The symmetry of ω entails that $|\psi_-(\gamma)| = |\psi_+(\gamma)|$ and we can also identify the energy density directly with the norm-density of ψ_+ :

$$(10) \quad e^\varepsilon(x) = \sum_{\gamma \in \mathbb{Z}^3} \delta(x - \varepsilon\gamma) |\psi_+(\gamma)|^2.$$

Thus also for all $\varepsilon > 0$,

$$(11) \quad H(u, v) = \int dx e^\varepsilon(x) = \|\psi_+\|_{\ell^2(\mathbb{Z}^3)}^2 = \|\hat{\psi}_+\|_{L^2(\mathbb{T}^3)}^2 = \|\hat{\psi}_-\|_{L^2(\mathbb{T}^3)}^2$$

which is conserved when $(u, v) = (u(t), v(t))$.

We have given an example of the time-evolution of the so defined energy density in Fig. 2. The last panel in the figure contains the most obvious features which are implied by the corresponding macroscopic evolution equation: the points of discontinuity of the solution. The macroscopic initial data is given by $\mu_0(dx, dk) = \delta(x)\frac{1}{2}|\omega(k)|^2 dx dk$, which has no concentration at $k = 0$. Thus only (2) is relevant. It is readily solved to yield as the energy density

$$(12) \quad e(x, t) = \int_{\mathbb{T}^3} dk \delta(x - t\frac{1}{2\pi}\nabla\omega(k)) = t^{-3} \int_{\mathbb{T}^3} dk \delta(\frac{x}{t} - \frac{1}{2\pi}\nabla\omega(k))$$

Evaluating such integrals has been considered, for instance, in Sec. 6.4 of.⁵ $|\nabla\omega(k)|$ has its maximum near the point of discontinuity of the gradient, at $k = 0$. This defines the outer circle outside which the solution must be zero. Inside the circle, the solution has a finite density, apart from points which correspond to values of k for which the Hessian of ω is not invertible. We have computed the positions of such points using Mathematica, and plotted the result in the last panel in Fig. 2.

We are interested in the limiting behavior of $e^\varepsilon[u(t/\varepsilon), v(t/\varepsilon)]$, as ε tends to 0. Since the velocity of the waves with wave vector k depends on k it is necessary to work with an object that encodes the density of waves with wave vector $k \in \mathbb{T}^3$ at $x \in \mathbb{R}^3$. This job is conveniently done by the Wigner-transform. In order to avoid certain technical difficulties we are going to define our Wigner-transform only in the sense of distributions, i.e., via a duality principle.

First we introduce the space of Schwartz functions.

Definition 2.2. Let $\mathcal{S}_d = \mathcal{S}(\mathbb{R}^d)$ denote the Schwartz space, and $\|\cdot\|_{\mathcal{S}_d, N}$ the corresponding N :th Schwartz norm. Explicitly, with α denoting an arbitrary multi-index and with $\langle x \rangle = \sqrt{1 + x^2}$, then

$$(13) \quad \|f\|_{\mathcal{S}_d, N} = \sup_{x \in \mathbb{R}^d} \max_{|\alpha| \leq N} |\langle x \rangle^N \partial^\alpha f(x)|.$$

We also employ the shorthand notation $\mathcal{S} = \mathcal{S}_3$.

To extract the relevant weak limits from the sequence ψ^ε as ε tends to 0 we have to specify a space of suitable test functions. Since we want to track the evolution of three different kinds of lattice vibrations (short-, medium- and long-wavelength) we require a somewhat involved and non-standard notion of multiscale test functions.

Definition 2.3. We call a test function $a \in C^\infty(\mathbb{R}^3 \times \mathbb{T}^3 \times \mathbb{R}^3)$ *admissible*, if it satisfies the following properties:

1. $\sup_{k,q,|\alpha|\leq N} \|\partial^\alpha a(\cdot, k, q)\|_{\mathcal{S},N} < \infty$, for all $N \geq 0$,
2. $q \mapsto a(x, k, q)$ is constant for all $\text{mod } k_\infty \geq \frac{1}{4}$ and $x \in \mathbb{R}^3$.
3. There is a function $b \in C^\infty(\mathbb{R}^3 \times \mathbb{T}^3 \times S^2)$ such that for any $N \geq 0$

$$(14) \quad \sup_{|q|\geq R, k \in \mathbb{T}^3} \|a(\cdot, k, q) - b(\cdot, k, \frac{q}{|q|})\|_{\mathcal{S},N} \rightarrow 0, \quad \text{when } R \rightarrow \infty.$$

The first condition can be summarized as follows: we assume the test-functions to be Schwartz in x and smooth with bounded derivatives in k and q . The above requirements are not minimal. The second condition is only needed in order to guarantee that

$k \mapsto a(x, k, k/\varepsilon)$ would always be smooth on \mathbb{T}^3 . Also, taking arbitrarily large N in the last step is not necessary, most likely $N = d + 3 = 6$ would suffice.

Having the notion of admissible test functions at our disposal we can define the central object of this paper: the Wigner transform.

Definition 2.4. Let $\psi \in \ell_2(\mathbb{Z}^3)$. We define the lattice Wigner transform $W^\varepsilon[\psi]$ at scale $\varepsilon > 0$ by

$$(15) \quad \langle a, W^\varepsilon[\psi] \rangle = \int_{\mathbb{R}^3} dp \int_{\mathbb{T}^3} dk \overline{\hat{a}(p, k, \frac{k}{\varepsilon})} \hat{\psi}(k - \varepsilon \frac{p}{2}) \hat{\psi}(k + \varepsilon \frac{p}{2}),$$

where a is an admissible test function and $\hat{a} = \mathcal{F}_{x \rightarrow p} a$, i.e.,

$$(16) \quad \hat{a}(p, k, q) = \int_{\mathbb{R}^3} dx e^{-2\pi i p \cdot x} a(x, k, q).$$

The L^2 -Wigner transform $W_{\text{cont}}^{(\varepsilon)}[\phi]$ of a function $\phi \in L^2(\mathbb{R}^3)$ at the scale $\varepsilon > 0$ is given by the distribution

$$(17) \quad b \mapsto \langle b, W_{\text{cont}}^{(\varepsilon)}[\phi] \rangle = \int_{\mathbb{R}^3 \times \mathbb{R}^3} dp dq \overline{\hat{b}(p, q)} \hat{\phi}(q - \varepsilon \frac{p}{2}) \hat{\phi}(q + \varepsilon \frac{p}{2})$$

for all $b \in \mathcal{S}(\mathbb{R}^3, C^\infty(\mathbb{R}^3))$, and with $\hat{b} = \mathcal{F}_{x \rightarrow p} b$.

The results in⁴ can be used to show that many of the basic properties of the usual Wigner transform carry over to the multi-scale Wigner transform. Particularly important for us is the following relation:

Prop 2.1. For any $f \in \mathcal{S}(\mathbb{R}^3)$, the test function $a_f(x, k, q) = f(x)$ is admissible, and for all $\varepsilon > 0$ and for all $(u, v) \in X$,

$$(18) \quad \langle f, e^\varepsilon \rangle = \langle a_f, W^\varepsilon[\psi] \rangle$$

where $e^\varepsilon = e^\varepsilon[u, v]$ and $\psi = \psi_+[u, v]$.

The above Proposition can be formally summarized by the formula

$$(19) \quad e^\varepsilon(x) = \int_{\mathbb{T}^3} dk \int_{\mathbb{R}^3} dq W^\varepsilon[\psi](x, k, q)$$

which implies also (in the sense of choosing any suitable test-function sequence approaching pointwise 1)

$$(20) \quad \int_{\mathbb{R}^3 \times \mathbb{T}^3 \times \mathbb{R}^3} dx dk dq W^\varepsilon[\psi](x, k, q) = \|\psi\|_{\ell_2(\mathbb{Z}^3)}^2.$$

3. Main results

The macroscopic evolution is obtained by sending ε to 0. Our objective is to characterize the asymptotic behavior of the Wigner function $W^\varepsilon[\psi^\varepsilon]$. The limit strongly depends on the dispersion relation ω . We will consider here regular acoustic dispersion relations, keeping in mind that in the case of a scalar field and nearest neighbor interactions in \mathbb{Z}^3 the dispersion relation ω is given by $\omega_{\text{nn}}(k) = \left[\sum_{\nu=1}^3 2(1 - \cos(2\pi k^\nu)) \right]^{\frac{1}{2}}$ which is regular acoustic with $\omega_0(q) = 2\pi|q|$. The main achievement of this paper is that complicated assumptions concerning the concentrations of the Wigner transform W^ε in wave-number space as ε tends to 0 are no longer needed. The only remaining requirements are boundedness and tightness of the sequence of initial excitations.

Assumption 3.1. *We consider a sequence of values $\varepsilon > 0$ such that $\varepsilon \rightarrow 0$. For each ε in the sequence we assume that there is given an initial data vector $\psi_0^\varepsilon \in \ell_2(\mathbb{Z}^3)$ such that*

1. $\sup_\varepsilon \|\psi_0^\varepsilon\| < \infty$.
2. The sequence ψ_0^ε is tight on the scale ε^{-1} :

$$(1) \quad \lim_{R \rightarrow \infty} \limsup_{\varepsilon \rightarrow 0} \sum_{|\gamma| > R/\varepsilon} |\psi_0^\varepsilon(\gamma)|^2 = 0.$$

After these preparations we are in a position to state our result. The main point is that if ω is a regular acoustic dispersion relation the asymptotic behavior of the energy density is characterized by precisely three different objects: the weak limit (macroscopic waves), the H-measure (short macroscopic waves) and the Wigner measure (microscopic waves) and no assumption concerning energy concentrations except those stated in Assumption 3.1 are required.

Theorem 3.2. *Let $\psi_0^\varepsilon \in \ell_2(\mathbb{Z}^3)$ be a sequence which satisfies Assumption 3.1. Let ω be a regular acoustic dispersion relation and define $\psi_t^\varepsilon \in \ell_2(\mathbb{Z}^3)$ for all $t \in \mathbb{R}$ by the formula*

$$(2) \quad \hat{\psi}_t^\varepsilon(k) = e^{-it\omega(k)} \hat{\psi}_0^\varepsilon(k).$$

Let also $\mathbb{T}_^3 = \mathbb{T}^3 \setminus \{0\}$. Then there are positive, bounded Radon measures μ_0, μ_0^H on $\mathbb{R}^3 \times \mathbb{T}_*^3$ and $\mathbb{R}^3 \times S^2$, respectively, a function $\phi_0 \in L^2(\mathbb{R}^3)$ and a subsequence (not relabelled) such that for all admissible test functions a and $t \in \mathbb{R}$,*

$$(3) \quad \lim_{\varepsilon \rightarrow 0} \langle a, W^\varepsilon[\psi_{t/\varepsilon}^\varepsilon] \rangle = \int_{\mathbb{R}^3 \times \mathbb{T}_*^3} d\mu_t(x, k) \overline{b(x, k, \frac{k}{|k|})} \\ + \int_{\mathbb{R}^3 \times S^2} d\mu_t^H(x, q) \overline{b(x, 0, q)} + \langle a_0, W_{\text{cont}}^{(1)}[\phi_t] \rangle,$$

where $b(x, k, q) = \lim_{R \rightarrow \infty} a(x, k, Rq)$ for $|q| = 1$, $a_0(x, q) = a(x, 0, q)$, and ϕ_t , μ_t and μ_t^H are given by

$$(4) \quad \hat{\phi}_t(q) := e^{-it\omega_0(q)} \hat{\phi}_0(q),$$

$$(5) \quad \int_{\mathbb{R}^3 \times \mathbb{T}_*^3} a(x, k) d\mu_t(x, k) := \int_{\mathbb{R}^3 \times \mathbb{T}_*^3} a(x + t\frac{1}{2\pi}\nabla\omega(k), k) d\mu_0(x, k),$$

$$(6) \quad \int_{\mathbb{R}^3 \times S^2} b(x, q) d\mu_t^H(x, q) := \int_{\mathbb{R}^3 \times S^2} b(x + t\frac{1}{2\pi}\nabla\omega_0(q), q) d\mu_0^H(x, q).$$

Moreover, for all t the energy equality

$$(7) \quad \lim_{\varepsilon \rightarrow 0} \|\psi_0^\varepsilon\|^2 = \mu_t(\mathbb{R}^3 \times \mathbb{T}_*^3) + \mu_t^H(\mathbb{R}^3 \times S^2) + \|\phi_t\|_{L^2(\mathbb{R}^3)}^2$$

holds.

Remark 3.1. It is immediate from the definition that ϕ , μ and μ^H are weak solutions of the set of decoupled linear transport equations (2-4).

The subsequences which are extracted in the statement of the theorem can be characterized by a simple condition. In particular, if equation (3) holds for $t = 0$, then no subsequence has to be extracted.

Corollary 3.3. Let (ψ_0^ε) be a sequence which satisfies Assumption 3.1. Suppose that ϕ_0^ε converges weakly to ϕ_0 , and that $\lim_{\varepsilon \rightarrow 0} \langle a, W^\varepsilon[\psi_0^\varepsilon] \rangle$ exists for every admissible testfunction a . Then there are unique positive, bounded Radon measures μ_0, μ_0^H on $\mathbb{R}^3 \times \mathbb{T}_*^3$ and $\mathbb{R}^3 \times S^2$, respectively, such that for every admissible testfunction a

$$(8) \quad \lim_{\varepsilon \rightarrow 0} \langle a, W^\varepsilon[\psi_0^\varepsilon] \rangle = \int_{\mathbb{R}^3 \times \mathbb{T}_*^3} d\mu_0(x, k) \overline{b(x, k, \frac{k}{|k|})} + \int_{\mathbb{R}^3 \times S^2} d\mu_0^H(x, q) \overline{b(x, 0, q)} + \langle a_0, W_{cont}^{(1)}[\phi_0] \rangle,$$

where a_0 and b are defined as in Theorem 3.2. In addition, then (3) holds for all $t \in \mathbb{R}$ along the original sequence ε with the initial macroscopic data determined by the triplet (μ_0, μ_0^H, ϕ_0) .

The measure μ^H is closely related to H-measures which have been introduced in the context of oscillatory solutions of partial differential equations by L. Tartar⁷ and P. Gérard.¹ The proofs of Theorem 3.2 and Corollary 3.3, together with a discussion illuminating the precise relation between μ^H and the H-measures can be found in.²

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