Energy transport by acoustic modes of harmonic lattices

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Abstract

We study the large scale evolution of a scalar lattice excitation u which satisfies a discrete 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. We assume that the dispersion relation ω associated to the elastic coupling constants $\alpha(\gamma - \gamma')$ is acoustic, i.e., it has a singularity of the type $|k|$ near the vanishing wave vector, $k = 0$.

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 continuum limit, which is achieved by sending the parameter ε 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 relations.

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

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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, as will be discussed in Sec. 1.1. 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" denoting a discrete Fourier transform. If ω is not smooth, then depending on the wavelength different types of continuum energy transport equations can arise. We follow the basic ideas of Luc Tartar who developed in the 1980s a mathematical framework that can be used to analyze the weak limits of certain nonlinear quantities, the energy density being one of them.

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. Let us leave the details for Sec. 2.1, and only summarize the main findings here. 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

$$e^\varepsilon(x) = \int_{\mathbb{T}^3} \mathrm{d}k\, W^\varepsilon(x,k), \tag{1.1}$$

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 $\int_{\mathbb{R}^3} \mathrm{d}q \int_{\mathbb{T}^3} \mathrm{d}k\, W^\varepsilon(x,k) = H(u_{t=0}, \dot{u}_{t=0})$ 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 $\mu \in M_+$. For such limit measures to form a sensible approximation for the original dynamical system, the convergence property needs to be retained in the time-evolution. In addition, for such a description to be useful, μ_t should also satisfy an autonomous evolution equation. However, this is typically not possible if the initial measure concentrates to the singular set of ω, i.e., to 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. With some effort, it is likely that our results could be extended to cover any dispersion relation for which the singular set consists of isolated points. However, we will not explicitly spell out the general result here.

Our result can be seen as a generalization of the analysis in [1] 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.

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^{H}_t 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 $(\mu_t, \mu^{\mathrm{H}}_t, \phi_t)$ 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, $(\mu_0, \mu^{\mathrm{H}}_0, \phi_0)$. For all other times $t \in \mathbb{R}$, the measures $\mu_t, \mu^{\mathrm{H}}_t$ and the L^2-function ϕ_t can be determined using the transport equations

$$\partial_t \mu_t(x,k) + \tfrac{1}{2\pi}\nabla\omega(k)\cdot\nabla_x\mu_t(x,k) = 0, \qquad k \in \mathbb{T}^3_*\,, \tag{1.2}$$

$$\partial_t \mu^{\mathrm{H}}_t(x,q) + \tfrac{1}{2\pi}\nabla\omega_0(q)\cdot\nabla_x\mu^{\mathrm{H}}_t(x,q) = 0, \quad q \in S^2\,, \tag{1.3}$$

$$\partial_t^2\phi = \operatorname{div}\!\left(\tfrac{1}{(2\pi)^2}A_0\nabla\phi\right), \tag{1.4}$$

together with the initial conditions

$$\mu|_{t=0} = \mu_0, \quad \mu^{\mathrm{H}}\big|_{t=0} = \mu^{\mathrm{H}}_0, \quad \phi|_{t=0} = \phi_0, \quad \partial_t\hat\phi(t,q)|_{t=0} = -i\omega_0(q)\hat\phi_0(q). \tag{1.5}$$

Here the constant matrix A_0 and the function ω_0 are determined by the Hessian of the square of the dispersion relation ω (defined in (2.6)) at $k = 0$, explicitly

$$A_0 = \frac{1}{2}D^2\omega^2(0), \qquad \omega_0(q) = \sqrt{q\cdot A_0 q}. \tag{1.6}$$

Equation (1.2) describes the propagation of energy along the harmonic lattice with the group velocity $\nabla\omega(k)/(2\pi)$. Equation (1.4) is the wave equation which describes the evolution of macroscopic fluctuations. Equation (1.3) 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.

Standard results in semi-classical analysis show that the Wigner measure μ and $\int_{\mathbb{R}^3} \mathrm{d}q\, W^1[\phi](x,q)$ are non-negative. Hence, a key step in our analysis is to demonstrate that also μ^{H} has a sign. The measure μ^{H} is closely related to the H-measure which was introduced by L. Tartar in [2] and P. Gérard in [3], 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 [4, 5]. In particular, the method of calculating continuous, macroscopic energy by finding the limit object of a sequence of energies e^{ε} on rescaled lattice models is one that has been widely used and justified in, for example, [1, 6, 7]. In [1], the Wigner transform of the normal modes is employed in solving the macroscopic transport of energy in the above harmonic systems for deterministic initial data. The same system is considered in [8] with random initial data and in a larger function space, however, excluding the type of concentration effects we study here.

The main use of the Wigner transform is that, unlike the energy density e^{ε} itself, it contains enough information so that it satisfies a closed equation in the limit $\varepsilon \to 0$. Indeed, it was shown in [1] that, as long as there is no concentration on the singular set of the dispersion relation faster than $\varepsilon^{1/2}$, the Wigner transform of the time-evolved state vector $\psi(t/\varepsilon)$ converges to a limit measure $\tilde{\mu}_t$ on $\mathbb{R} \times \mathbb{K}$. Here $\mathbb{K}$ is a suitable compactification of $\mathbb{T}^3 \setminus \mathbb{S}$, $\mathbb{S} =$ the singular set, which allows a continuous extension of the group velocity $\nabla\omega$. The measure $\tilde{\mu}_t$ is then proven to satisfy the transport equation

$$\partial_t \tilde{\mu}_t(x,k) + \tfrac{1}{2\pi} \nabla\omega(k) \cdot \nabla_x \tilde{\mu}_t(x,k) = 0. \tag{1.7}$$

It was also shown in [1], that if the weak limit of the rescaled initial data exists, then the limit satisfies the continuum wave equation. However, removing the assumption about the rate of concentration, as well as combining the result with a non-zero weak limit for the initial data remain open questions.

In this paper we will show how to overcome the above difficulties in a physically relevant class of models with a singular dispersion relation. In Section 2 we will first present the microscopic dynamical model in detail. In Section 2.1 we will define the Wigner transform, and discuss its relation to the energy of the microscopic lattice model. The main results will be presented in Section 3.

1.1 Relation with solid state physics

A crystal in solid state physics is a state of matter in which the atoms retain a nearly perfect periodic structure over macroscopic times. The Hamiltonian model used for the time-evolution in such a crystal is, to the first order accuracy, harmonic. If we assume that each periodic cell of the idealized perfectly periodic crystal structure contains n atoms, then we can form a vector $q(\gamma) \in \mathbb{R}^{3n}$ out of the displacements of the atoms in the periodic cell labeled by $\gamma \in \mathbb{Z}^3$. The (classical) Hamiltonian equations of motion of this harmonic model are then

$$\dot{q}_i(\gamma, t) = \frac{1}{m_i} p_i(\gamma, t), \qquad \dot{p}_i(\gamma, t) = -\sum_{\gamma', i'} \mathbb{A}(\gamma - \gamma')_{i,i'} q_{i'}(\gamma', t) \tag{1.8}$$

where $\gamma \in \mathbb{Z}^3$, $i = 1, \dots, 3n$, and m_i denotes the mass of the atom whose displacement q_i measures.

By the change of variables to $\tilde{q}_i(\gamma) = m_i^{\frac{1}{2}} q_i(\gamma)$, $\tilde{p}_i(\gamma) = m_i^{-\frac{1}{2}} p_i(\gamma)$, these equations can be transformed into a standard form whose force matrix is given by $\tilde{\mathbb{A}}(\gamma)_{i,i'} = m_i^{-1/2} \mathbb{A}(\gamma)_{i,i'} m_{i'}^{-1/2}$. The standard form equations can then be solved by Fourier transform, and a diagonalization of the remaining multiplicative evolution equations decomposes the $3n$ vector degrees of freedom into independent *normal modes*, called *phonons* in solid state physics. Each normal mode is a complex scalar field on the crystal lattice, and its time-evolution is unitary and uniquely determined by the corresponding dispersion relation $\omega_i(k)$ on $\mathbb{T}^3$. More details about the related mathematical issues can be found in [1, 8].

From the physical perspective it is highly relevant to understand energy transport in the case where ω is acoustic in the sense that it contains a $|k|$ singularity. In this case ω is degenerate for large wave-numbers in the sense that the velocity at which long waves propagate converges to the speed of sound. In other words, the energy density can travel ballistically over large distance without experiencing dilution effects due to dispersion.

Acoustic dispersion relations arise in general from atomistic Hamiltonians with short range harmonic interactions. For instance, for the type of interactions considered in [1] all dispersion relations are Lipschitz continuous and piecewise analytic. In solid state physics, the modes are accordingly divided into *optical* and *acoustic* depending on this regularity: if the dispersion relation is regular at $k = 0$, then the mode is called optical, if it behaves as $|k|$ at $k = 0$, then the mode is called acoustic. The latter name arises as these modes are believed to be responsible for the propagation of sound waves in the crystal.

The simplicity of the Fourier-picture is the reason that the dispersion relation is the starting point of most of the more physically oriented publications. Obviously, within the context of harmonic defect-free crystals both approaches are completely equivalent. In the beginning of Section 2 we will provide the mathematical details which establish this equivalence on an elementary level.

Finally, let us remark that the discrete *linear* wave equation alone does not suffice to determine the physically relevant properties of the crystal, such as its thermal conductivity. However, it forms the basis for perturbative treatments using which these questions can be addressed. We refer to [9, 10, 11] for further details on the physical aspects of the topic and to [12] for a review about related open problems.

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2 The microscopic model

There are two mathematically equivalent descriptions of harmonic crystals. On the one hand, one can work with the Hamiltonian equations of motion and analyze the properties of the solutions. At least formally anharmonic crystals can be discussed in the same way. On the other hand, one can utilize the periodicity and linearity to condense the Hamiltonian into the dispersion relation. While this approach is very elegant, it cannot be used to directly analyze nonlinear models.

We will show in this chapter how for harmonic lattices the first approach reduces to the second one. Then we demonstrate how the tool of Wigner functions can be brought to bear on the reduced description.

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

$$\frac{\partial^2}{\partial t^2} u_t(\gamma) = -\sum_{\gamma' \in \mathbb{Z}^3} \alpha(\gamma - \gamma') u(\gamma') \tag{2.1}$$

with initial data $(u|_{t=0}, \partial_t u|_{t=0}) \in X = \ell_2 \times \ell_2$. The numbers $\alpha(\gamma - \gamma')$ are the elastic coupling constants between the sites γ and γ'. We assume that α is real and symmetric ($\alpha(-\gamma) = \alpha(\gamma)$). Clearly system (2.1) can be written in a Hamiltonian form and the energy

$$E(u) = H(u, \dot{u}) = \frac{1}{2}\left(\sum_{\gamma \in \mathbb{Z}^3} |\dot{u}(\gamma)|^2 + \sum_{\gamma \in \mathbb{Z}^3} \left[\sum_{\gamma' \in \mathbb{Z}^3} u(\gamma)\alpha(\gamma - \gamma')u(\gamma') \right] \right) \tag{2.2}$$

is constant along solutions. Depending on the initial conditions the solutions of system (2.1) may develop large scale oscillations which carry a finite amount of energy, cf. Fig. 1 where snapshots of u at several times are plotted.

Since system (2.1) is linear and invariant under discrete translations, we can write the solutions in a closed form using the Fourier transform.

Definition 2.1 *We define the Fourier transform $\ell_2(\mathbb{Z}^3) \to L^2(\mathbb{T}^3)$ by extending*

$$(\mathcal{F}_{\gamma \to k} \psi)(k) = \hat{\psi}(k) = \sum_{\gamma \in \mathbb{Z}^3} \mathrm{e}^{-2\pi \mathrm{i} k \cdot \gamma} \psi(\gamma) \tag{2.3}$$

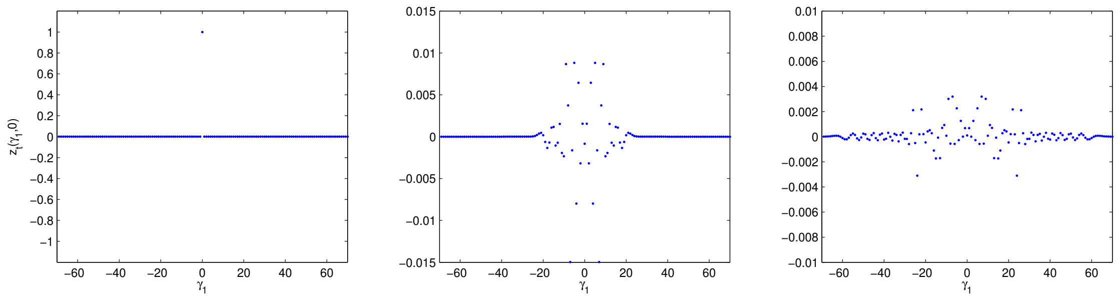

Figure 1: Values of $u(\gamma, t)$ along the axis $\gamma_2 = \gamma_3 = 0$ for $t = 0$, $t = 0.1/\varepsilon$, $t = 0.9/\varepsilon$ with $\varepsilon = \frac{1}{7} * 10^{-1}$. The evolution is given by (2.1) with the nearest neighbor elastic couplings (2.12), and the initial conditions are $u_{t=0}(0) = 1$, $u_{t=0}(\gamma) = 0$ for all $\gamma \neq 0$ and $\dot{u}_{t=0} \equiv 0$.

from ψ with finite support to all of $\ell_2(\mathbb{Z}^3)$. Here $\mathbb{T}^3 = \mathbb{R}^3/\mathbb{Z}^3$ denotes the unit 3-torus. The inverse transform is pointwise convergently defined by the integral

$$(\mathcal{F}_{k\to\gamma}\hat{\psi})(\gamma) = \int_{\mathbb{T}^3} \mathrm{d}k\, \mathrm{e}^{2\pi \mathrm{i} k\cdot\gamma}\hat{\psi}(k) = \psi(\gamma). \tag{2.4}$$

where the measure $\mathrm{d}k$ is induced by the Lebesgue measure on $[-\frac{1}{2}, \frac{1}{2}]^3$. In particular, $\int_{\mathbb{T}^3} \mathrm{d}k = 1$.

If one applies the Fourier transform to equation (2.1) one obtains the simpler system

$$\frac{\partial}{\partial t}\begin{pmatrix}\hat{u}(k,t)\\ \hat{v}(k,t)\end{pmatrix} = \begin{pmatrix}0 & 1\\ -\omega^2(k) & 0\end{pmatrix}\begin{pmatrix}\hat{u}(k,t)\\ \hat{v}(k,t)\end{pmatrix}. \tag{2.5}$$

The function $\omega : \mathbb{T}^3 \to \mathbb{R}$ is the dispersion relation and is related to the atomistic Hamiltonian via the following formula

$$\omega(k) = \sqrt{\hat{\alpha}(k)} = \sqrt{\sum_{\gamma\in\mathbb{Z}^3} \alpha(\gamma)\cos(2\pi\gamma\cdot k)}. \tag{2.6}$$

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

Now diagonalizing the matrix on the right hand side of (2.5) 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

$$\hat{\psi}_\sigma(k) = \frac{1}{\sqrt{2}}\left(\omega(k)\hat{u}(k) + \mathrm{i}\sigma\hat{v}(k)\right) \tag{2.7}$$

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

$$\hat{v} = -\frac{\mathrm{i}}{\sqrt{2}}(\hat{\psi}_+ - \hat{\psi}_-), \quad \hat{u} = \frac{1}{\omega\sqrt{2}}(\hat{\psi}_+ + \hat{\psi}_-). \tag{2.8}$$

These fields are normal modes of the harmonic system, since (2.5) implies that $\psi_\pm(\gamma, t) = \psi_\pm[u(t), v(t)](\gamma)$ satisfy the evolution equations

$$\frac{\partial}{\partial t}\begin{pmatrix}\hat{\psi}_+(k,t)\\ \hat{\psi}_-(k,t)\end{pmatrix} = -\mathrm{i}\begin{pmatrix}\omega(k) & 0\\ 0 & -\omega(k)\end{pmatrix}\begin{pmatrix}\hat{\psi}_+(k,t)\\ \hat{\psi}_-(k,t)\end{pmatrix}, \tag{2.9}$$

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

$$\hat{\psi}_\pm(k,t) = \mathrm{e}^{\mp\mathrm{i}\omega(k)t}\hat{\psi}_\pm(k,0)\,. \tag{2.10}$$

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

After these reduction steps it is obvious that the dispersion relation ω fully determines the properties of the solutions. We will assume throughout this paper that ω is of acoustic type in the following precise sense:

Definition 2.2 *We call $\omega \in C(\mathbb{T}^3, [0,\infty))$ an* acoustic dispersion relation *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 in [1] $\omega = \sqrt{\lambda}$ is Lipschitz continuous.

A prototype for the kind of dispersion relations we will consider here is the dispersion relation of the nearest neighbor square lattice:

$$\omega_{\mathrm{nn}}(k) = \Big[\sum_{\nu=1}^{3} 2(1 - \cos(2\pi k^\nu))\Big]^{\frac{1}{2}}. \tag{2.11}$$

This is clearly a regular acoustic dispersion relation, in the sense of Definition 2.2, and for it A_0 is proportional to a unit matrix and $\omega_0(q) = 2\pi|q|$. The corresponding elastic couplings are given by $\alpha_{\rm nn}(\gamma' - \gamma) = -\Delta_{\gamma'\gamma}$, where Δ is the discrete Laplacian of the square lattice. Explicitly,

$$\alpha_{\rm nn}(\gamma) = \begin{cases} 6, & \text{if } \gamma = 0, \\ -1, & \text{if } |\gamma| = 1, \\ 0, & \text{otherwise.} \end{cases} \tag{2.12}$$

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

From now we will focus on analyzing asymptotic behavior of the fields $\psi_\pm$ as ε tends to 0. As is carefully discussed in [1], 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 in [7] which will allow us to rely on the properties proven in Appendix B of that reference. However, we wish to keep in mind that this choice might not be optimal for all purposes, and we refer the interested reader to the discussion and to the references in [1, 13] for further possibilities.

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 (2.7):

$$e^\varepsilon(x) = \sum_{\gamma\in\mathbb{Z}^3} \delta(x - \varepsilon\gamma) \frac{1}{2} \sum_{\sigma=\pm 1} |\psi_\sigma(\gamma)|^2 \tag{2.13}$$

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:

$$\begin{aligned} \int {\rm d}x\, e^\varepsilon(x) &= \sum_{\gamma\in\mathbb{Z}^3} \frac{1}{2} \sum_{\sigma=\pm 1} |\psi_\sigma(\gamma)|^2 = \frac{1}{2} \sum_{\sigma=\pm 1} \|\psi_\sigma\|^2 \\ &= \frac{1}{4} \sum_{\sigma=\pm 1} \int {\rm d}k\, |\omega(k)\hat{u}(k) + {\rm i}\sigma\hat{v}(k)|^2 = H(u, \dot{u}) < \infty. \end{aligned} \tag{2.14}$$

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 implies that $|\psi_-(\gamma)| =$

$|\psi_+(\gamma)|$ and thus we can also identify the energy density directly with the norm-density of ψ_+:

$$e^\varepsilon(x) = \sum_{\gamma\in\mathbb{Z}^3} \delta(x-\varepsilon\gamma)|\psi_+(\gamma)|^2. \tag{2.15}$$

Then also for all $\varepsilon > 0$,

$$H(u,v) = \int \mathrm{d}x\, e^\varepsilon(x) = \|\psi_+\|^2_{\ell_2(\mathbb{Z}^3)} = \|\hat{\psi}_+\|^2_{L^2(\mathbb{T}^3)} = \|\hat{\psi}_-\|^2_{L^2(\mathbb{T}^3)} \tag{2.16}$$

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 $\mu_0(\mathrm{d}x, \mathrm{d}k) = \delta(x)\frac{1}{2}|\omega(k)|^2\mathrm{d}x\mathrm{d}k$, which has no concentration at $k = 0$. Thus only (1.2) is relevant. It is readily solved to yield as the energy density

$$e(x,t) = \int_{\mathbb{T}^3} \mathrm{d}k\, \delta(x - t\tfrac{1}{2\pi}\nabla\omega(k)) = t^{-3}\int_{\mathbb{T}^3} \mathrm{d}k\, \delta(\tfrac{x}{t} - \tfrac{1}{2\pi}\nabla\omega(k)) \tag{2.17}$$

Evaluating such integrals has been considered, for instance, in Sec. 6.4 of [1]. $|\nabla\omega(k)|$ 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. For a reader interested in the details of the computation, we point out that considering the case $x_3 = 0$ simplifies the problem, as it implies that either $k_3 = 0$ or $k_3 = \frac{1}{2}$.

We are interested in the limiting behavior of $e^\varepsilon[u(t/\varepsilon), \dot{u}(t/\varepsilon)]$, 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 2.3 *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*

$$\|f\|_{\mathcal{S}_d,N} = \sup_{x\in\mathbb{R}^d} \max_{|\alpha|\le N} |\langle x\rangle^N \partial^\alpha f(x)|. \tag{2.18}$$

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

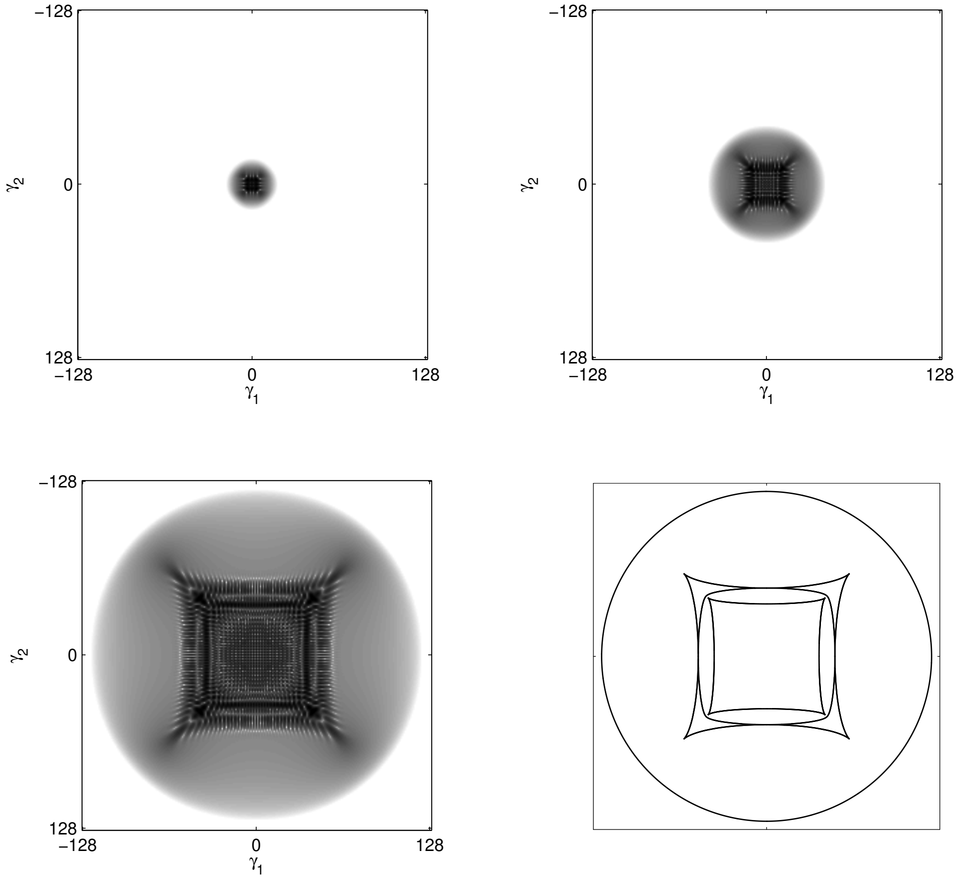

Figure 2: First three panels: Snapshots of the energy density $|\psi_+(\gamma, t)|^2$ in the plane $\gamma_3 = 0$ at $t = 0.1/\varepsilon$, $t = 0.3/\varepsilon$ and $t = 0.95/\varepsilon$, $\varepsilon = \frac{1}{128}$, with initial data and elastic constants as in Fig. 1. The plot is of the logarithm of the density, with all values less than a fixed cut-off shown white. Last panel: Plot of the restriction to the plane $x_3 = 0$ of the singular set of the solution to the transport equation (1.2) with the corresponding macroscopic initial data. As the solution is scale-invariant, no explicit length scale has been denoted.

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 2.4 *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. $\sup_{k,q,|\alpha|\le N} \|\partial^\alpha a(\cdot,k,q)\|_{\mathcal{S},N} < \infty$*, for all* $N \ge 0$*,*
2. $q \mapsto a(x,k,q)$ *is constant for all* $|k|_\infty \ge \frac{1}{4}$ *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* $N \ge 0$

$$\sup_{|q|\ge R, k\in\mathbb{T}^3} \|a(\cdot,k,q) - b(\cdot,k,\tfrac{q}{|q|})\|_{\mathcal{S},N} \to 0, \quad \text{when } R \to \infty. \tag{2.19}$$

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

$$\langle a, W^\varepsilon[\psi]\rangle = \int_{\mathbb{R}^3} \mathrm{d}p \int_{\mathbb{T}^3} \mathrm{d}k\, \overline{\hat{a}(p,k,\tfrac{k}{\varepsilon})}\, \overline{\hat{\psi}(k - \varepsilon\tfrac{p}{2})} \hat{\psi}(k + \varepsilon\tfrac{p}{2}), \tag{2.20}$$

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

$$\hat{a}(p,k,q) = \int_{\mathbb{R}^3} \mathrm{d}x\, \mathrm{e}^{-2\pi \mathrm{i} p\cdot x} a(x,k,q). \tag{2.21}$$

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

$$b \mapsto \langle b, W^{(\varepsilon)}_{cont}[\phi]\rangle = \int_{\mathbb{R}^3\times\mathbb{R}^3} \mathrm{d}p\, \mathrm{d}q\, \overline{\hat{b}(p,q)}\, \overline{\hat{\phi}(q - \varepsilon\tfrac{p}{2})} \hat{\phi}(q + \varepsilon\tfrac{p}{2}) \tag{2.22}$$

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

The test-function space $\mathcal{S}(\mathbb{R}^3, C^{(\infty)}(\mathbb{R}^3))$ used above to define $W_{\rm cont}$ is obtained via the family of seminorms $p_N(b) = \sup_{|\alpha|,|x|,|q|\le N} |\langle x\rangle^N D^\alpha b(x,q)|$ with $b \in C^{(\infty)}(\mathbb{R}^3 \times \mathbb{R}^3)$. This is a Fréchet-space, and $W_{\rm cont}[\phi]$ is a continuous functional on it for any $\phi \in L^2(\mathbb{R}^3)$, as the following estimate reveals:

$$|\langle b, W^{(\varepsilon)}_{\rm cont}[\phi]\rangle| \le \sup_{p,q} |\langle p\rangle^4 \hat{b}(p,q)|\, \|\phi\|^2 \int_{\mathbb{R}^3} {\rm d}p\, \langle p\rangle^{-4}. \tag{2.23}$$

Although $\mathcal{S}_6$ is not dense in this test-function space, it is nevertheless enough to know how $W_{\rm cont}$ acts on it. More precisely, if $W_i = W^{(\varepsilon)}_{\rm cont}[\phi_i]$, $i = 1,2$, and $\langle b, W_1\rangle = \langle b, W_2\rangle$ for all $b \in \mathcal{S}_6$, then $W_1 = W_2$. This follows straightforwardly from an estimate similar to (2.23) using smooth cutoff functions to cut out the infinity of the q-variable. In addition, we will also need the property that, if $b(x,q) = f(x)$, with $f \in \mathcal{S}_3$, then

$$\langle b, W^{(\varepsilon)}_{\rm cont}[\phi]\rangle = \int_{\mathbb{R}^3} {\rm d}x \overline{f(x)} |\phi(x)|^2. \tag{2.24}$$

That is, at least formally, $\int_{\mathbb{R}^3} {\rm d}q\, W^{(\varepsilon)}_{\rm cont}[\phi](x,q) = |\phi(x)|^2$.

In [7] the Wigner transform of a lattice state was defined as a distribution $W^\varepsilon_{\rm latt} \in \mathcal{S}'(\mathbb{R}^3 \times \mathbb{T}^3)$. The above definition is simply a refinement of this definition: formally for any ψ

$$W^\varepsilon(x,k,q) = \delta\big(q - \tfrac{k}{\varepsilon}\big) W^\varepsilon_{\rm latt}(x,k). \tag{2.25}$$

This follows immediately from Eq. (B.6) of [7], after one realizes that if a is an admissible test function, then $(x,k) \mapsto a(x,k,k/\varepsilon)$ belongs to $\mathcal{S}(\mathbb{R}^3 \times \mathbb{T}^3)$ for any $\varepsilon > 0$. This identification immediately allows us to use the results in [7] and to prove 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:

Proposition 2.6 *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 $(u,v) \in X$,*

$$\langle f, e^\varepsilon\rangle = \langle a_f, W^\varepsilon[\psi]\rangle \tag{2.26}$$

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

Proof: By inspection, we find that a is a well-defined test-function, and $\psi \in \ell_2$. Then, by the above mentioned relation, $\langle a_f, W^\varepsilon[\psi]\rangle = \langle J_f, W^\varepsilon_{\rm latt}[\psi]\rangle$ with

$J_f(x,k) = f(x)$. On the other hand, it follows directly from the definition of $W^\varepsilon_{\mathrm{latt}}$ (equation (B.2) in [7]) that

$$\begin{aligned}\langle J_f, W^\varepsilon_{\mathrm{latt}}[\psi]\rangle &= \sum_{\gamma,\gamma'\in\mathbb{Z}^3} \psi(\gamma)\overline{\psi(\gamma')} \int_{\mathbb{T}^3} \mathrm{d}k\, \mathrm{e}^{2\pi \mathrm{i}k\cdot(\gamma'-\gamma)}\overline{f(\varepsilon(\gamma'+\gamma)/2)} \\ &= \sum_{\gamma\in\mathbb{Z}^3} \overline{f(\varepsilon\gamma)}|\psi(\gamma)|^2 = \langle f, e^\varepsilon\rangle. \end{aligned} \tag{2.27}$$

This proves (2.26). □

The above Proposition can be formally summarized by the formula

$$e^\varepsilon(x) = \int_{\mathbb{T}^3} \mathrm{d}k \int_{\mathbb{R}^3} \mathrm{d}q\, W^\varepsilon[\psi](x,k,q) \tag{2.28}$$

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

$$\int_{\mathbb{R}^3\times\mathbb{T}^3\times\mathbb{R}^3} \mathrm{d}x\, \mathrm{d}k\, \mathrm{d}q\, W^\varepsilon[\psi](x,k,q) = \|\psi\|^2_{\ell_2(\mathbb{Z}^3)}. \tag{2.29}$$

As noted earlier, analogous results hold for the L^2-Wigner transform. Let us also remark here that, if the sequence $W^\varepsilon_{\mathrm{latt}}[\psi^\varepsilon](\cdot,\cdot)$ converges, then the limit is given by a non-negative Radon-measure [7]. The results of the next section will show that also $W^\varepsilon_{\mathrm{latt}}[\psi^\varepsilon](\cdot,\cdot/\varepsilon)$ has such a limit property.

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 (2.11) 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 $\varepsilon \to 0$. For each ε in the sequence we assume that there is given an initial data vector $\psi^\varepsilon_0 \in \ell_2(\mathbb{Z}^3)$ such that*

1. $\sup_\varepsilon \|\psi_0^\varepsilon\| < \infty$.

2. The sequence ψ_0^ε is tight on the scale ε^{-1}:

$$\lim_{R\to\infty} \limsup_{\varepsilon\to 0} \sum_{|\gamma|>R/\varepsilon} |\psi_0^\varepsilon(\gamma)|^2 = 0. \tag{3.1}$$

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*

$$\hat{\psi}_t^\varepsilon(k) = \mathrm{e}^{-\mathrm{i}t\omega(k)} \hat{\psi}_0^\varepsilon(k). \tag{3.2}$$

Let also $\mathbb{T}_*^3 = \mathbb{T}^3 \setminus \{0\}$. Then there are positive, bounded Radon measures $\mu_0, \mu_0^{\mathrm{H}}$ 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 relabeled) such that for all admissible test functions a and $t \in \mathbb{R}$,

$$\begin{aligned}\lim_{\varepsilon\to 0} \langle a, W^\varepsilon[\psi_{t/\varepsilon}^\varepsilon]\rangle = &\int_{\mathbb{R}^3\times\mathbb{T}_*^3} \mathrm{d}\mu_t(x,k)\, \overline{b(x,k,\tfrac{k}{|k|})} \\ &+ \int_{\mathbb{R}^3\times S^2} \mathrm{d}\mu_t^{\mathrm{H}}(x,q)\, \overline{b(x,0,q)} + \langle a_0, W_{cont}^{(1)}[\phi_t]\rangle\,,\end{aligned} \tag{3.3}$$

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

$$\hat{\phi}_t(q) := \mathrm{e}^{-\mathrm{i}t\omega_0(q)} \hat{\phi}_0(q), \tag{3.4}$$

$$\int_{\mathbb{R}^3\times\mathbb{T}_*^3} a(x,k)\, \mathrm{d}\mu_t(x,k) := \int_{\mathbb{R}^3\times\mathbb{T}_*^3} a(x + t\tfrac{1}{2\pi}\nabla\omega(k), k)\, \mathrm{d}\mu_0(x,k), \tag{3.5}$$

$$\int_{\mathbb{R}^3\times S^2} b(x,q)\, \mathrm{d}\mu_t^{\mathrm{H}}(x,q) := \int_{\mathbb{R}^3\times S^2} b(x + t\tfrac{1}{2\pi}\nabla\omega_0(q), q)\, \mathrm{d}\mu_0^{\mathrm{H}}(x,q)\,. \tag{3.6}$$

Moreover, for all t the energy equality

$$\lim_{\varepsilon\to 0} \|\psi_0^\varepsilon\|^2 = \mu_t(\mathbb{R}^3 \times \mathbb{T}_*^3) + \mu_t^{\mathrm{H}}(\mathbb{R}^3 \times S^2) + \|\phi_t\|_{L^2(\mathbb{R}^3)}^2 \tag{3.7}$$

holds.

Remark 3.3 *It is immediate from the definition that ϕ, μ and μ^{H} are weak solutions of the set of decoupled linear transport equations (1.2–1.4).*

The proof of Theorem 3.2 also shows that the subsequences which are extracted in the statement of the theorem can be characterized by a simple condition. In particular, the initial state of the wave-equation, ϕ_0, is determined as the weak-$L^2(\mathbb{R}^3)$ limit of the sequence of the functions (ϕ_0^ε) with Fourier-transforms

$$\hat{\phi}_0^\varepsilon(q) = \begin{cases} \varepsilon^{\frac{3}{2}} \hat{\psi}_0^\varepsilon(\varepsilon q) & \text{if } \|q\|_\infty \le \frac{1}{2\varepsilon}, \\ 0 & \text{otherwise.} \end{cases} \tag{3.8}$$

The exact characterization is contained in the following Corollary whose proof will be given in Section 5.

Corollary 3.4 *Let (ψ_0^ε) be a sequence which satisfies Assumption 3.1. Suppose that ϕ_0^ε converges weakly to ϕ_0, and that $\lim_{\varepsilon\to 0}\langle a, W^\varepsilon[\psi_0^\varepsilon]\rangle$ exists for every admissible testfunction a. Then there are unique positive, bounded Radon measures $\mu_0, \mu_0^{\mathrm{H}}$ on $\mathbb{R}^3 \times \mathbb{T}_*^3$ and $\mathbb{R}^3 \times S^2$, respectively, such that for every admissible testfunction a*

$$\begin{aligned} \lim_{\varepsilon\to 0}\langle a, W^\varepsilon[\psi_0^\varepsilon]\rangle = & \int_{\mathbb{R}^3\times\mathbb{T}_*^3} \mathrm{d}\mu_0(x,k)\, \overline{b(x,k,\tfrac{k}{|k|})} \\ & + \int_{\mathbb{R}^3\times S^2} \mathrm{d}\mu_0^{\mathrm{H}}(x,q)\, \overline{b(x,0,q)} + \langle a_0, W^{(1)}_{cont}[\phi_0]\rangle\,, \end{aligned} \tag{3.9}$$

where a_0 and b are defined as in Theorem 3.2. In addition, then (3.3) holds for all $t \in \mathbb{R}$ along the original sequence ε with the initial macroscopic data determined by the triplet $(\mu_0, \mu_0^{\mathrm{H}}, \phi_0)$.

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. Tartar [2] and P. Gérard [3]. The precise nature of the connection of between μ^{H} and H-measures is irrelevant for the purpose of this paper, but for the convenience of the reader we include a brief discussion.

Definition 3.5 (H-measures) *Let $\phi^\varepsilon \in L^2(\mathbb{R}^d)$ be a sequence which converges weakly to 0 as $\varepsilon \to 0$ and let $\nu \in \mathcal{M}_+(\mathbb{R}^d \times S^{d-1})$ be a nonnegative Radon measure. If*

$$\lim_{\varepsilon\to 0}\int_{\mathbb{R}^d} \overline{\mathcal{F}_{x\to q}(a_1\phi^\varepsilon)}\mathcal{F}_{x\to q}(a_2\phi^\varepsilon)\psi(\tfrac{q}{|q|})\,\mathrm{d}k = \int_{\mathbb{R}^d}\int_{S^{d-1}} \mathrm{d}\nu(x,q)\, a_1(x)a_2(x)\psi(q)$$

for all $a_1, a_2 \in C_c^\infty(\mathbb{R}^d)$ and $\psi \in C(S^{d-1})$, then ν is the H-measure generated by the sequence ϕ^ε.

The connection between μ^{H} and H-measures is established by the following

Proposition 3.6 *Let $\phi^\varepsilon \in L^2(\mathbb{R}^d)$ be a tight sequence converging weakly to 0 as $\varepsilon \to \infty$ such that*

$$\lim_{\rho\to 0}\lim_{\varepsilon\to 0}\int_{\varepsilon|k|\geq\rho} \mathrm{d}k\,|\hat{\phi}^\varepsilon(k)|^2 = 0. \tag{3.10}$$

If ϕ^ε generates an H-measure ν as $\varepsilon \to 0$ and a is an admissible testfunction, then

$$\lim_{\varepsilon\to 0}\int_{\mathbb{R}^3}\mathrm{d}x\int_{\mathbb{R}^3}\mathrm{d}q\,\overline{\hat{a}(p,\varepsilon q,q)}\,\overline{\hat{\phi}^\varepsilon(q-\tfrac{p}{2})}\hat{\phi}^\varepsilon(q+\tfrac{p}{2}) = \int_{\mathbb{R}^3\times S^2}\mathrm{d}\nu(x,q)\,a(x,0,q). \tag{3.11}$$

Proof: See [14] □

Note that we will never assume that ϕ^ε converges weakly to 0, hence we cannot define the H-measure associated to ϕ^ε. Moreover, unlike the H-measure ν the measure μ^{H} does not take the contribution of oscillations with wavelength $1/\varepsilon$ into account. For these reasons μ^{H} differs from ν in general.

4 Proof of Theorem 3.2

Let a be an admissible testfunction and consider a fixed $t \in \mathbb{R}$, when we need to inspect the $\varepsilon \to 0$ limit of

$$\langle a, W^\varepsilon[\psi^\varepsilon_{t/\varepsilon}]\rangle = \int_{\mathbb{R}^3}\mathrm{d}p\int_{\mathbb{T}^3}\mathrm{d}k\,\overline{\hat{a}(p,k,\tfrac{k}{\varepsilon})}\,\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}\left(\omega(k+\varepsilon\frac{p}{2})-\omega(k-\varepsilon\frac{p}{2})\right)}\,\overline{\hat{\psi}^\varepsilon_0(k-\varepsilon\tfrac{p}{2})}\,\hat{\psi}^\varepsilon_0(k+\varepsilon\tfrac{p}{2})\,. \tag{4.1}$$

First we identify the function ϕ_0 which contains the contributions of the long-wave excitations. Let $\hat{\phi}^\varepsilon_0$ be defined by (3.8). Since $\limsup_{\varepsilon\to 0}\|\hat{\phi}^\varepsilon_0\|_{L^2} = \limsup_{\varepsilon\to 0}\|\psi^\varepsilon_0\|_{\ell_2}$ is bounded by Assumption 3.1 there exists a subsequence and a function $\phi_0 \in L^2(\mathbb{R}^3)$ such that ϕ^ε_0 converges weakly to ϕ_0 in $L^2(\mathbb{R}^3)$.

Using a localization function χ which will be specified later we split the rhs of (4.1) into three parts and an error term so that the contributions short-, medium- and long-wave excitation can be analyzed separately:

$$\begin{aligned}
I_> &= \int_{\mathbb{R}^3}\mathrm{d}p\int_{\mathbb{T}^3}\mathrm{d}k\,\overline{\hat{a}(p,k,\tfrac{k}{\varepsilon})}\,\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}\left(\omega(k+\varepsilon\frac{p}{2})-\omega(k-\varepsilon\frac{p}{2})\right)}\,\overline{\hat{\psi}^\varepsilon_0(k-\varepsilon\tfrac{p}{2})}\,\hat{\psi}^\varepsilon_0(k+\varepsilon\tfrac{p}{2})(1-\chi),\\
I^{\mathrm{H}}_< &= \int_{\mathbb{R}^3}\mathrm{d}p\int_{\mathbb{T}^3}\mathrm{d}k\,\overline{\hat{a}(p,k,\tfrac{k}{\varepsilon})}\,\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}\left(\omega(k+\varepsilon\frac{p}{2})-\omega(k-\varepsilon\frac{p}{2})\right)}\,\overline{(\hat{\psi}^\varepsilon_0(k-\varepsilon\tfrac{p}{2})-\varepsilon^{-\frac{3}{2}}\hat{\phi}_0(\tfrac{k}{\varepsilon}-\tfrac{p}{2}))}\\
&\qquad\times(\hat{\psi}^\varepsilon_0(k+\varepsilon\tfrac{p}{2})-\varepsilon^{-\frac{3}{2}}\hat{\phi}_0(\tfrac{k}{\varepsilon}+\tfrac{p}{2}))\chi,\\
I^{\mathrm{wv}}_< &= \varepsilon^{-3}\int_{\mathbb{R}^3}\mathrm{d}p\int_{\mathbb{T}^3}\mathrm{d}k\,\overline{\hat{a}(p,k,\tfrac{k}{\varepsilon})}\,\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}\left(\omega(k+\varepsilon\frac{p}{2})-\omega(k-\varepsilon\frac{p}{2})\right)}\,\overline{\hat{\phi}_0(\tfrac{k}{\varepsilon}-\tfrac{p}{2})}\,\hat{\phi}_0(\tfrac{k}{\varepsilon}+\tfrac{p}{2})\chi,\\
R &= I - I_> - I^{\mathrm{H}}_< - I^{\mathrm{wv}}_<.
\end{aligned}$$

The definition of R implies that

$$\langle a, W^\varepsilon[\psi^\varepsilon_{t/\varepsilon}]\rangle = I_> + I^{\mathrm{H}}_< + I^{\mathrm{wv}}_< + R. \tag{4.2}$$

To localize the oscillations in Fourier-space we need smooth cutoff-functions.

Definition 4.1 *Let $f \in C^{(\infty)}(\mathbb{R}, [0,1])$ denote a fixed function which is symmetric, $f(-x) = f(x)$, strictly monotonically decreasing on $[1,2]$, and*

$$f(x) = \begin{cases} 1 & \text{if } |x| \le 1, \\ 0 & \text{if } |x| \ge 2. \end{cases} \tag{4.3}$$

We define further $\varphi \in C^{(\infty)}(\mathbb{R}^3, [0,1])$ by $\varphi(k) = f(|k|)$.

Let $0 < \rho \le \frac{1}{4}$ be arbitrary and set $\chi(k) = \varphi\left(\frac{k_+}{\rho}\right)\varphi\left(\frac{k_-}{\rho}\right)$ where $k_\pm = k \pm \varepsilon\frac{p}{2}$. We will continue to use this shorthand notation, under the tacit assumption that $k_\pm$ is always really a function of k and εp. All four terms depend on ε and ρ, although we do not denote this explicitly in general.

The first term containing $1-\chi$ in (4.2) is zero, if $|k_\pm| \le \rho$, while the remainder is zero, if $|k_+|$ or $|k_-| \ge 2\rho$. Thus the chosen decomposition splits the integration over k and p into "large", "intermediate" and "small" wave numbers. We will demonstrate that the following convergences hold: there is a sequence of ρ and a subsequence of ε such that

$$\lim_{\rho\to 0}\lim_{\varepsilon\to 0} I_> = \int_{\mathbb{R}^3\times\mathbb{T}^3_*} \mathrm{d}\mu_t(x,k)\,\overline{b(x,k,\tfrac{k}{|k|})}, \tag{4.4}$$

$$\lim_{\rho\to 0}\lim_{\varepsilon\to 0} I^{\mathrm{H}}_< = \int_{\mathbb{R}^3\times S^2} \mathrm{d}\mu^{\mathrm{H}}_t(x,q)\,\overline{b(x,0,q)}, \tag{4.5}$$

$$\lim_{\rho\to 0}\limsup_{\varepsilon\to 0} \left| I^{\mathrm{wv}}_< - \langle a_0, W^{(1)}_{\mathrm{cont}}[\phi_t]\rangle \right| = 0, \tag{4.6}$$

$$\lim_{\rho\to 0}\limsup_{\varepsilon\to 0} |R| = 0. \tag{4.7}$$

Clearly, equations (4.4 - 4.7) imply (3.3).

Large wave numbers.

We split $I_>$ further into two parts using

$$\begin{aligned} 1 - \varphi\left(\tfrac{k_-}{\rho}\right)\varphi\left(\tfrac{k_+}{\rho}\right) &= 1 - \varphi\left(\tfrac{k}{\rho}\right)^2 + \left(\varphi\left(\tfrac{k}{\rho}\right) - \varphi\left(\tfrac{k_+}{\rho}\right)\right)\varphi\left(\tfrac{k}{\rho}\right) \\ &\quad + \left(\varphi\left(\tfrac{k}{\rho}\right) - \varphi\left(\tfrac{k_-}{\rho}\right)\right)\varphi\left(\tfrac{k_+}{\rho}\right). \end{aligned} \tag{4.8}$$

Letting $h_\rho(k) = 1 - \varphi\left(\frac{k}{\rho}\right)^2$, which is a smooth function, the integral then becomes $I_> = I^1_> + R_1$, where

$$I^1_> = \int_{\mathbb{R}^3} \mathrm{d}p \int_{\mathbb{T}^3} \mathrm{d}k\, \overline{\hat{a}(p,k,\tfrac{k}{\varepsilon})} h_\rho(k)\, \mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}\left(\omega(k+\varepsilon\frac{p}{2}) - \omega(k-\varepsilon\frac{p}{2})\right)}\, \overline{\hat{\psi}^\varepsilon_0(k-\varepsilon\tfrac{p}{2})}\, \hat{\psi}^\varepsilon_0(k+\varepsilon\tfrac{p}{2})\,. \tag{4.9}$$

The remainder R_1 can be estimated using $|\varphi| \le 1$ and

$$\varphi\left(\tfrac{k_\pm}{\rho}\right) - \varphi\left(\tfrac{k}{\rho}\right) = \pm\tfrac{\varepsilon}{2\rho} \int_0^1 \mathrm{d}s\, p \cdot \nabla\varphi\Big(\tfrac{1}{\rho}(k \pm s\tfrac{\varepsilon}{2}p)\Big), \tag{4.10}$$

which yield the bound, with a universal constant C,

$$|R_1| \le C\tfrac{\varepsilon}{\rho} \sup_{k,q} \|a(\cdot,k,q)\|_{\mathcal{S},d+2} \|\hat{\psi}^\varepsilon_0\|^2 \|\nabla\varphi\|_\infty. \tag{4.11}$$

Therefore, there is a constant c' such that $|R_1| \le c'\varepsilon/\rho$ and thus $R_1 \to 0$ when $\varepsilon \to 0$ for all ρ.

We then consider $I^1_>$. The presence of h_ρ guarantees that the integrand is zero unless $|k| \ge \rho$. Thus we can change $\hat{a}(p,k,k/\varepsilon)$ to $\hat{b}(p,k,k/|k|)$ in the integrand with an error R_2 bounded by

$$|R_2| \le C \sup_{k,|q|\ge\rho/\varepsilon} \|a(\cdot,k,q) - b(\cdot,k,\tfrac{q}{|q|})\|_{\mathcal{S},d+1} \|\hat{\psi}^\varepsilon_0\|^2 \tag{4.12}$$

where C is a universal constant. Therefore, the assumptions imply that $R_2 \to 0$ when $\varepsilon \to 0$ for all ρ. On the other hand, for $|k| \ge \rho$ and $|p| < \rho/\varepsilon$, inequality (A.2) implies that

$$\left|\tfrac{1}{\varepsilon}\left(\omega(k+\varepsilon\tfrac{p}{2}) - \omega(k-\varepsilon\tfrac{p}{2})\right) - p\cdot\omega(k)\right| \le C_3\varepsilon\tfrac{|p|^2}{|k|} \le C_3\tfrac{\varepsilon}{\rho}|p|^2. \tag{4.13}$$

Therefore, using the estimate $|\mathrm{e}^{\mathrm{i}x} - \mathrm{e}^{\mathrm{i}y}| \le \min(|x-y|, 2)$, valid for all $x, y \in \mathbb{R}$, we find that we can further change the t-dependent exponential in the integrand to $\mathrm{e}^{-\mathrm{i}tp\cdot\nabla\omega(k)}$ with a error R_3 bounded by

$$|R_3| \le C \sup_{k,q} \|b(\cdot,k,q)\|_{\mathcal{S},d+3} \left(\tfrac{\varepsilon}{\rho}|t| + \int_{|p|\ge\rho/\varepsilon} \mathrm{d}p \langle p\rangle^{-d-3}\right) \tag{4.14}$$

for some constant C. Therefore, also $\lim_{\varepsilon\to 0} R_3 = 0$ for all ρ. In summary, $I^1_> = I^2_> + R_2 + R_3$, where R_2, R_3 are negligible, and

$$I^2_> = I^2_>(\varepsilon,\rho) = \int_{\mathbb{R}^3} \mathrm{d}p \int_{\mathbb{T}^3} \mathrm{d}k\, \overline{\hat{b}(p,k,\tfrac{k}{|k|})} h_\rho(k) \mathrm{e}^{-\mathrm{i}tp\cdot\nabla\omega(k)}\, \overline{\hat{\psi}^\varepsilon_0(k-\varepsilon\tfrac{p}{2})}\, \hat{\psi}^\varepsilon_0(k+\varepsilon\tfrac{p}{2})\,. \tag{4.15}$$

Let us for a moment consider the lattice Wigner transform $W^\varepsilon_{\text{latt}}$ of ψ^ε_0, as defined in [7]. As pointed out after Definition 2.5, then for any testfunction $f \in \mathcal{S}(\mathbb{R}^3\times\mathbb{T}^3)$, we get an admissible test-function by the formula $a_f(x,k,q) = f(x,k)$ and then also $\langle f, W^\varepsilon_{\text{latt}}\rangle = \langle a_f, W^\varepsilon[\psi^\varepsilon_0]\rangle$. Since ψ^ε_0 is a norm-bounded sequence, the sequence $W^\varepsilon_{\text{latt}}$ is weak-$*$ bounded, and thus there is $W^0_{\text{latt}} \in \mathcal{S}'(\mathbb{R}^3 \times \mathbb{T}^3)$ and a subsequence along which $W^\varepsilon_{\text{latt}} \overset{*}{\rightharpoonup} W^0_{\text{latt}}$.

Since the sequence ψ^ε_0 is by assumption also tight on the scale ε^{-1}, we can then apply Theorems B.4 and B.5 of [7] and conclude that W^0_{latt} is given by a positive, bounded Radon measure μ on $\mathbb{R}^3 \times \mathbb{T}^3$ such that for all *continuous* functions $f \in C(\mathbb{T}^3)$ and $p \in \mathbb{R}^3$,

$$\lim_{\varepsilon\to 0}\int_{\mathbb{T}^3} \mathrm{d}k\, f(k)\overline{\hat{\psi}^\varepsilon_0(k-\varepsilon\tfrac{p}{2})}\,\hat{\psi}^\varepsilon_0(k+\varepsilon\tfrac{p}{2}) = \int_{\mathbb{R}^3\times\mathbb{T}^3} \mathrm{d}\mu(x,k)\, f(k)\mathrm{e}^{-2\pi \mathrm{i} p\cdot x}. \tag{4.16}$$

As $\nabla\omega(k)$ and $k/|k|$ are continuous apart from $k = 0$, the function $k \mapsto h_\rho(k)\overline{\hat{b}(p,k,\frac{k}{|k|})}\mathrm{e}^{-\mathrm{i}tp\cdot\nabla\omega(k)}$ is everywhere continuous for all $\rho > 0$ and $p \in \mathbb{R}^3$. Therefore, by the dominated convergence theorem, for all ρ we find

$$\begin{aligned}\lim_{\varepsilon\to 0} I^2_> &= \int_{\mathbb{R}^3}\mathrm{d}p \int_{\mathbb{R}^3\times\mathbb{T}^3} \mathrm{d}\mu(x,k)\,\overline{\hat{b}(p,k,\tfrac{k}{|k|})}h_\rho(k)\mathrm{e}^{-2\pi\mathrm{i}p\cdot(x+t\nabla\omega(k)(2\pi)^{-1})}\\ &= \int_{\mathbb{R}^3\times\mathbb{T}^3} \mathrm{d}\mu(x,k)\, h_\rho(k)\overline{b(x+t\tfrac{1}{2\pi}\nabla\omega(k),k,\tfrac{k}{|k|})}\,. \end{aligned}\tag{4.17}$$

When $\rho \to 0$, the integrand approaches pointwise $\overline{b(x+t\frac{1}{2\pi}\nabla\omega(k),k,\frac{k}{|k|})}$ apart from $k = 0$, when the limit is 0. Therefore, by the dominated convergence theorem

$$\begin{aligned}&\lim_{\rho\to 0}\int_{\mathbb{R}^3\times\mathbb{T}^3} \mathrm{d}\mu(x,k)\, h_\rho(k)\overline{b(x+t\tfrac{1}{2\pi}\nabla\omega(k),k,\tfrac{k}{|k|})}\\ &\quad= \int_{\mathbb{R}^3\times\mathbb{T}^3_*} \mathrm{d}\mu(x,k)\,\overline{b(x+t\tfrac{1}{2\pi}\nabla\omega(k),k,\tfrac{k}{|k|})} = \int_{\mathbb{R}^3\times\mathbb{T}^3_*}\mathrm{d}\mu_t(x,k)\,\overline{b(x,k,\tfrac{k}{|k|})}. \end{aligned}\tag{4.18}$$

where we have defined the bounded, positive Radon measure μ_t using $\mu_0 = \mu|_{\mathbb{R}^3\times\mathbb{T}^3_*}$ in the formula (3.5). We have shown that equation (4.4) holds.

Small wave-numbers and the remainder

After a change of variables $q = \frac{k}{\varepsilon}$ one obtains that

$$I^{\text{wv}}_< = \int_{\mathbb{R}^3}\mathrm{d}p\int_{\mathbb{T}^3/\varepsilon}\mathrm{d}q\,\overline{\hat{a}(p,\varepsilon q,q)}\,\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}(\omega(\varepsilon q_+)-\omega(\varepsilon q_-))}\,\overline{\hat{\phi}_0(q_-)}\,\hat{\phi}_0(q_+)\,\varphi(\tfrac{\varepsilon q_+}{\rho})\,\varphi(\tfrac{\varepsilon q_-}{\rho})\,, \tag{4.19}$$

where $q_\pm = q \pm \frac{p}{2}$. We can immediately replace the integration region for the q-integral by $\mathbb{R}^3$. To see this, note that the integrand is zero, unless $|q \pm \frac{p}{2}| \leq \frac{2\rho}{\varepsilon}$ for both signs. Since $2q = q_+ + q_-$, this can happen only if also $|q| \leq \frac{2\rho}{\varepsilon} \leq \frac{1}{2\varepsilon}$, which implies that the integrand is zero if $\|q\|_\infty > \frac{1}{2\varepsilon}$.

However, if $|\varepsilon q| \leq 2\rho$, then

$$|\hat{a}(p, \varepsilon q, q) - \hat{a}(p, 0, q)| \leq \sup_k |\nabla_k \hat{a}(p, k, q)|\, 2\rho, \tag{4.20}$$

and thus we can replace in the integrand the function $\hat{a}(p, \varepsilon q, q)$ by $\hat{a}(p, 0, q)$, with an error R_1' which is bounded by $C\rho$ with a constant C independent of ε and ρ. Thus we only need to consider the integral

$$I_<^1 = \int_{\mathbb{R}^3} \mathrm{d}p \int_{\mathbb{R}^3} \mathrm{d}q\, \overline{\hat{a}(p,0,q)}\, \mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}(\omega(\varepsilon q_+) - \omega(\varepsilon q_-))}\, \overline{F^{\varepsilon,\rho}(q_-)} F^{\varepsilon,\rho}(q_+), \tag{4.21}$$

where $F^{\varepsilon,\rho}(q) = \hat{\phi}_0(q)\varphi(\frac{\varepsilon q}{\rho})$. Next we use estimate (A.3), which implies that, if now $|p| \leq \frac{1}{2\varepsilon}$, then

$$\left|\tfrac{1}{\varepsilon}(\omega(\varepsilon q_+) - \omega(\varepsilon q_-)) - \omega_0(q_+) + \omega_0(q_-)\right| \leq C_4 \varepsilon |p|\, |q|\,. \tag{4.22}$$

Following the same argument as earlier, we can then conclude that the t-dependent exponential can be changed to $\mathrm{e}^{-\mathrm{i}t(\omega_0(q_+) - \omega_0(q_-))}$, with an error R_2' which satisfies the estimate

$$|R_2'| \leq C \sup_q \|a(\cdot, 0, q)\|_{\mathcal{S}, d+2} \left(|t|\rho + \int_{|p| \geq (2\varepsilon)^{-1}} \mathrm{d}p\, \langle p \rangle^{-d-2} \right). \tag{4.23}$$

Thus $\lim_{\rho\to 0} \limsup_{\varepsilon \to 0} |R_2'| = 0$ for all t. Finally, we need to change $F^{\varepsilon,\rho}$ to ϕ_0, with an error R_3' which can be bounded by $C\|F^{\varepsilon,\rho} - \phi_0\|$. Since the bound goes to zero when $\varepsilon \to 0$ and

$$I_<^{\mathrm{wv}} = \int_{\mathbb{R}^3} \mathrm{d}p \int_{\mathbb{R}^3} \mathrm{d}q\, \overline{\hat{a}(p,0,q)}\, \mathrm{e}^{-\mathrm{i}t(\omega_0(q_+) - \omega_0(q_-))}\, \overline{\hat{\phi}_0(q_-)} \hat{\phi}_0(q_+) + R_1' + R_2' + R_3', \tag{4.24}$$

equation (4.6) has been established.

Similar estimates can be employed to demonstrate the vanishing of the remainder, equation (4.7). From the definition of R we get

$$\begin{aligned} R = & \int_{\mathbb{R}^3} \mathrm{d}p \int_{\mathbb{T}^3/\varepsilon} \mathrm{d}q\, \overline{\hat{a}(p, \varepsilon q, q)}\, \mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}(\omega(\varepsilon q_+) - \omega(\varepsilon q_-))}\, \overline{\left(\hat{\phi}_0^\varepsilon(q_-) - \hat{\phi}_0(q_-)\right)}\, \hat{\phi}_0(q_+) \\ & \times \varphi(\tfrac{\varepsilon q_+}{\rho})\, \varphi(\tfrac{\varepsilon q_-}{\rho}) + \int_{\mathbb{R}^3} \mathrm{d}p \int_{\mathbb{T}^3/\varepsilon} \mathrm{d}q\, \overline{\hat{a}(p, \varepsilon q, q)}\, \mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}(\omega(\varepsilon q_+) - \omega(\varepsilon q_-))} \\ & \times \overline{\hat{\phi}_0(q_-)} \left(\hat{\phi}_0^\varepsilon(q_+) - \hat{\phi}_0(q_+)\right) \varphi(\tfrac{\varepsilon q_+}{\rho})\, \varphi(\tfrac{\varepsilon q_-}{\rho}). \end{aligned} \tag{4.25}$$

We then apply the above estimates to remove the ε-dependence from all other terms in the integrands, apart from the differences $\hat{\phi}_0^\varepsilon - \hat{\phi}_0$. The error has a bound which vanishes when $\rho \to 0$. We are then left with

$$\int_{\mathbb{R}^3} \mathrm{d}\eta \int_{\mathbb{R}^3} \mathrm{d}\xi\, \overline{\hat{a}(\eta-\xi, 0, \tfrac{1}{2}(\eta+\xi))}\, \mathrm{e}^{-\mathrm{i}t(\omega_0(\eta)-\omega_0(\xi))}\, \overline{\left(\hat{\phi}_0^\varepsilon(\xi) - \hat{\phi}_0(\xi)\right)}\, \hat{\phi}_0(\eta)$$
$$+ \int_{\mathbb{R}^3} \mathrm{d}\eta \int_{\mathbb{R}^3} \mathrm{d}\xi\, \overline{\hat{a}(\eta-\xi, 0, \tfrac{1}{2}(\eta+\xi))}\, \mathrm{e}^{-\mathrm{i}t(\omega_0(\eta)-\omega_0(\xi))}\, \overline{\hat{\phi}_0(\xi)}\left(\hat{\phi}_0^\varepsilon(\eta) - \hat{\phi}_0(\eta)\right), \tag{4.26}$$

which vanishes as $\varepsilon \to 0$, since ϕ_0^ε converges weakly to ϕ_0. This establishes (4.7).

Intermediate wave-numbers

Changing coordinates $q = \frac{k}{\varepsilon}$ yields that

$$I_<^{\mathrm{H}} = \int_{\mathbb{R}^3} \mathrm{d}p \int_{\mathbb{T}^3/\varepsilon} \mathrm{d}q\, \overline{\hat{a}(p, \varepsilon q, q)}\, \mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}(\omega(\varepsilon q_+)-\omega(\varepsilon q_-))}\, \overline{\hat{f}^{\varepsilon,\rho}(q_-)}\hat{f}^{\varepsilon,\rho}(q_+)\,,$$

where $\hat{f}^{\varepsilon,\rho}(q) = \varphi\left(\frac{\varepsilon q}{\rho}\right)(\hat{\phi}_0^\varepsilon(q) - \hat{\phi}_0(q))$. Let $M > 0$ be arbitrary. We split off the values $|p| > M$ from the integral defining $I_<^3$. The difference $R_4' = R_4'(\varepsilon, \rho, M)$ can be bounded by $C\int_{|p|>M} \mathrm{d}p\, \langle p\rangle^{-d-1}$ and thus $\lim_{M\to\infty} \sup_{\rho,\varepsilon} |R_4'| = 0$. We divide the remaining integral over $|p| \le M$ further into two parts using the identity

$$1 = \tilde{\varphi}\left(\tfrac{q_-}{2M}\right)\tilde{\varphi}\left(\tfrac{q_+}{2M}\right) + 1 - \tilde{\varphi}\left(\tfrac{q_-}{2M}\right)\tilde{\varphi}\left(\tfrac{q_+}{2M}\right), \tag{4.27}$$

where $\tilde{\varphi} = 1 - \varphi$. If $|q| \ge 5M$, then $|q_\pm| \ge 4M$ and the second part is zero. It can be checked by inspection that the sequence $(f^{\varepsilon,\rho})_\varepsilon$ is bounded and tight, and it has a weak limit zero. Of these properties only the tightness is non-obvious, but this can also be easily deduced from the formula

$$f^{\varepsilon,\rho}(x) = \rho^3\varepsilon^{-3/2}\sum_{\gamma\in\mathbb{Z}^3} \psi_0^\varepsilon(\gamma)\hat{\varphi}(\rho(\gamma - \tfrac{1}{\varepsilon}x)) - \int_{\mathbb{R}^3} \mathrm{d}y\, \phi_0(x + \tfrac{\varepsilon}{\rho}y)\hat{\varphi}(y). \tag{4.28}$$

Therefore, by Lemma A.2, $\lim_{\varepsilon\to0} \|\hat{f}^{\varepsilon,\rho}\|_{L^2(B_{6M})} = 0$ for all M, ρ. This implies that the contribution of the second term, denoted by R_5', satisfies $\lim_{\varepsilon\to0} |R_5'| = 0$ for all M, ρ.

We are thus a left with

$$I_<^4 = \int_{|p|\le M} \mathrm{d}p \int_{\mathbb{R}^3} \mathrm{d}q\, \overline{\hat{a}(p, 0, q)}\, \mathrm{e}^{-\mathrm{i}t(\omega_0(q_+)-\omega_0(q_-))}\, \overline{\hat{g}^{\varepsilon,\rho,M}(q_-)}\hat{g}^{\varepsilon,\rho,M}(q_+), \tag{4.29}$$

where $\hat{g}^{\varepsilon,\rho,M}(q) = \tilde{\varphi}\left(\frac{q}{2M}\right) \hat{f}^{\varepsilon,\rho}(q)$ and the integrand can be non-zero only for $|q| \geq M$. We thus only need to consider $|q| \geq M$ and $|p| \leq M$. First we replace in the integrand $\hat{a}(p, 0, q)$ by $\hat{b}(p, 0, \hat{q})$, $\hat{q} = \frac{q}{|q|}$, with an error R'_6 which is bounded by

$$|R'_6| \leq C \sup_{k,|q|\geq M} \|a(\cdot, k, q) - b(\cdot, k, \tfrac{q}{|q|})\|_{\mathcal{S},d+1} \tag{4.30}$$

for some constant C. Then we change $\mathrm{e}^{-\mathrm{i}t(\omega_0(q_+)-\omega_0(q_-))}$ to $\mathrm{e}^{-\mathrm{i}tp\cdot\nabla\omega_0(\hat{q})}$ with an error, R'_7 which can be estimated using (A.4) which proves that there is a constant C such that

$$|R'_7| \leq C\tfrac{|t|}{M} \sup_{k,q} \|b(\cdot, k, q)\|_{\mathcal{S},d+3}. \tag{4.31}$$

Therefore, $I^4_< = I^5_< + R'_6 + R'_7$, where

$$I^5_< = \int_{|p|\leq M} \mathrm{d}p \int_{\mathbb{R}^3} \mathrm{d}q\, \overline{\hat{b}(p, 0, \hat{q})}\, \mathrm{e}^{-\mathrm{i}tp\cdot\nabla\omega_0(\hat{q})}\, \overline{\hat{g}^{\varepsilon,\rho,M}(q_-)} \hat{g}^{\varepsilon,\rho,M}(q_+). \tag{4.32}$$

and $\lim_{M\to\infty} \sup_{\rho,\varepsilon} |R'_6 + R'_7| = 0$ for all t.

Let

$$b_t(x, \hat{q}) = b(x + t\tfrac{1}{2\pi}\nabla\omega_0(\hat{q}), 0, \hat{q}). \tag{4.33}$$

Then $b_t \in \mathcal{S}(\mathbb{R}^3 \times S^2)$, and it has an extension to a function $J_t \in \mathcal{S}_6$, i.e., there is J_t such that $J_t(x, q) = b_t(x, q)$ for all $|q| = 1$. On the other hand, then

$$I^5_< = \int_{|p|\leq M} \mathrm{d}p \int_{\mathbb{R}^3} \mathrm{d}q\, \overline{\hat{b}_t(p, \hat{q})}\, \overline{\hat{g}^{\varepsilon,\rho,M}(q_-)} \hat{g}^{\varepsilon,\rho,M}(q_+) = \langle J_t, \Lambda^{\varepsilon,\rho,M}\rangle \tag{4.34}$$

where $\Lambda^{\varepsilon,\rho,M} \in \mathcal{S}'_6$ denotes the distribution

$$J \mapsto \langle J, \Lambda^{\varepsilon,\rho,M}\rangle = \int_{|p|\leq M} \mathrm{d}p \int_{\mathbb{R}^3} \mathrm{d}q\, \overline{\hat{J}(p, \hat{q})}\, \overline{\hat{g}^{\varepsilon,\rho,M}(q_-)} \hat{g}^{\varepsilon,\rho,M}(q_+). \tag{4.35}$$

Clearly, each $\Lambda^{\varepsilon,\rho,M}$ has support in $\mathbb{R}^3 \times S^2$, and there is a constant C such that for all J, ε, ρ, M

$$|\langle J, \Lambda^{\varepsilon,\rho,M}\rangle| \leq C\|\hat{g}^{\varepsilon,\rho,M}\|^2 \|J\|_{\mathcal{S},d+1}. \tag{4.36}$$

However, since we have $\|\hat{g}^{\varepsilon,\rho,M}\| \leq \|\hat{f}^{\varepsilon,\rho}\|$, where $\|\hat{f}^{\varepsilon,\rho}\|$ is bounded in ε, Banach-Alaoglu theorem implies that the family $(\Lambda^{\varepsilon,\rho,M})_{\varepsilon,\rho,M}$ belongs to a weak-$*$ sequentially compact set. Therefore, for every ρ, M there is a subsequence of (ε) and $\Lambda^{\rho,M}$ such that $\Lambda^{\varepsilon,\rho,M} \overset{*}{\rightharpoonup} \Lambda^{\rho,M}$ along this subsequence. In addition, for every ρ

there is Λ^ρ and a sequence of integers M such that $\Lambda^{\rho,M} \overset{*}{\rightharpoonup} \Lambda^\rho$ along this sequence. Finally, there is $\Lambda \in \mathcal{S}_6'$ and a sequence of integers $N \geq 4$ such that for $\rho = \frac{1}{N}$, $\Lambda^\rho \overset{*}{\rightharpoonup} \Lambda$.

All of the above distributions clearly must have support on $\mathbb{R}^3 \times S^2$. We will soon prove that, in addition, for all $f \in \mathcal{S}_6$ and ρ

$$\langle |f|^2, \Lambda^\rho \rangle \geq 0. \tag{4.37}$$

This implies then that also $\langle |f|^2, \Lambda \rangle \geq 0$. Therefore, by the Bochner-Schwartz theorem, there is a positive Radon measure $\mu^{\rm H}$ on $\mathbb{R}^6$ such that for all testfunctions J, $\langle J, \Lambda \rangle = \int \mu^{\rm H}({\rm d}x, {\rm d}k)\, J(x,k)$. Since also $\mu^{\rm H}$ must have support on $\mathbb{R}^3 \times S^2$, we can thus identify it with a positive Radon measure $\mu_0^{\rm H}$ on $\mathbb{R}^3 \times S^2$. By considering testfunctions $J(x,k) = {\rm e}^{-\delta^2 x^2}$ in the limit $\delta \to 0$, it is also clear that $\mu_0^{\rm H}$ must be bounded. We then define the positive, bounded Radon measures $\mu_t^{\rm H}$, $t \in \mathbb{R}$, by the formula (3.6). It follows from the construction of $\mu_t^{\rm H}$ that equation (4.5) holds along the above sequences ρ, ε.

The main missing ingredient is provided by the following Lemma

Lemma 4.2 *For $p, q \in \mathbb{R}^3$, let us denote $q_\pm = q \pm \frac{p}{2}$, $\hat{q}_\pm = q_\pm/|q_\pm|$, and $\hat{q} = q/|q|$. There is a constant C such that for all $q, q' \in \mathbb{R}^3$, and $f \in \mathcal{S}_6$*

$$\left| \int_{\mathbb{R}^3} {\rm d}x\, {\rm e}^{-2\pi {\rm i} p\cdot x} \overline{f(x,q')} f(x,q) \right| \leq C \langle p \rangle^{-d-1} \|f\|^2_{\mathcal{S},d+1}. \tag{4.38}$$

If, in addition, $|q| \geq M$ and $|p| \leq M$, then also

$$\left| \mathcal{F}_{x\to p}(|f|^2)(p,\hat{q}) - \int_{\mathbb{R}^3} {\rm d}x\, {\rm e}^{-2\pi {\rm i} p\cdot x} \overline{f(x,\hat{q}_+)} f(x,\hat{q}_-) \right| \leq \tfrac{1}{M} C \langle p \rangle^{-d-1} \|f\|^2_{\mathcal{S},d+2}. \tag{4.39}$$

Before proving the lemma we demonstrate that it implies inequality (4.37). Let then $f \in \mathcal{S}_6$ be arbitrary. Define $q_\pm, \hat{q}_\pm$ as in Lemma 4.2, except that let here also $\hat{0} = 0$, and let

$$I^{\varepsilon,\rho,M,f} = \int_{\mathbb{R}^3} {\rm d}p \int_{\mathbb{R}^3} {\rm d}q \left[\int_{\mathbb{R}^3} {\rm d}x\, {\rm e}^{2\pi {\rm i} p\cdot x} f(x,\hat{q}_+) \overline{f(x,\hat{q}_-)} \right] \overline{\hat{g}^{\varepsilon,\rho,M}(q_-)} \hat{g}^{\varepsilon,\rho,M}(q_+). \tag{4.40}$$

Note that this integral is well-defined by (4.38). Then, by estimate (4.39) and uniform boundedness of $g^{\varepsilon,\rho,M}$, there is a constant c such that

$$\left| \langle |f|^2, \Lambda^{\varepsilon,\rho,M} \rangle - I^{\varepsilon,\rho,M,f} \right| \leq c \|f\|^2_{\mathcal{S},d+2} \left(\int_{|p|\geq M} {\rm d}p\, \langle p \rangle^{-d-1} + \tfrac{1}{M} \right). \tag{4.41}$$

On the other hand, always $I^{\varepsilon,\rho,M,f} \geq 0$. To see this, consider first the case when $g^{\varepsilon,\rho,R} \in \mathcal{S}$. Then $\hat{g}^{\varepsilon,\rho,R} \in \mathcal{S}$, and by changing variables from (q,p) to (q_+,q_-) in (4.40), and then using Fubini's theorem to reorder the integrals, we find that

$$I^{\varepsilon,\rho,M,f} = \int_{\mathbb{R}^3} \mathrm{d}x |G(x)|^2, \qquad \text{with } G(x) = \int_{\mathbb{R}^3} \mathrm{d}q\, \mathrm{e}^{2\pi \mathrm{i} q\cdot x} f(x,\hat{q}) \hat{g}^{\varepsilon,\rho,R}(q) \in L^2. \tag{4.42}$$

Since $I^{\varepsilon,\rho,M,f}$ depends L^2-continuously on $g^{\varepsilon,\rho,R}$ this implies that also for general $g^{\varepsilon,\rho,R} \in L^2$ we have $I^{\varepsilon,\rho,M,f} \geq 0$. Since the right hand side of (4.41) vanishes if first $\varepsilon \to 0$ and then $M \to \infty$, we must thus also have $\langle |f|^2, \Lambda^\rho\rangle \geq 0$. This proves (4.37).

The only remaining task is to prove Lemma 4.2. Consider first (4.38). If $|p| \leq 1$, we have trivially a bound

$$\int_{\mathbb{R}^3} \mathrm{d}x\, |f(x,q')|\, |f(x,q)| \leq \|f\|^2_{\mathcal{S},d+1} \int_{\mathbb{R}^3} \mathrm{d}x\, \langle x\rangle^{-2d-2} \leq c\|f\|^2_{\mathcal{S},d+1}. \tag{4.43}$$

If $|p| \geq 1$, we perform N partial integrations in the direction of p, that is in the direction $\hat{p} = \frac{p}{|p|}$, yielding

$$\int_{\mathbb{R}^3} \mathrm{d}x\, \mathrm{e}^{-2\pi \mathrm{i} p\cdot x} \overline{f(x,q')} f(x,q) = \tfrac{1}{(2\pi \mathrm{i}|p|)^N} \int_{\mathbb{R}^3} \mathrm{d}x \mathrm{e}^{-2\pi \mathrm{i} p\cdot x} (\hat{p}\cdot\nabla)^N \left(\overline{f(x,q')} f(x,q)\right). \tag{4.44}$$

By the Leibniz rule,

$$(\hat{p}\cdot\nabla)^N \left(\overline{f(x,q')} f(x,q)\right) = \sum_{n=0}^{N} \binom{N}{n} (\hat{p}\cdot\nabla)^n \overline{f(x,q')} (\hat{p}\cdot\nabla)^{N-n} f(x,q) \tag{4.45}$$

which is bounded by $c'_N \langle x\rangle^{-N} \|f\|^2_{\mathcal{S},N}$. Choosing $N = d+1$ then yields (4.38) for some constant. Adjusting the constant C so that the bound is true also for $|p| \leq 1$ proves that (4.38) is valid.

To prove (4.39), consider q,p as required in the Lemma. Let $q(s) = q + \frac{s}{2}p$, when $|q(s)| \geq |q|/2 > 0$ for all $|s| \leq 1$, and $\hat{q}(s)$ is thus well-defined and smooth. Therefore, for any $g \in \mathcal{S}_6$ and $s_0 \in [-1,1]$,

$$\begin{aligned} g(x,\hat{q}(s_0)) - g(x,\hat{q}) &= \int_0^{s_0} \mathrm{d}s\, \tfrac{\mathrm{d}}{\mathrm{d}s} g(x,\hat{q}(s)) \\ &= \int_0^{s_0} \mathrm{d}s\, \left(\tfrac{1}{2|q(s)|} p - \tfrac{p\cdot\hat{q}(s)}{2|q(s)|} \hat{q}(s)\right) \cdot \nabla_q g(x,q)\big|_{q=\hat{q}(s)} \end{aligned} \tag{4.46}$$

implying

$$|g(x,\hat{q}_\pm) - g(x,\hat{q})| \le 2\tfrac{|p|}{|q|} \sup_{|q|=1} |\nabla_q g(x,q)|. \tag{4.47}$$

Also for all $g_1, g_2 \in \mathcal{S}_6$,

$$\begin{aligned}&\overline{g_1(x,\hat{q})} g_2(x,\hat{q}) - \overline{g_1(x,\hat{q}_-)} g_2(x,\hat{q}_+)\\ &\quad = \overline{(g_1(x,\hat{q}) - g_1(x,\hat{q}_-))} g_2(x,\hat{q}) + \overline{g_1(x,\hat{q}_-)} \left(g_2(x,\hat{q}) - g_2(x,\hat{q}_+)\right).\end{aligned} \tag{4.48}$$

Following the steps made in the first part of the proof, and replacing the earlier estimates with the above more accurate ones when necessary, we can conclude that the constant C can be adjusted so that for these values of q, p also (4.39) holds. This completes the proof of equation (4.5).

Energy equality

The energy equality (3.7) follows by considering a sequence of testfunctions $a^\delta = \mathrm{e}^{-\delta^2 x^2}$ and taking $\delta \to 0$. To see this, first note that the right hand side of (3.7) is clearly independent of t, and thus it is enough to consider $t = 0$. Thanks to equation (2.26) and to the tightness of the sequence ψ_0^ε we obtain for this particular testfunction that

$$\lim_{\delta\to 0}\lim_{\varepsilon\to 0} \langle a^\delta, W^\varepsilon[\psi_0^\varepsilon]\rangle = \lim_{\delta\to 0}\lim_{\varepsilon\to 0} \langle a^\delta, e^\varepsilon\rangle = \lim_{\varepsilon\to 0} \|\psi_0^\varepsilon\|^2$$

Equation (3.3) implies that

$$\lim_{\varepsilon\to 0} \langle a^\delta, W^\varepsilon[\psi_0^\varepsilon]\rangle = \int_{\mathbb{R}^3} \mathrm{d}x\, a^\delta |\phi_0(x)|^2 + \int_{\mathbb{R}^3}\int_{\mathbb{T}^3} a^\delta(x)\, \mathrm{d}\mu_0(x,k) + \int_{\mathbb{R}^3}\int_{S^2} a^\delta(x)\, \mathrm{d}\mu_0^{\mathrm{H}}(x,k).$$

Sending δ to 0 yields that

$$\lim_{\varepsilon\to 0} \|\hat{\psi}_0^\varepsilon\|^2 = \|\phi_0\|^2_{L^2(\mathbb{R}^3)} + \mu_0(\mathbb{R}^3 \times \mathbb{T}^3) + \mu_0^{\mathrm{H}}(\mathbb{R}^3 \times S^2),$$

and the energy equality has been established. This finishes the proof of Theorem 3.2.

5 Proof of Corollary 3.4

Let I_0 denote the original sequence of ε, and consider an arbitrary subsequence I of I_0. Since $(\psi_0^\varepsilon)_{\varepsilon\in I}$ then also satisfies Assumption 3.1, we can conclude from Theorem 3.2 that for every I there is a subsequence I' such that (3.3) holds for all t

with the initial conditions given by some triplet $(\mu_I, \mu_I^{\mathrm{H}}, \phi_I)$. From the construction of the subsequence in the proof of Theorem 3.2, we know that ϕ_I can be chosen as the weak limit of ϕ_0^ε along the subsequence I'. The first assumption thus implies that we can always choose $\phi_I = \phi_0$. Let us also denote $\mu_0 = \mu_{I_0}$ and $\mu_0^{\mathrm{H}} = \mu_{I_0}^{\mathrm{H}}$, and to prove the stated uniqueness, we will prove that $\mu_I = \mu_0$ and $\mu_I^{\mathrm{H}} = \mu_0^{\mathrm{H}}$ for all I.

Consider first an arbitrary $\tilde{a} \in C_c^{(\infty)}(\mathbb{R}^3 \times \mathbb{T}_*^3)$. Let $a(x,k,q) = \tilde{a}(x,k)$ for $k \neq 0$ and define $a(x,0,q) = 0$. Then a is an admissible test-function with $a_0 = 0 = b(k,0,q)$ and for any subsequence I we thus obtain, using the second assumption

$$\int_{\mathbb{R}^3\times\mathbb{T}_*^3} \mathrm{d}\mu_I(x,k)\, \overline{\tilde{a}(x,k)} = \lim_{\varepsilon\in I} \langle a, W^\varepsilon[\psi_0^\varepsilon]\rangle = \int_{\mathbb{R}^3\times\mathbb{T}_*^3} \mathrm{d}\mu_0(x,k)\, \overline{\tilde{a}(x,k)}. \tag{5.1}$$

Such $\tilde{a}$ are dense in $C_c(\mathbb{R}^3 \times \mathbb{T}_*^3)$, and thus $\mu_I = \mu_0$ on $\mathbb{R}^3 \times \mathbb{T}_*^3$.

Consider then an arbitrary $b \in C_c^{(\infty)}(\mathbb{R} \times S^2)$. Let φ be a smooth cutoff function as in Definition 4.1, and define $a(x,k,q) = b(x, q/|q|)\,(1-\varphi(2q))$. Then a is an admissible testfunction and indeed $\lim_{R\to\infty} a(x,k,Rq) = b(x,q)$ for all $|q| = 1$. By the already proven results we then find that for any subsequence I

$$\begin{aligned}\int_{\mathbb{R}^3\times S^2} \mathrm{d}\mu_I^{\mathrm{H}}(x,q)\, \overline{b(x,q)} &= \lim_{\varepsilon\to 0} \langle a, W^\varepsilon[\psi_0^\varepsilon]\rangle - \int_{\mathbb{R}^3\times\mathbb{T}_*^3} \mathrm{d}\mu_0(x,k)\, \overline{b(x, \tfrac{k}{|k|})} \\ &- \langle a_0, W_{\mathrm{cont}}^{(1)}[\phi_0]\rangle = \int_{\mathbb{R}^3\times S^2} \mathrm{d}\mu_0^{\mathrm{H}}(x,q)\, \overline{b(x,q)}\,. \end{aligned}\tag{5.2}$$

Therefore, also $\mu_I^{\mathrm{H}} = \mu_0^{\mathrm{H}}$, which concludes the uniqueness part of the proof of the Corollary.

Finally, define for $t \neq 0$ the triplet $(\mu_t, \mu_t^{\mathrm{H}}, \phi_t)$ using $(\mu_0, \mu_0^{\mathrm{H}}, \phi_0)$ as the initial data. By the above proved uniqueness, for any subsequence I, (3.3) holds along the subsubsequence I'. As the right hand side is thus independent of I, this proves that the limit also holds along the original sequence I_0. This completes the proof of the Corollary.

A Technicalities

The proof of Theorem 3.2 relies on two simple lemmas which are provided here. The first lemma summarizes several properties of regular acoustic dispersion relations.

Lemma A.1 *Let ω be a regular acoustic dispersion relation and recall the definitions of λ, A_0 and ω_0. Then the following assertions are true.*

1. $\omega \in C^{(3)}(\mathbb{T}^3 \setminus \{0\}, \mathbb{R})$.

2. $\nabla\lambda(0) = 0$ *and* $A_0 > 0$.

3. *There are constants* $C_1, C_2 > 0$ *such that for all* $|k|_\infty \le \frac{3}{4}$,
$$\omega(k) \ge C_1|k|, \qquad |\nabla\lambda(k)| \le C_2|k|\,. \tag{A.1}$$
In addition, $\|\nabla\omega\|_\infty < \infty$.

4. *There is* C_3 *such that, if* $\varepsilon > 0$, $p \in \mathbb{R}^3$, *and* $|k|_\infty \le \frac{1}{2}$, *with* $|k| > \varepsilon|p|$, *then*
$$|\omega(k + \tfrac{1}{2}\varepsilon p) - \omega(k - \tfrac{1}{2}\varepsilon p) - \varepsilon p \cdot \nabla\omega(k)| \le C_3\varepsilon^2 \tfrac{|p|^2}{|k|}. \tag{A.2}$$

5. *There is* C_4 *such that, if* $\varepsilon > 0$ *and* $p, q \in \mathbb{R}^3$ *with* $|p|, \|q\|_\infty \le \frac{1}{2}\varepsilon^{-1}$, *then for* $q_\pm = q \pm \frac{1}{2}p$,
$$|\omega(\varepsilon q_+) - \omega(\varepsilon q_-) - \omega_0(\varepsilon q_+) + \omega_0(\varepsilon q_-)| \le C_4\varepsilon^2|p|\,|q|\,. \tag{A.3}$$

6. *There is* C_5 *such that, if* $p, q \in \mathbb{R}^3$ *with* $q \neq 0$ *and* $|p| \le |q|$, *then for* $q_\pm = q \pm \frac{1}{2}p$,
$$|\omega_0(q_+) - \omega_0(q_-) - p \cdot \nabla\omega_0(\tfrac{q}{|q|})| \le C_5 \tfrac{|p|^2}{|q|}. \tag{A.4}$$

Proof: The first item is obvious, and the second one follows from the assumptions, since 0 is a minimum. The second inequality in (A.1) follows by using item 2 and $\|D^2\lambda\|_\infty < \infty$, when by Taylor expansion $|\nabla\lambda(k)| \le C_2|k|$ for all $k \in \mathbb{R}$. To prove the first inequality, we first note that, by continuity, also $\|D^3\lambda\|_\infty < \infty$. Thus there is c' such that for all $k \in \mathbb{R}^3$
$$|\lambda(k) - \lambda_0(k)| \le c'|k|^3, \tag{A.5}$$
where $\lambda_0(k) = \frac{1}{2}k \cdot A_0 k$. Since $A_0 > 0$, there is $c > 0$ such that $\lambda_0(k) \ge c^2k^2$ for all k. Thus there is $\delta' > 0$ such that for all $|k| < \delta'$, we have $|1 - \lambda(k)/\lambda_0(k)| \le \frac{3}{4}$, and for these k therefore also $\omega(k) = \sqrt{\lambda(k) - \lambda_0(k) + \lambda_0(k)} \ge \frac{1}{2}\sqrt{\lambda_0(k)} \ge \frac{c}{2}|k|$. Since λ has no zeroes in the complement set, the constant can then be adjusted so that (A.1) holds for all k with $|k|_\infty \le \frac{3}{4}$.

We still need to prove the third property, boundedness of $\nabla\omega$. For later use, let us, more generally, consider a non-negative $f \in C^{(2)}(\mathbb{R}^3)$, $q \in \mathbb{R}^3$, and k such that $f(k) \neq 0$. Then we have
$$(q \cdot \nabla)\sqrt{f(k)} = \frac{1}{2\sqrt{f(k)}} q \cdot \nabla f(k), \tag{A.6}$$
$$(q \cdot \nabla)^2\sqrt{f(k)} = -\frac{1}{4f(k)^{3/2}}(q \cdot \nabla f(k))^2 + \frac{1}{2\sqrt{f(k)}}(q \cdot \nabla)^2 f(k). \tag{A.7}$$

This implies that there is a constant C such that for all $q \in \mathbb{R}^3$ and $k \neq 0$, with $|k|_\infty \leq \frac{3}{4}$,

$$|q \cdot \nabla\omega(k)|, |q \cdot \nabla\omega_0(k)| \leq C|q|\,, \tag{A.8}$$

$$|(q \cdot \nabla)^2\omega(k)|, |(q \cdot \nabla)^2\omega_0(k)| \leq C\frac{|q|^2}{|k|}\,. \tag{A.9}$$

In particular, by periodicity therefore $\|\nabla\omega\|_\infty < \infty$.

To prove item 4, consider k, p, ε as in the claim, and define a function $f(s) = \omega(k_+) - \omega(k_-)$ with $k_\pm = k \pm s\frac{1}{2}p$ and $s \in [-\varepsilon, \varepsilon]$. Then $|k_\pm|_\infty \leq \frac{3}{2}|k|_\infty$ and $|k_\pm| \geq |k| - \varepsilon\frac{1}{2}p \geq \frac{1}{2}|k| > 0$, and thus f belongs to $C^{(3)}$. In particular, $f(0) = 0$, $f'(0) = p \cdot \nabla\omega(k)$, and

$$\begin{aligned} f''(s) = \frac{1}{2}\Big[&\frac{1}{\omega(k_+)}\Big(\frac{p}{2}\cdot\nabla\Big)^2\lambda(k_+) - \frac{1}{\omega(k_-)}\Big(\frac{p}{2}\cdot\nabla\Big)^2\lambda(k_-) \\ &- \frac{1}{2\omega(k_+)^3}\Big(\frac{p}{2}\cdot\nabla\lambda(k_+)\Big)^2 + \frac{1}{2\omega(k_-)^3}\Big(\frac{p}{2}\cdot\nabla\lambda(k_-)\Big)^2\Big]. \end{aligned} \tag{A.10}$$

Using item 3, we find that there is C such that this is uniformly bounded by $C|p|^2/|k|$. Then a Taylor expansion at the origin proves item 4.

Since for all $k \neq 0$,

$$\omega(k) - \omega_0(k) = \sqrt{\lambda(k)} - \sqrt{\lambda_0(k)} = \frac{\lambda(k) - \lambda_0(k)}{\sqrt{\lambda(k)} + \sqrt{\lambda_0(k)}}\,, \tag{A.11}$$

and then also

$$\begin{aligned} &q \cdot \nabla(\omega(k) - \omega_0(k)) \\ &\quad = \frac{q \cdot \nabla\lambda(k) - q \cdot \nabla\lambda_0(k)}{\omega(k) + \omega_0(k)} - (\lambda(k) - \lambda_0(k))\frac{q \cdot \nabla\omega(k) + q \cdot \nabla\omega_0(k)}{(\omega(k) + \omega_0(k))^2}\,. \end{aligned} \tag{A.12}$$

By Taylor expansion at the origin, we find that there is C' such that for all $q \in \mathbb{R}^3$,

$$|\lambda(k) - \lambda_0(k)| \leq C'|k|^3, \qquad |q \cdot \nabla\lambda(k) - q \cdot \nabla\lambda_0(k)| \leq C'|k|^2|q|, \tag{A.13}$$

$$|(q \cdot \nabla)^2\lambda(k) - (q \cdot \nabla)^2\lambda_0(k)| \leq C'|k|\,|q|^2\,. \tag{A.14}$$

Thus there is also C such that for all $q \in \mathbb{R}^3$, and $|k|_\infty \leq \frac{3}{4}$, with $k \neq 0$,

$$|q \cdot \nabla(\omega(k) - \omega_0(k))| \leq C|k|\,|q|\,, \qquad |(q \cdot \nabla)^2(\omega(k) - \omega_0(k))| \leq C|q|^2. \tag{A.15}$$

Let us then consider q, p, ε satisfying the assumptions made in the final item. Since then $\|\varepsilon q_\pm\|_\infty \leq \frac{3}{4}$, we can apply the previous estimates. If $p = 0$, then $q_- = q_+$ and the bound in (A.3) is trivially valid for any C_4. Consider thus

$p \neq 0$, and assume first that p is not proportional to q. Since then the line segment $[0,1] \ni s \mapsto \varepsilon q + s\varepsilon p/2$ does not pass through the origin, the function $s \mapsto \omega(\varepsilon q + s\varepsilon p/2) - \omega_0(\varepsilon q + s\varepsilon p/2)$ is in $C^{(3)}([0,1])$. We make a Taylor expansion of this function at $s = 0$, yielding

$$\omega(\varepsilon q + \varepsilon \tfrac{p}{2}) - \omega_0(\varepsilon q + \varepsilon \tfrac{p}{2}) = \omega(\varepsilon q) - \omega_0(\varepsilon q) + \varepsilon \tfrac{p}{2} \cdot (\nabla\omega(\varepsilon q) - \nabla\omega_0(\varepsilon q)) + R\,. \tag{A.16}$$

Here (A.15) implies $|R| \leq C\varepsilon^2|p|^2$, since

$$R = \int_0^1 \mathrm{d}s\,(1-s)\Big(\varepsilon\tfrac{p}{2}\cdot\nabla\Big)^2 (\omega(\varepsilon q + s\varepsilon\tfrac{p}{2}) - \omega_0(\varepsilon q + s\varepsilon\tfrac{p}{2}))\,. \tag{A.17}$$

This proves that (A.3) holds in this case for some constant C_4. In final remaining case $p \propto q$, we choose a direction u orthogonal to q, and use the previous estimate with $p + \delta u$ instead of p for an arbitrary $0 < \delta \leq 1$. Since the left hand side of (A.3) is continuous in δ, the bound must then hold also for $\delta = 0$, proving the validity of the estimate also in this case.

To prove (A.4), we use the fact that by assumption $|q_\pm| \geq \frac{1}{2}|q| > 0$, and thus denoting $\hat{q} = q/|q|$, we get

$$\omega_0(q_+) - \omega_0(q_-) = |q| \left(\omega_0(\hat{q} + \frac{p}{2|q|}) - \omega_0(\hat{q} - \frac{p}{2|q|})\right) = p\cdot\nabla\omega_0(\hat{q}) + R \tag{A.18}$$

where $|R| \leq C|p|^2/|q|$. We have thus completed the proof of the Lemma. □

The second lemma recalls a well-known fact in Fourier analysis: the Fourier transform of a bounded and tight sequence of L^2 functions converges strongly on compact sets. For the convenience of the reader we give a proof.

Lemma A.2 *Let $f^\varepsilon \in L^2(\mathbb{R}^d)$ be a bounded and tight sequence of functions such that $f^\varepsilon \rightharpoonup 0$ as $\varepsilon \to 0$. Then*

$$\lim_{\varepsilon\to 0} \|\hat{f}^\varepsilon\|_{L^2(\Omega)} = 0. \tag{A.19}$$

for every $\Omega \subset \mathbb{R}^d$ with a finite measure.

Proof: Choose an arbitrary number $\beta > 0$. By tightness of f^ε there exists a number $R_\beta > 0$ such that

$$\limsup_{\varepsilon\to 0} \int_{|x|\geq R_\beta} \mathrm{d}x\,|f^\varepsilon(x)|^2 \leq \beta^2. \tag{A.20}$$

Define now

$$f^{\varepsilon,\beta}(x) = \begin{cases} f^{\varepsilon}(x) & \text{if } |x| \le R_\beta, \\ 0 & \text{else.} \end{cases} \tag{A.21}$$

By the boundedness of $f^{\varepsilon,\beta}$ in $L^2(\mathbb{R}^d)$ there exists g^β and a subsequence (ε') such that $f^{\varepsilon',\beta} \rightharpoonup g^\beta$ in $L^2(\mathbb{R}^d)$ as $\varepsilon' \to 0$. Estimate (A.20) implies that $\limsup_{\varepsilon\to 0} \|f^\varepsilon - f^{\varepsilon,\beta}\|^2_{L^2(\mathbb{R}^3)} \le \beta^2$. Since also $f^\varepsilon \rightharpoonup 0$, we have

$$\|g^\beta\|^2 = \lim_{\varepsilon'} |\langle g^\beta, f^{\varepsilon',\beta}\rangle| \le \|g^\beta\| \limsup_{\varepsilon\to 0} \|f^\varepsilon - f^{\varepsilon,\beta}\| \tag{A.22}$$

and, therefore, $\|g^\beta\|_{L^2(\mathbb{R}^d)} \le \beta$.

Since g^β has support in a ball of radius R_β, also $g_1^\beta(x) = -2\pi \mathrm{i} x g^\beta(x) \in L^2(\mathbb{R}^d)$. Therefore, $\hat{g}^\beta \in H^1(\mathbb{R}^d)$, and $\nabla \hat{g}^\beta = \hat{g}_1^\beta$. Similarly, also $\hat{f}^{\varepsilon,\beta} \in H^1(\mathbb{R}^d)$ and it is straightforward to check that $\nabla \hat{f}^{\varepsilon',\beta} \rightharpoonup \nabla \hat{g}^\beta$ in L^2. Since Ω is assumed to be a set of finite measure, we have then $\lim_{\varepsilon'\to 0} \|\hat{f}^{\varepsilon',\beta} - \hat{f}^\beta\|_{L^2(\Omega)} = 0$ (for a proof, see for instance Theorem 8.6. in [15]). This result yields the following estimate for the original sequence $\hat{f}^\varepsilon$:

$$\begin{aligned} &\limsup_{\varepsilon'\to 0} \|\hat{f}^{\varepsilon'}\|_{L^2(\Omega)} \\ &\quad \le \limsup_{\varepsilon'\to 0} \|\hat{f}^{\varepsilon'} - \hat{f}^{\varepsilon',\beta}\|_{L^2(\Omega)} + \limsup_{\varepsilon'\to 0} \|\hat{f}^{\varepsilon',\beta} - \hat{f}^\beta\|_{L^2(\Omega)} + \|\hat{f}^\beta\|_{L^2(\Omega)} \le 2\beta. \end{aligned}$$

Since β can be arbitrarily small, we obtain that there must be a subsequence ε'' such that $\lim_{\varepsilon''\to 0} \|\hat{f}^{\varepsilon''}\|_{L^2(\Omega)} = 0$.

Since the assumptions on the sequence f^ε are preserved for subsequences, we can consider an arbitrary subsequence and apply the above result to it. Then we can conclude that for every subsequence there is a subsubsequence along which (A.19) holds. This implies that the limit (A.19) actually holds also along the original sequence. □

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