Lecture Notes on Kinetic Models for Waves in Random Media: the Vienna version

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Chapter 1

Random geometric optics I: short time asymptotics

1.1 Rays without the wave equation – the formal theory

We consider in this section the very basic ray theory in a random emdium without any references to the wave equation – this material is based on the classical paper by J.B. Keller [38].

1.1.1 Perturbative ray theory

Fermat's principle postulates that light goes from point A to B as fast as possible. Such fastest path is called a ray connecting points A and B. The medium in which light is propagating is described in terms of the local speed of light $c(x)$. Let Γ be a ray from A to B, then

$$\int_{\Gamma} \frac{dl}{c(X)} = \inf_{\gamma} \int_{\gamma} \frac{dl}{c(X)}.$$

Here the infimum is taken over all continuous curves γ connecting A and B. Equivalently, parameterizing γ by $x(t) = (x_1(t), x_2(t), x_3(t))$, $0 \leq t \leq 1$, we need to minimize the functional

$$\int_0^1 n(x(s))|\dot{x}(s)|ds \tag{1.1}$$

with $n(x) = c_0/c(x)$ being the refractive index. Here $c_0 = \mathrm{const}$ is a reference speed that is some typical speed of propagation in the medium. This will be sometimes formalized by requiring that $n(x)$ does not deviate from $n_0 = 1$ too much but that is not required a priori. The Euler-Lagrange equations for the functional (1.1) are

$$\frac{d}{dt}\frac{\partial F}{\partial \dot{x}_j} - \frac{\partial F}{\partial x_j} = 0$$

with $F(x, \dot{x}) = n(x(s))|\dot{x}(s)|$. This may be rewritten as

$$\frac{d}{dt}\left(\frac{n\dot{x}_j}{|\dot{x}|}\right) - |\dot{x}|\frac{\partial n}{\partial x_j} = 0.$$

Let θ be the unit vector along the ray: $\theta = \dot{x}/|\dot{x}|$, then the above equations take the form

$$\frac{d}{dt}(n\theta) - |\dot{x}|\nabla n = 0. \tag{1.2}$$

A convenient way to parameterize the path is to use the arclength parameter l along the curve $x(t)$, then $dl = |\dot{x}|dt$ and we obtain the ray equation

$$\frac{d}{dl}(n\theta) - \nabla n = 0. \tag{1.3}$$

It may be also written as

$$\frac{d}{dl}\left(n\frac{dx}{dl}\right) - \nabla n = 0. \tag{1.4}$$

Equation (1.4) should be supplemented by the initial conditions:

$$x(0) = 0,\ \frac{dx}{dl}(0) = \theta_0,\ |\theta_0| = 1. \tag{1.5}$$

This is the fundamental equation of the ray optics that describes the geometry of rays connecting different points in an inhomogeneous medium. Observe that if $n(x) = \text{const}$, then $d\theta/dl = 0$ and the direction θ doesn't change along the ray. Therefore rays in a homogeneous medium are straight lines. Similarly, if the medium is layered, that is, the refraction variable depends only on the variable x_1: $n = n(x_1)$ then rays that point initially in the direction of x_1 are straight lines – this also follows immediately from (1.5) with $n = n(x_1)$ and the initial data $\theta_0 = e_1$.

Let us now consider the case when index of refraction deviates slightly from unity:

$$n(x) = 1 + \varepsilon\mu(x).$$

We assume that ε is a small parameter: $\varepsilon \ll 1$ and employ the formal perturbation theory to determine the perturbed path $x(l,\varepsilon)$ expanding it as

$$x(l,\varepsilon) = x_0(l) + \varepsilon x_1(l) + \varepsilon^2 x_2(l) + \dots$$

We insert this expansion in the ray equations (1.4) and get in the order ε^0:

$$\frac{d^2x_0}{dl^2} = 0$$

so that $x_0(l) = l\theta_0$. The first order correction in ε is determined by the equation

$$\frac{d^2x_1}{dl^2} = \nabla\mu(x_0) - \left(\frac{dx_0}{dl}\cdot\nabla\mu(x_0)\right)\frac{dx_0}{dl} \tag{1.6}$$

with the initial condition $x_1(0) = dx_1/dl(0) = 0$. The right side of (1.6) is the component of $\nabla\mu$ normal to θ_0. We will denote it by $\nabla_\perp\mu$ below. The solution of (1.6) is given by

$$x_1(l) = \int_0^l (l-s)\nabla_\perp\mu(\theta_0 s)ds. \tag{1.7}$$

It follows that $(x_1 \cdot x_0) = 0$ – this is typical for a first order correction in the perturbation series. A straightforward computation using the fact that x_1 is perpendicular to θ_0 shows that the second order term x_2 satisfies a lengthy equation

$$\frac{d^2x_2}{dl^2} = (x_1\cdot\nabla_\perp)\nabla_\perp\mu(x_0) - \frac{1}{2}\nabla_\perp\mu^2 - \left(\frac{dx_1}{dl}\cdot\nabla_\perp\mu(x_0)\right)\frac{dx_0}{dl} - \left(\frac{dx_0}{dl}\cdot\nabla\mu(x_0)\right)\frac{dx_1}{dl} \tag{1.8}$$

with the initial data $x_2(0) = dx_2/dl(0) = 0$. Its solution is given by

$$x_2(l) = \int\limits_0^l ds(l-s)\left[(x_1(s)\cdot\nabla_\perp)\nabla_\perp\mu(s\theta_0) - \frac{1}{2}\nabla_\perp\mu^2(s\theta_0) - \theta_0\int\limits_0^s(\nabla_\perp\mu(s\theta_0)\cdot\nabla_\perp\mu(\tau\theta_0))d\tau\right.$$
$$\left. - (\theta_0\cdot\nabla\mu(s\theta_0))\int\limits_0^s\nabla_\perp\mu(\tau\theta_0)d\tau\right]. \tag{1.9}$$

1.1.2 Weakly perturbed rays in a random medium

Expressions for the corrections x_1 and x_2 obtained above are valid for any perturbation $\mu(x)$. Let us now specify that $\mu(x)$ is a random function that has mean zero and its statistics is spatially homogeneous and isotropic:

$$\langle\mu(x)\rangle = 0, \quad \langle\mu(x)\mu(y)\rangle = R(|x-y|), \quad \langle\mu(p)\mu(q)\rangle = (2\pi)^n\hat{R}(p)\delta(p+q). \tag{1.10}$$

The correlation function $R(|x|)$ is smooth, has maximum at zero, is a decreasing and rapidly decaying function of $|x|$, and the power spectrum $\hat{R}(p)$ is its Fourier transform.

The mean ray position

Let us first compute the average ray position using expressions obtained in Section 1.1. The first order correction has mean zero: $\langle x_1\rangle = 0$ so that

$$\langle x(l)\rangle = l\theta_0 + \varepsilon^2\langle x_2\rangle + O(\varepsilon^3).$$

The expected value of of x_2 may be computed explicitly using expression (1.9).

$$\langle x(l)\rangle = l\theta_0 - \varepsilon^2\theta_0\int\limits_0^l ds(l-s)\int\limits_0^s d\tau\,\langle(\nabla_\perp\mu(s\theta_0)\cdot\nabla_\perp\mu(\tau\theta_0))\rangle + O(\varepsilon^3).$$

A rather lengthy computation leads to

$$\langle x(l)\rangle = \theta_0\left(l + \frac{(n-1)\varepsilon^2}{2}\int\limits_0^l(l-r)^2\frac{R'(r)}{r}\right)dr + O(\varepsilon^3). \tag{1.11}$$

We see that the mean location of the endpoint of a ray of length l which starts from the origin is in the direction θ_0. However, its distance from the origin is less than when the ray is not perturbed since $R'(r) < 0$. Physically this is expected because the presence of the inhomogeneities slows down the propagation as light no longer propagates along a straight line.

The mean square fluctuations

Let us denote by ρ deviation of the ray from the straight line $x = \theta_0 l$: $\rho(l) = x_\varepsilon(l) - \theta_0 l$. Then we have

$$\langle\rho(l)^2\rangle = \varepsilon^2\langle x_1^2\rangle + o(\varepsilon^2).$$

We set now space dimension $n = 3$ and compute the above average in the same manner as before:

$$\langle x_1^2(l)\rangle = -\int_0^l R'(r)\left[\frac{2r^2}{3} - 2l^2 + \frac{4l^3}{3r}\right]dr.$$

For l large compared to the correlation length a the last term above dominates so that

$$\langle \rho(l)^2 \rangle \approx -\frac{4\varepsilon^2 l^3}{3} \int_0^\infty \frac{R'(r)}{r} dr + O(\varepsilon^3) \text{ for } l \gg a. \tag{1.12}$$

Similarly one may compute the average deviation α of the direction of the ray from the mean direction θ_0:

$$\langle \alpha^2(l) \rangle = \left\langle \left(\frac{dx}{dl} - \theta_0 \right)^2 \right\rangle = 4\varepsilon^2 \left[R(l) - R(0) - l \int_0^l \frac{R'(r)}{r} dr \right] + O(\varepsilon^3).$$

For l large compared to the correlation length a this becomes

$$\left\langle \alpha^2(l) \right\rangle \approx -4\varepsilon^2 l \int_0^\infty \frac{R'(r)}{r} dr + O(\varepsilon^3) \text{ for } l \gg a. \tag{1.13}$$

Expressions (1.12) and (1.13) may be written as

$$\left\langle \rho^2(l) \right\rangle \approx \frac{1}{3} D l^3 + O(\varepsilon^3) \tag{1.14}$$

and

$$\left\langle \alpha^2(l) \right\rangle \approx Dl + O(\varepsilon^3). \tag{1.15}$$

Here we introduced the ray diffusion coefficient

$$D = -4\varepsilon^2 \int_0^\infty \frac{R'(r)}{r} dr. \tag{1.16}$$

Expressions (1.14) and (1.15) may also be obtained by treating the ray direction $\alpha(l)$ as a Brownian motion with the diffusion coefficient D and $\rho(l)$ as its time integral:

$$d\alpha = \sqrt{D} dB, \quad d\rho = \alpha(l) dl.$$

Here $B(l)$ is the standard Brownian motion. Then a simple calculation shows that

$$\langle \rho(l)^2 \rangle = D \left\langle \int_0^l \int_0^l B(s) B(s') ds' ds \right\rangle = 2D \left\langle \int_0^l \int_0^{s'} B(s) B(s') ds ds' \right\rangle = 2D \int_0^l \int_0^s s ds ds' = \frac{Dl^3}{3}.$$

However, the a priori assumption that ray direction may be described in terms of such Markov process is not easy to justify unlike the derivation presented above. Nevertheless, this concept is important and the ray direction does behave as a Markov process in a certain asymptotic limit that we will discuss in the rest of this chapter.

1.1.3 Random Liouville equations: small time formal asymptotics

Reduction to a time-dependent stochastic accelaration problem

In order to make the above discussion of the diffusive ray behavior somewhat more careful (albeit not yet rigorous) we consider the Liouville equations in phase space

$$\frac{\partial \phi}{\partial t} + c(x)\hat{k} \cdot \nabla_x \phi - |k| \nabla c(x) \cdot \nabla_k \phi = 0 \tag{1.17}$$

with the speed $c(x) = 1 + \delta\mu(x)$. Here $\mu(x)$ is a spatially homogeneous random process with the correlation function as in (1.10). Then (1.17) becomes

$$\frac{\partial \phi}{\partial t} + [1 + \delta\mu(x)]\hat{k} \cdot \nabla_x \phi - \delta \nabla\mu(x)|k| \cdot \nabla_k \phi = 0 \tag{1.18}$$

and solutions are close to those of

$$\frac{\partial \phi}{\partial t} + \hat{k} \cdot \nabla_x \phi = 0 \tag{1.19}$$

for times $t = O(1)$. In order to see some more interesting phenomena, in particular, the ray diffusion mentioned above, we look at the bicharacteristics of (1.18):

$$\dot{X}(t) = -(1 + \delta\mu(X))\hat{K}(t), \quad \dot{K}(t) = \delta\nabla\mu(X(t))|K(t)|, \quad X(0) = x_0, \quad K(0) = k_0. \tag{1.20}$$

It is convenient to re-write this system in terms of the unit vector $\hat{K}(t) = K(t)/|K(t)|$ as

$$\frac{dX(t)}{dt} = -(1 + \delta\mu(X))\hat{K}(t), \quad \frac{d\hat{K}(t)}{dt} = \delta[\nabla\mu(X(t)) - (\hat{K} \cdot \nabla\mu(X))\hat{K}]. \tag{1.21}$$

Let us introduce the rescaled quantities $Y(t) = X(t) + \hat{k}_0 t - x_0$ and $P = (\hat{K}(t) - \hat{k}_0)/\delta^\alpha$ with $\alpha > 0$ to be chosen. Naively, one would expect that over a time T the direction $\hat{K}$ deviates from its initial value by δT which means that the trajectory deviates from $X_0(t) = -\hat{k}_0 t$ by $T \cdot \delta T = \delta T^2$. Hence we would expect that $Y(t)$ behaves non-trivially on the time scale $O(\delta^{-1/2})$. We will see, however, that because the random perturbation has mean zero, the effect takes place on a longer time scale.

In the slow time variable $t' = \delta^\alpha t$ with $\alpha = 2/3$ so that $\delta^{1-2\alpha} = \delta^{-\alpha/2}$ and setting $\varepsilon = \delta^{1/3}$ we get:

$$\begin{aligned} \frac{d\tilde{Y}(t')}{dt'} &= -\tilde{P}(t') - \varepsilon\mu\left(x_0 - \frac{k_0 t'}{\varepsilon^2} + \tilde{Y}(t')\right)\hat{k}_0 - \varepsilon^3\mu\left(x_0 - \frac{k_0 t'}{\varepsilon^2} + \tilde{Y}(t')\right)\tilde{P}(t'), \\ \frac{d\tilde{P}(t')}{dt'} &= \frac{1}{\varepsilon}\left[I - (\hat{k}_0 + \varepsilon^2\tilde{P}(t')) \otimes (\hat{k}_0 + \varepsilon^2\tilde{P}(t'))\right]\nabla\mu\left(x_0 - \frac{k_0 t'}{\varepsilon^2} + \tilde{Y}(t')\right). \end{aligned} \tag{1.22}$$

Let us keep only the leading order terms in (1.22). The analysis that we perform on the simplified system may be applied to the full problem as well albeit at the price of somewhat lengthier calculations that we are not willing to pay at the moment. Then (1.22) becomes (we now drop both the primes and tildes)

$$\begin{aligned} &\dot{Y}(t) = -P(t), \quad Y(0) = 0 \\ &\dot{P}(t) = \frac{1}{\varepsilon}\left[I - (\hat{k}_0 \otimes \hat{k}_0)\right]\nabla\mu\left(x_0 - \frac{k_0 t}{\varepsilon^2} + Y(t)\right), \quad P(0) = 0, \end{aligned} \tag{1.23}$$

which is the system we will study. The vector $\dot{P}(t)$ is orthogonal to k_0 for all $t \geq 0$ – hence so is $P(t)$ and thus $(Y(t) \cdot k_0) = 0$ for all $t \geq 0$ as well. This is a familiar phenomenon for the perturbation theory – the first order correction is orthogonal to the mean dispalcement. It is convenient to set $x_0 = 0$ and choose the coordinate axes so that $k_0 = e_n$, the unit vector in the direction of x_n. Then $Y(t) = (Y_1, \ldots, Y_{n-1}, 0)$, $P(t) = (P_1, \ldots, P_{n-1}, 0)$ and (1.23) may be re-written as the following system for $Z(t) = (Y_1(t), \ldots, Y_{n-1}(t))$ and $Q(t) = (P_1(t), \ldots, P_{n-1}(t))$:

$$\begin{aligned} &\dot{Z}(t) = -Q(t), \quad Z(0) = 0 \\ &\dot{Q}(t) = \frac{1}{\varepsilon}G\left(\frac{t}{\varepsilon^2}, Z(t)\right), \quad Q(0) = 0, \end{aligned} \tag{1.24}$$

where

$$G(x_n, x') = \left(\frac{\partial \mu(x', -x_n)}{\partial x_1}, \dots, \frac{\partial \mu(x', -x_n)}{\partial x_{n-1}}\right), \quad x' \in \mathbb{R}^{n-1}.$$

This system also happens to describe the motion of a classical particle moving in a random time-dependent force field $\varepsilon^{-1} G(t/\varepsilon^2, x)$ and is called the stochastic acceleration problem in this context.

A very formal derivation of the diffusive limit

We now describe a very formal but quick and effective way to obtain the limit of (1.24) as $\varepsilon \to 0$. Let us write the corresponding Liouville equation

$$\frac{\partial \phi}{\partial t} + q \cdot \nabla_z \phi - \frac{1}{\varepsilon} G\left(\frac{t}{\varepsilon^2}, z\right) \cdot \nabla_q \phi = 0. \tag{1.25}$$

Instead of assuming that the random function $G(s, x)$ is as in (1.24) we make a more general hypothesis that for each $x \in \mathbb{R}^n$ the process $G(s, x) \in \mathbb{R}^n$ is stationary in time with the two-point correlation tensor

$$R_{ml}(s, x) = \langle G_m(t, x) G_p(t + s, x) \rangle.$$

We seek the solution as a multiple time scale expansion

$$\phi = \phi_0(t, z) + \varepsilon \phi_1(t, \tau, z) + \varepsilon^2 \phi_2(t, \tau, z) + \dots, \quad \tau = t/\varepsilon^2. \tag{1.26}$$

As usual in such expansions in random media we assume that the leading order term is independent of the fast variable and is deterministic. The higher order corrections are assumed to be stationary in the fast variable τ. These assumptions are typically very hard to justify rigorously – nevertheless they often provide the correct answer. We insert the expansion into (1.25) and obtain in the leading order $O(1/\varepsilon)$

$$\frac{\partial \phi_1}{\partial \tau} = G(\tau, z) \cdot \nabla_q \phi_0(t, z)$$

so that

$$\phi_1(t, z, \tau) = \chi(\tau, z) \cdot \nabla_q \phi_0(t, z) \tag{1.27}$$

with the corrector $\chi(\tau, z)$ that solves $\dot{\chi} = G(\tau, z)$. It is very convenient to introduce a regularization parameter θ that we will send to zero later and write

$$\chi_m(\tau, z) = \int_{-\infty}^{\tau} e^{\theta s} G_m(s, z) ds. \tag{1.28}$$

The terms of the order $O(1)$ in (1.25) are

$$\frac{\partial \phi_0}{\partial t} + q \cdot \nabla_z \phi_0 - G(\tau, z) \cdot \nabla_q \phi_1 + \frac{\partial \phi_2}{\partial \tau} = 0.$$

We take the expectation of this equation using the fact that ϕ_0 is deterministic and argue that because ϕ_2 is stationary in τ we have

$$\left\langle \frac{\partial \phi_2}{\partial \tau} \right\rangle = 0.$$

With these two closure assumptions we obtain

$$\frac{\partial \phi_0}{\partial t} + q \cdot \nabla_z \phi_0 = \langle G(\tau, z) \cdot \nabla_q \phi_1 \rangle.$$

The term on the right side is computed explicitly using expression (1.27)-(1.28) for ϕ_1:

$$\begin{aligned}\langle G(\tau, z) \cdot \nabla_q \phi_1 \rangle &= \left\langle G_m(\tau, z) \frac{\partial}{\partial q_m} \left[\int_{-\infty}^{\tau} e^{\theta s} G_p(s, z) ds \frac{\partial \phi_0}{\partial q_p} \right] \right\rangle \\ &= \int_{-\infty}^{\tau} e^{\theta s} R_{mp}(s - \tau, z) ds \frac{\partial^2 \phi_0}{\partial q_m \partial q_p} \to \int_{-\infty}^{0} R_{mp}(s, z) ds \frac{\partial^2 \phi_0}{\partial q_m \partial q_p} \text{ as } \theta \to 0.\end{aligned}$$

Therefore, the function $\phi_0(t, q, z)$ satisfies a degenerate parabolic equation

$$\frac{\partial \phi_0}{\partial t} + q \cdot \nabla_z \phi_0 = D_{mp}(z) \frac{\partial^2 \phi_0}{\partial q_m \partial q_p} \tag{1.29}$$

with the symmetrized diffusion coefficient

$$D_{mp}(z) = \frac{1}{2} \left[\int_{-\infty}^{0} R_{mp}(s, z) ds + \int_{-\infty}^{0} R_{pm}(s, z) ds \right] = \frac{1}{2} \int_{-\infty}^{\infty} R_{mp}(s, z) ds.$$

If the statistics of $G(s, x)$ is identical for all $x \in \mathbb{R}^n$ then the diffusion matrix is constant in space. This means that in the limit $\varepsilon \to 0$ the process $Q(t)$ becomes a diffusion while $Z(t)$ is its integral in time.

Going back to the short time asymptotics for the geomtric optics we see that the rescaled deviation of the wave vector from its original value k_0 converges to a diffusion process $Q(t)$ and the deviation of the spatial position from its average $k_0 t$ converges to the time integral of $Q(t)$ on a time scale of the order $O(\delta^{-2/3})$. This time is much longer than the naive prediction $O(\delta^{-1/2})$ discussed below (1.21). Here δ is the relative size of the variations of the refraction index. This provides a formalization of the ray diffusion we have discussed in Section 1.1.2, at least for short times. It turns out that the randomization of the wave vector on the time scale $O(\delta^{-2/3})$ is related to the appearance of a caustic. kIt has been shown by B. White [62] appears on this time scale with probability one. This means that the ray approach in a random medium works only on a very short time scale as caustics appear very qucikly. On the other hand, one may follow the solutions of the Liouville equations for arbitrarily long times.

1.2 A limit theorem for a particle in a random flow

The rigorous approach to this problem lies via understanding the more general problem of the behavior of a particle in a rapidly varying in time random flow:

$$\dot{X} = \frac{1}{\varepsilon} V\left(\frac{t}{\varepsilon^2}, X\right), \quad X(0) = x, \tag{1.30}$$

with a random function V when $\varepsilon \ll 1$. This question goes back to the papers by Khasminskii [74] from the 60's with subsequent contributions by various authors: without any attempt at completeness we mention the work of Papanicolaou and Kohler [77], and Kesten and Papanicolaou [73]. We present a version of the limit theorem due to T. Komorowski [75].

When does one expect the trajectories of (1.30) to behave diffusively? First of all, V has to have mean zero so that the mean displacement would not be clearly biased. Second, V should "mix things around" which means that the flow should be incompressible. It helps if dynamics at "far away" points is nearly independent: this is formalized by the mixing assumption below that eliminates the memory effect. Finally, there should be no distinguished times – this requires stationarity of V in time.

The ray equations are not quite of the form (1.30): one should consider a slightly more general dynamics with an additional slow component $F(t,x)$:

$$\frac{dX}{dt} = \frac{1}{\varepsilon}G\left(\frac{t}{\varepsilon^2}, X\right) + F(t,X), \quad X(0) = x, \tag{1.31}$$

with a function F which we will assume to be deterministic for simplicity but we will not do that here.

Assumptions on the random field

Stationarity. The random field $V(t,x)$ is strictly stationary in time and space. This means that for any $t_1, t_2, \ldots, t_m \in \mathbb{R}$, $x_1, \ldots, x_m \in \mathbb{R}^n$, and each $h \in \mathbb{R}$ and $y \in \mathbb{R}^n$ the joint distirbution of $V(t_1+h, x+y), V(t_2+h, x+y), \ldots, V(t_m+h, x+y)$ is the same as that of $V(t_1,x), V(t_2,x), \ldots, V(t_m,x)$. We will denote by $R_{nm}(t,x)$ the two-point correlation tensor of $V(t,x)$:

$$R_{nm}(t,x) = \mathbb{E}\left\{V_n(s,y)V_m(t+s,y+x)\right\}. \tag{1.32}$$

Mixing. Given $C > 0$ and $\rho > 0$ let us denote by $\mathcal{V}_a^b(C,\rho)$ the σ-algebra generated by the sets of the form $\{\omega : V(t,x,\omega) \in A\}$ where $a \le t \le b$, $|x| \le C(1+t^\rho)$ and A is a Borel set in $\mathbb{R}^n$. We will assume that there exists $C > 0$ and $1/2 < \rho < 1$ such that for any $m \ge 0$ the mixing coefficient

$$\beta(h; C, \rho) = \sup_t \sup_{A \in \mathcal{V}_{t+h}^\infty(C,\rho), B \in \mathcal{V}_0^t(C,\rho)} \frac{|P(A \cap B) - P(A)P(B)|}{P(B)} \tag{1.33}$$

satisfies

$$h^m \beta(h; C, \rho) \le C_m \text{ for all } h \ge 0.$$

Boundedness. The random field $V(t,x)$ has three spatial derivatives and there exists a deterministic constant $C > 0$ so that with probability one we have

$$|V(t,x)| + \left|\frac{\partial V(t,x)}{\partial x_j}\right| + \left|\frac{\partial^2 V}{\partial x_i \partial x_j}\right| + \left|\frac{\partial^3 V}{\partial x_l \partial x_i \partial x_j}\right| \le C < +\infty$$

for all $1 \le i, j, l \le n$.

Incompressibility. The field V is divergence free, that is, almost surely

$$\nabla \cdot V(t,x) = \sum_{j=1}^n \frac{\partial V_j}{\partial x_j} = 0.$$

The mixing assumption is sometimes strengthened considering larger σ-algebras $\tilde{\mathcal{V}}_a^b$ generated by the sets of the form $\{\omega : V(t,x,\omega) \in A\}$ where $a \le t \le b$, $x \in \mathbb{R}^n$ (there is no restriction on x now) and A is a Borel set in $\mathbb{R}^n$ with the corresponding mixing coefficient

$$\tilde{\beta}(h) = \sup_t \sup_{A \in \tilde{\mathcal{V}}_{t+h}, B \in \tilde{\mathcal{V}}_0^t} \frac{|P(A \cap B) - P(A)P(B)|}{P(B)}.$$

The stronger assumption does not apply to shifts by a mean flow, that is, random fields of the form $V(t,x) = U(x - \bar{u}t)$, where $U(x)$ is a field that is mixing in space and $\bar{u}$ is a mean flow.

This is an important and interesting class of random fields that we would like to include in our consideration. The small price to pay for its inclusion is the modification of the mixing condition as in (1.33).

The spatial stationarity of $V(t,x)$ is not a necessary assumption but it allows to simplify a few expressions in what follows. This can be seen already from the formal computation in Section 1.1.3. It can, however, be dropped and we adopt it here simply for convenience. On the other hand, stationarity in time is essential for the limit theorem.

The limit theorem

Let us define the diffusion matrix

$$a_{pq} = \int_0^\infty E\left\{V_q(t,0)V_p(0,0) + V_p(t,0)V_q(0,0)\right\} dt = \int_0^\infty \left[R_{pq}(t,0) + R_{qp}(t,0)\right] dt$$

and its symmetric non-negative definite square-root matrix σ: $\sigma^2 = a$. Then the following theorem holds.

Theorem 1.2.1 *Suppose that the random field $V(t,x)$ satisfies the assumptions above. Then the process $X_\varepsilon(t)$ converges weakly as $\varepsilon \to 0$ to the limit process $\bar{X}(t)$ that satisfies a stochastic differential equation*

$$d\bar{X}(t) = F(t, \bar{X}(t))dt + \sigma dW_t.$$

Here W_t is the standard Brownian motion.

The main result of [75] is actually much more general – it applies also to non-divergence free velocities. Then the large time behavior is a sum of a large (order $1/\varepsilon$) deterministic component that comes from the flow compressibility and an order one diffusive process. Komorowski also accounts for the possible small scale variations of the random field looking at equations of the form

$$\frac{dX}{dt} = \frac{1}{\varepsilon} V\left(\frac{t}{\varepsilon^2}, \frac{X(t)}{\varepsilon^\alpha}\right)$$

with $0 \le \alpha < 1$. When $\alpha = 1$ a new regime arises – the time it takes the particle to pass one spatial correlation length is no longer much larger than the correlation time of the random fluctuations. This seriously changes the analysis.

We will not present the proof of Theorem 1.2.1 but simply discuss a couple of crucial points. The proof proceeds in several steps. First, we establish a mixing lemma that translates the mixing properties of the random field into a "loss-of-memroy" effect for the trajectories. Second, using the mixing lemma we establish the tightness of the family of processes $X_\varepsilon(t)$. In the last step one identifies the limit as a Brownian motion multiplied by the matrix σ by means of the martingale characterization of the Brownian motion.

The proof of tightness

The mixing lemmas

A crucial component in many proofs of this kind is some sort of a mixing lemma. It translates the mixing properties of the random field into the mixing properties of the trajectories. At the end of the day this allows us to split expectations into product of expectations and either "justify", or explain away the closure assumptions that are often made formally. In our particular problem it explains why the formal assumption that the leading order term in the asymptotic expansion (1.26) is deterministic produced the correct answer.

We set $G_0(s_1,x)=V(s_1,x)$ and

$$G_{1,j}(s_1,s_2,x)=\sum_{p=1}^{n} V_p(s_2,x)\frac{\partial V_j(s_1,x)}{\partial x_p}, \quad j=1,\ldots,n.$$

Incompressibility of $V(t,x)$ and its spatial stationarity imply that $\mathbb{E}\{G_1(s_1,s_2,x)\}=0$. In the next lemma we drop C and ρ in the notation for the σ-algebras $\mathcal{V}_0^s(C,\rho)$.

Lemma 1.2.2 *Fix $T\geq 0$ and let $0\leq u\leq s\leq T$. Assume that Y is a $\mathcal{V}_0^{s/\varepsilon^2}$-measurable random vector function. Then there exists $\varepsilon_0>0$ and a constant $C>0$ such that for any $0\leq u\leq s\leq s_2\leq s_1\leq T$ and $0<\varepsilon<\varepsilon_0$ we have*

$$\left|\mathbb{E}\left\{V\left(\frac{s_1}{\varepsilon^2},X_\varepsilon(u)\right)Y\left(\frac{s}{\varepsilon^2}\right)\right\}\right|\leq C\beta(s_1-s)\mathbb{E}\left|Y\left(\frac{s}{\varepsilon^2}\right)\right|, \tag{1.34}$$

$$\left|\mathbb{E}\left\{\frac{\partial}{\partial x_k}\left[V\left(\frac{s_1}{\varepsilon^2},X_\varepsilon(u)\right)\right]Y\left(\frac{s}{\varepsilon^2}\right)\right\}\right|\leq C\beta(s_1-s)\mathbb{E}\left|Y\left(\frac{s}{\varepsilon^2}\right)\right|, \tag{1.35}$$

and

$$\left|\mathbb{E}\left\{G_1\left(\frac{s_1}{\varepsilon^2},\frac{s_2}{\varepsilon^2},X_\varepsilon(u)\right)Y\left(\frac{s}{\varepsilon^2}\right)\right\}\right|\leq C\beta^{1/2}(s_1-s_2)\beta^{1/2}(s_2-s)\mathbb{E}\left|Y\left(\frac{s}{\varepsilon^2}\right)\right|, \tag{1.36}$$

$$\left|\mathbb{E}\left\{\frac{\partial}{\partial x_k}\left[G_1\left(\frac{s_1}{\varepsilon^2},\frac{s_2}{\varepsilon^2},X_\varepsilon(u)\right)\right]Y\left(\frac{s}{\varepsilon^2}\right)\right\}\right|\leq C\beta^{1/2}(s_1-s_2)\beta^{1/2}(s_2-s)\mathbb{E}\left|Y\left(\frac{s}{\varepsilon^2}\right)\right|, \tag{1.37}$$

for all $1\leq k\leq n$.

The proof of tightness

We will establish the inequality

$$\mathbb{E}\left\{|X_\varepsilon(t)-X_\varepsilon(s)|^2|X_\varepsilon(s)-X_\varepsilon(u)|^2\right\}\leq C(t-u)^{1+\nu} \tag{1.38}$$

with $\nu>0$. This is a criterion for tightness in the space D of cadlag functions. The main step in the proof is to find $\gamma\in(1,2)$ such that for all times t and s such that $t-s>10\varepsilon^\gamma$ we have an estimate for the conditional expectation

$$\mathbb{E}\left\{|X_\varepsilon(t)-X_\varepsilon(s)|^2\middle|\,\mathcal{F}_s\right\}\leq C(t-s) \text{ for } t-s>10\varepsilon^\gamma. \tag{1.39}$$

Step 0. Nearby times. As we have explained before, the estimate (1.39) itself is sufficient to establish tightness in D for the family $X_\varepsilon(t)$ if it were to hold for all $t>s$. As we will prove it only for pairs of time with a gap: $t-s>10\varepsilon^\gamma$, we may at the moment conclude only that

$$\mathbb{E}\left\{|X_\varepsilon(t)-X_\varepsilon(s)|^2|X_\varepsilon(s)-X_\varepsilon(u)|^2\right\}\leq C(t-u)^{1+\nu} \text{ for } t-s>10\varepsilon^\gamma \text{ and } s-u>10\varepsilon^\gamma.$$

Our first step is to establish that, with an appropriate choice of $\gamma\in(1,2)$, if either $t-s\leq 10\varepsilon^\gamma$ or $s-u\leq 10\varepsilon^\gamma$, the estimate (1.38) follows from (1.39) together with the dynamical system (1.31) governing $X_\varepsilon(t)$. If both $t-s\leq 10\varepsilon^\gamma$ and $s-u\leq 10\varepsilon^\gamma$ then we have directly from (1.31):

$$\begin{aligned}&\mathbb{E}\left\{|X_\varepsilon(t)-X_\varepsilon(s)|^2|X_\varepsilon(s)-X_\varepsilon(u)|^2\right\}\leq C\varepsilon^{-4}(t-s)^2(s-u)^2\\&\leq C\varepsilon^{11\gamma/4-4}(t-u)^{5/4}\leq C(t-u)^{5/4}\end{aligned}$$

provided that $\gamma>16/11$. On the other hand, if, say, $t-s\leq 10\varepsilon^\gamma$ but $s-u>10\varepsilon^\gamma$, (1.39) implies that

$$\mathbb{E}\left\{|X(s)-X(u)|^2\right\}\leq C(s-u),$$

and (1.31) implies that with probability one

$$|X(t) - X(s)| \le \frac{C(t-s)}{\varepsilon}.$$

Therefore, the following estimate holds for such times t, s and u:

$$\begin{aligned}
&\mathbb{E}\left\{|X_\varepsilon(t) - X_\varepsilon(s)|^2 |X_\varepsilon(s) - X_\varepsilon(u)|^2\right\} \le \frac{C}{\varepsilon^2}(t-s)^2(s-u) \\
&\le C\varepsilon^{7\gamma/4-2}(t-u)^{5/4} \le C(t-u)^{5/4},
\end{aligned}$$

provided that $\gamma > 8/7$. We see that, indeed, (1.39) together with (1.31) are sufficient to prove the tightness criterion (1.38). The rest of the proof of tightness of the processes $X_\varepsilon(t)$ is concerned with verifying (1.39).

Step 1. Taking a time-step backward. We start with a pair of times $t > s$ with a gap between them: $t - s > 10\varepsilon^\gamma$. Consider a partition of the interval $[s,t]$ into subintervals of the length

$$\Delta t = l_\varepsilon = (t-s)\left(\left[\frac{t-s}{\varepsilon^\gamma}\right]\right)^{-1},$$

where $[x]$ is the integer part of x. Then the time step l_ε is such that $\varepsilon^\gamma/2 \le l_\varepsilon \le 2\varepsilon^\gamma$ and the partition is $s = t_0 < t_1 < \cdots < t_{M+1} = t$ with a time step $\Delta t = t_{i+1} - t_i = l_\varepsilon$. The parameter $\gamma \in (1,2)$ is to be defined later. The important aspect is that $\gamma < 2$ so that Δt is much larger than the velocity correlation time ε^2. The basic idea in the proof of (1.39) is "to expand $X_\varepsilon(t) - X_\varepsilon(s)$ in a Taylor series" with a "large" time step $O(\Delta t)$. This will produce explicitly computable terms which are the first two terms in this expansion. The error terms which are nominally large are shown to be small using the mixing Lemma 1.2.2.

Dropping the subscript ε of X_ε we write for $t > s$:

$$X(t) - X(s) = \frac{1}{\varepsilon}\int_s^t V\left(\frac{u}{\varepsilon^2}, X(u)\right)du = \frac{1}{\varepsilon}\sum_{i=0}^{M}\int_{t_i}^{t_{i+1}} V\left(\frac{u}{\varepsilon^2}, X(u)\right)du \tag{1.40}$$

Therefore our task is to estimate the integral inside the summation in the right side of (1.40). In the preparation for the application of the mixing lemma the integrand on the interval $t_i \le u \le t_{i+1}$ can be rewritten as

$$\begin{aligned}
V\left(\frac{u}{\varepsilon^2}, X(u)\right) &= V\left(\frac{u}{\varepsilon^2}, X(t_{i-1})\right) + \int_{t_{i-1}}^u \frac{d}{du_1}V\left(\frac{u}{\varepsilon^2}, X(u_1)\right)du \\
&= V\left(\frac{u}{\varepsilon^2}, X(t_{i-1})\right) + \int_{t_{i-1}}^{u}\sum_{p=1}^{n}\frac{\partial}{\partial x_p}\left[V\left(\frac{u}{\varepsilon^2}, X(u_1)\right)\right]\left(\frac{1}{\varepsilon}V_p\left(\frac{u_1}{\varepsilon^2}, X(u_1)\right)\right)du_1 \\
&= V\left(\frac{u}{\varepsilon^2}, X(t_{i-1})\right) + \frac{1}{\varepsilon}\int_{t_{i-1}}^u G_1\left(\frac{u}{\varepsilon^2}, \frac{u_1}{\varepsilon^2}, X(u_1)\right)du_1.
\end{aligned}$$

The next step is to expand G_1 as well, also around the "one-step-backward" time t_{i-1}:

$$G_1\left(\frac{u}{\varepsilon^2}, \frac{u_1}{\varepsilon^2}, X(u_1)\right) = G_1\left(\frac{u}{\varepsilon^2}, \frac{u_1}{\varepsilon^2}, X(t_{i-1})\right) + \frac{1}{\varepsilon}\int_{t_{i-1}}^{u_1} G_2\left(\frac{u}{\varepsilon^2}, \frac{u_1}{\varepsilon^2}, \frac{u_2}{\varepsilon^2}, X(u_2)\right)du_2$$

with

$$G_2(u, u_1, u_2, x) = \sum_{q=1}^{n}\frac{\partial}{\partial x_q}\left[G_1(u, u_1, x)\right]V_q(u_2, x).$$

Putting together the above calculations we see that

$$X(t)-X(s)=\frac{1}{\varepsilon}\sum_{i=0}^{M}\int_{t_i}^{t_{i+1}}V\left(\frac{u}{\varepsilon^2},X(u)\right)du=\frac{1}{\varepsilon}\sum_{i=0}^{M}\int_{t_i}^{t_{i+1}}V\left(\frac{u}{\varepsilon^2},X(t_{i-1})\right)du$$
$$+\frac{1}{\varepsilon^2}\sum_{i=0}^{M}\int_{t_i}^{t_{i+1}}\left[\int_{t_{i-1}}^{u}G_1\left(\frac{u}{\varepsilon^2},\frac{u_1}{\varepsilon^2},X(u_1)\right)du_1\right]du$$
$$=\frac{1}{\varepsilon}\sum_{i=0}^{M}\int_{t_i}^{t_{i+1}}V\left(\frac{u}{\varepsilon^2},X(t_{i-1})\right)du+\frac{1}{\varepsilon^2}\sum_{i=0}^{M}\int_{t_i}^{t_{i+1}}\left[\int_{t_{i-1}}^{u}G_1\left(\frac{u}{\varepsilon^2},\frac{u_1}{\varepsilon^2},X(t_{i-1})\right)du_1\right]du$$
$$+\frac{1}{\varepsilon^3}\sum_{i=0}^{M}\int_{t_i}^{t_{i+1}}\left[\int_{t_{i-1}}^{u}\left[\int_{t_{i-1}}^{u_1}G_2\left(\frac{u}{\varepsilon^2},\frac{u_1}{\varepsilon^2},\frac{u_2}{\varepsilon^2},X(u_2)\right)du_2\right]du_1\right]du.$$

The triple integral on the last line is deterministically small with an appropriate choice of γ: the time interval in each integration is smaller than ε^γ and the total number of terms is at most $2(t-s)/\varepsilon^\gamma$ as we have assumed that $t-s\geq 10\varepsilon^\gamma$. Therefore, the last integral is bounded by

$$\frac{1}{\varepsilon^3}\left|\sum_{i=0}^{M}\int_{t_i}^{t_{i+1}}\left[\int_{t_{i-1}}^{u}\left[\int_{t_{i-1}}^{u_1}G_2\left(\frac{u}{\varepsilon^2},\frac{u_1}{\varepsilon^2},\frac{u_2}{\varepsilon^2},X(u_2)\right)du_2\right]du_1\right]du\right|\leq C\varepsilon^{2\gamma-3}(t-s)$$

which is small if $\gamma>3/2$. This is a general idea in proofs of weak coupling limits: pull back one time step and expand the integrands until they become almost surely small, then compute the limit of the (very) finite number of surviviing terms. In our present case we have shown that, for $3/2<\gamma<2$,

$$X(t)-X(s)=L_1(s,t)+L_2(s,t)+E(s,t)$$

where

$$L_1(s,t)=\frac{1}{\varepsilon}\sum_{i=0}^{M}\int_{t_i}^{t_{i+1}}V\left(\frac{u}{\varepsilon^2},X(t_{i-1})\right)du$$

and

$$L_2(s,t)=\frac{1}{\varepsilon^2}\sum_{i=0}^{M}\int_{t_i}^{t_{i+1}}\left[\int_{t_{i-1}}^{u}G_1\left(\frac{u}{\varepsilon^2},\frac{u_1}{\varepsilon^2},X(t_{i-1})\right)du_1\right]du,$$

while $|E(s,t)|\leq C\varepsilon^\alpha(t-s)$ with some $\alpha>0$ and a deterministic constant $C>0$. This finishes the first preliminary step in the proof of tightness.

Step 2. Application of the tightness criterion. Now we are ready to prove (1.39). That is, we have to verify that for any non-negative and $\mathcal{V}_0^{s/\varepsilon^2}$-measurable random variable Y we have for all $0\leq s\leq t\leq T$ such that $t\geq s+10\varepsilon^\gamma$:

$$\mathbb{E}\left\{|X(t)-X(s)|^2Y\right\}\leq C(T)(t-s)\mathbb{E}\left\{Y\right\}.$$

Our estimates in Step 1 show that it is actually enough to verify that

$$\mathbb{E}\left\{(L_j(s,t))^2Y\right\}\leq C(t-s)\mathbb{E}\{Y\},\quad j=1,2.$$

An estimate for L_1. We first look at the term corresponding to L_1: it is equal to

$$\mathbb{E}\left\{(L_1(s,t))^2Y\right\} = \frac{2}{\varepsilon^2}\sum_{i<j}\sum_{p=1}^{n}\int\limits_{t_i}^{t_{i+1}}\int\limits_{t_j}^{t_{j+1}}\mathbb{E}\left\{V_p\left(\frac{u}{\varepsilon^2},X(t_{i-1})\right)V_p\left(\frac{u'}{\varepsilon^2},X(t_{j-1})\right)Y\right\}du'du$$

$$+\frac{1}{\varepsilon^2}\sum_{j}\sum_{p=1}^{n}\int\limits_{t_j}^{t_{j+1}}\int\limits_{t_j}^{t_{j+1}}\mathbb{E}\left\{V_p\left(\frac{u}{\varepsilon^2},X(t_{j-1})\right)V_p\left(\frac{u'}{\varepsilon^2},X(t_{j-1})\right)Y\right\}du'du = \sum_{i\le j}I_{ij}.$$

The idea is to use separation between t_{i-1} and t_{j-1} and apply the mixing lemma. Accordingly we look at the cases $i \le j-2$, $i = j-1$ and $i = j$ separately as the terms end up being of a different order. The terms with $i \le j-2$ may be estimated with the help of the mixing Lemma 1.2.2 using the time gap between the times u' and $t_{j-1} \ge t_{i+1} \ge u$ which is much larger than the correlation time ε^2:

$$\sum_{j=0}^{M}\sum_{i\le j-2}|I_{ij}| \le \frac{C}{\varepsilon^2}\sum_{j=0}^{M}\sum_{i\le j-2}\int\limits_{t_i}^{t_{i+1}}\int\limits_{t_j}^{t_{j+1}}\beta\left(\frac{u'-t_{j-1}}{\varepsilon^2}\right)\mathbb{E}\left\{Y\right\}du'du$$

$$\le \frac{C}{\varepsilon^2}\beta\left(\varepsilon^{2-\gamma}\right)(t-s)^2E\left\{Y\right\} \le C\varepsilon^p(t-s)E\left\{Y\right\}$$

for any $p > 0$ since $\gamma < 2$ and $\beta(s)$ decays faster than any power of s. The term I_3 corresponding to $i = j$ can be estimated using the mixing lemma again, using the fact that t_{j-1} is smaller than both u and u':

$$\sum_{j=0}^{M}|I_{jj}| \le \frac{C}{\varepsilon^2}\sum_{j=0}^{M}\int\limits_{t_j}^{t_{j+1}}\int\limits_{t_j}^{t_{j+1}}\mathbb{E}\left\{V_p\left(\frac{u}{\varepsilon^2},X(t_{j-1})\right)V_p\left(\frac{u'}{\varepsilon^2},X(t_{j-1})\right)Y\right\}du'du \tag{1.41}$$

$$\le \frac{2C}{\varepsilon^2}\sum_{j\in I}\int\limits_{t_j}^{t_{j+1}}\int\limits_{u'}^{t_{j+1}}\beta\left(\frac{u-u'}{\varepsilon^2}\right)dudu'E\left\{Y\right\} \le C(t-s)E\left\{Y\right\}\int_0^\infty\beta(u)du.$$

The integral I_2 with $i = j-1$ is estimated similarly.

A better estimate estimate for L_1. Let us now go one step further and actually identify the limit of $E\{L_{1,j}(s,t)L_{1,m}(s,t)Y\}$ with $1 \le j,m \le n$. The previous calculations already show that the term corresponding to the previous I_1 (but now with V_j and V_m replacing V_p and V_p) satisfies $|I_1| \le C\varepsilon^\alpha(t-s)E\{Y\}$ with $\alpha > 0$ so we are interested only in the limit of I_2 and I_3. The term I_3 is computed as in (1.41) with the help of the mixing lemma:

$$\sum_{j\in I}|I_{jj}| = \frac{1}{\varepsilon^2}\sum_{j=0}^{M}\int\limits_{t_j}^{t_{j+1}}\int\limits_{t_j}^{t_{j+1}}\mathbb{E}\left\{V_j\left(\frac{u}{\varepsilon^2},X(t_{j-1})\right)V_m\left(\frac{u'}{\varepsilon^2},X(t_{j-1})\right)Y\right\}du'du \tag{1.42}$$

$$= \frac{1}{\varepsilon^2}\sum_{j=0}^{M}\int\limits_{t_j}^{t_{j+1}}\int\limits_{t_j}^{t_{j+1}}R_{jm}\left(\frac{u-u'}{\varepsilon^2},0\right)dudu'E\left\{Y\right\} + o(1)(t-s)E\left\{Y\right\}$$

$$= \left[\int_{-\infty}^{\infty}R_{jm}(\tau,0)d\tau + o(1)\right](t-s)E\left\{Y\right\}.$$

Finally, I_2 corresponding to $i = j-1$ is computed as

$$\sum_{j\in I}|I_{j-1,j}| = \frac{1}{\varepsilon^2}\sum_{j=0}^{M}\int\limits_{t_j}^{t_{j+1}}\int\limits_{t_{j-1}}^{t_j}\mathbb{E}\left\{V_j\left(\frac{u}{\varepsilon^2},X(t_{j-1})\right)V_m\left(\frac{u'}{\varepsilon^2},X(t_{j-2})\right)Y\right\}du'du \tag{1.43}$$

$$= \frac{1}{\varepsilon^2}\sum_{j\in I}\int\limits_{t_j}^{t_{j+1}}\int\limits_{t_{j-1}}^{t_j}R_{jm}\left(\frac{u-u'}{\varepsilon^2},0\right)dudu'E\left\{Y\right\} + o(1)(t-s)E\left\{Y\right\} = o(1)(t-s)E\left\{Y\right\}.$$

because $t_{j+1}-t_j = \varepsilon^\gamma \gg \varepsilon^2$. Therefore we actually have a more precise estimate

$$\mathbb{E}\left\{(L_{1,j}(s,t)L_{1,m}(s,t))Y\right\} = \left[\int_{-\infty}^{\infty}R_{jm}(\tau,0)d\tau + o(1)\right](t-s)E\left\{Y\right\}. \tag{1.44}$$

An estimate for L_2. Following the above steps one also establishes the required estimate for L_2:

$$\mathbb{E}\left\{(L_2(s,t))^2Y\right\} \le C(t-s)E\{Y\}. \tag{1.45}$$

There is no reason to repeat these calculations separately for L_2 except that an even stronger estimate than (1.45) holds with an appropriate choice of γ:

$$\mathbb{E}\left\{(L_2(s,t))^2Y\right\} \le C\varepsilon^\alpha(t-s)E\{Y\} \tag{1.46}$$

with $\alpha > 0$. We will need (1.46) in the identification of the limit, thus we will show it now: $\mathbb{E}\left\{(L_2(s,t))^2Y\right\}$ is equal to

$$\frac{1}{\varepsilon^4}\sum_{i,j}\int\limits_{t_i}^{t_{i+1}}du\int\limits_{t_j}^{t_{j+1}}du'\int\limits_{t_{i-1}}^{u}du_1\int\limits_{t_{j-1}}^{u'}du_1'\mathbb{E}\left\{G_1\left(\frac{u}{\varepsilon^2},\frac{u_1}{\varepsilon^2},X(t_{i-1})\right)G_1\left(\frac{u'}{\varepsilon^2},\frac{u_1'}{\varepsilon^2},X(t_{j-1})\right)Y\right\}.$$

Once again, you split the sum above into terms with $i \le j-2$, $i = j-1$ and $i = j$: those with $i \le j-2$ add up to

$$\frac{1}{\varepsilon^4}\sum_{i\le j-2}\int\limits_{t_i}^{t_{i+1}}du\int\limits_{t_j}^{t_{j+1}}du'\int\limits_{t_{i-1}}^{u}du_1\int\limits_{t_{j-1}}^{u'}du_1'\mathbb{E}\left\{G_1\left(\frac{u}{\varepsilon^2},\frac{u_1}{\varepsilon^2},X(t_{i-1})\right)G_1\left(\frac{u'}{\varepsilon^2},\frac{u_1'}{\varepsilon^2},X(t_{j-1})\right)Y\right\}$$
$$\le C\varepsilon^{2\gamma-4}\beta\left(\varepsilon^{\gamma-2}\right)(t-s)^2\mathbb{E}\{Y\}.$$

We used in the above estimate the mixing lemma with the gap between t_{i-1} and t_{j-1} as well as the fact that the length of each time interval is ε^γ while the total number of terms in the sum is not more than $(2(t-s)/\varepsilon^\gamma)^2$. The important difference with L_1 is that the term with $i = j$ is also small:

$$\frac{1}{\varepsilon^4}\sum_{i}\int\limits_{t_i}^{t_{i+1}}du\int\limits_{t_i}^{t_{i+1}}du'\int\limits_{t_{i-1}}^{u}du_1\int\limits_{t_{i-1}}^{u'}du_1'\mathbb{E}\left\{G_1\left(\frac{u}{\varepsilon^2},\frac{u_1}{\varepsilon^2},X(t_{i-1})\right)G_1\left(\frac{u'}{\varepsilon^2},\frac{u_1'}{\varepsilon^2},X(t_{i-1})\right)Y\right\}$$
$$\le C\varepsilon^{3\gamma-4}(t-s)\mathbb{E}\{Y\}$$

simply because now the number of summands is bounded by $(2(t-s)/\varepsilon^\gamma)$ (without the square). This means that if we take $\gamma > 4/3$ this term is bounded by the right side of (1.46). The contribution of the terms with $i = j-1$ is estimated identically – hence (1.46) indeed holds.

Summarizing our work so far (and restoring the missing indices) we have shown that

$$\mathbb{E}\left\{(X_m(t) - X_m(s))(X_n(t) - X_n(s))Y\right\} = \left[\int_{-\infty}^{\infty} R_{mn}(\tau, 0)d\tau + o(1)\right](t-s)E\left\{Y\right\} \quad (1.47)$$

for all $t > s$ with $t - s \geq 10\varepsilon^{\gamma}$. This, of course, implies (1.39) and hence the tightness of the family $X_\varepsilon(t)$ follows.

Identification of the limit

In order to identify the limit, using the Levy theorem (the martingale characterization of the Brownian motion) (see, for instance, Theorem 3.16 in [37]) all we have to do is verify that the limit is continuous (that we already know) and the following two conditions hold: first,

$$\lim_{\varepsilon\to 0} \mathbb{E}\left\{\left[(X_j^\varepsilon(t) - X_j^\varepsilon(s))(X_m^\varepsilon(t) - X_m^\varepsilon(s)) - a_{jm}(t-s)\right]\Psi\right\} = 0$$

for all bounded non-negative continuous functions $\Psi = \Psi(X_\varepsilon(t_1), \ldots, X_\varepsilon(t_n))$ with $0 \leq t_1 \leq t_2 \leq \cdots \leq t_n \leq s < t \leq T$. Second, we need

$$\limsup_{\varepsilon\to 0} \mathbb{E}\left\{(X_j^\varepsilon(t))^4\right\} < +\infty$$

for all $t > 0$. These conditions allow us to conlude that the limit process is a martinagle. The former condition we have already verified in the previous section in the proof of tightness. The latter may be checked using very similar arguments. This finishes the proof of Theorem 1.2.1. $\square$

Chapter 2

Random geometric optics II: the long time limit, from rays to diffusion

Here we study the long time asymptotics of rays in a weakly random medium. This problem is analyzed in the general setting of a particle in a weakly random Hamiltonian field. This chapter is based on the results of [6] and [44].

2.1 A particle in a random Hamiltonian

We have considered in Chapter 1 the asymptotic behavior of a ray in a medium with weakly random sound speed and have seen that on a short time scale the rescaled deviation of the direction of the ray from its original value becomes a diffusion process. The long time behavior of this system is an example of the analysis of the long time, large distance behavior of a particle in a weakly random time-independent Hamiltonian flow. It turns out that this limit is also described by the momentum diffusion but now, of course, without rescaling of the momentum: the particle momentum itself undergoes the Brownian motion on the energy sphere. This intuitive result has been first proved in [40] for a classical particle in dimensions higher than two, and later extended to two dimensions with the Poisson distribution of scatterers in [22], and in a general two-dimensional setting in [45]. On the other hand, the long time limit of a momentum diffusion is the standard spatial Brownian motion. Hence, a natural question arises if it is possible to obtain such a Brownian motion directly as the limiting description in the original problem of a particle in a quenched random potential. This necessitates the control of the particle behavior over times longer than those when the momentum diffusion holds. This is what we do in this chapter.

We consider a particle that moves in an isotropic weakly random Hamiltonian flow with the Hamiltonian of the form $H_\delta(x,k) = H_0(k) + \sqrt{\delta} H_1(x,k)$, $k = |k|$, and $x, k \in \mathbb{R}^d$ with $d \geq 3$:

$$\frac{dX^\delta}{dt} = \nabla_k H_\delta, \quad \frac{dK^\delta}{dt} = -\nabla_x H_\delta, \quad X^\delta(0) = 0, \quad K^\delta(0) = k_0. \tag{2.1}$$

Here $H_0(k)$ is the background Hamiltonian and $H_1(x,k)$ is a random perturbation, while the small parameter $\delta \ll 1$ measures the relative strength of random fluctuations. One expects that the effect of the random fluctuation would be of order one on the time scale of the order

$t \sim O(\delta^{-1})$. And indeed, as we have mentioned, it has been shown in [40] that, when

$$H_\delta(x,k) = \frac{k^2}{2} + \sqrt{\delta} V(x),$$

and under certain mixing assumptions on the random potential $V(x)$, the momentum process $K^\delta(t/\delta)$ converges to a diffusion process $K(t)$ on the sphere $k = k_0$ and the rescaled spatial component $\tilde{X}^\delta(t) = \delta X^\delta(t/\delta)$ converges to $X(t) = \int_0^t K(s)ds$. This is the momentum diffusion mentioned above. Another special case,

$$H_\delta(x,k) = (c_0 + \sqrt{\delta} c_1(x))|k|, \tag{2.2}$$

arises in the geometrical optics limit of wave propagation and this is the problem we are mostly interested in these notes. Here c_0 is the background sound speed, and $c_1(x)$ is a random perturbation. This case has been considered in [6], where it has been shown that, once again, $K^\delta(t/\delta)$ converges to a diffusion process $K(t)$ on the sphere $\{k = k_0\}$ while $\tilde{X}^\delta(t) = \delta X^\delta(t/\delta)$ converges to $X(t) = c_0 \int_0^t \hat{K}(s)ds$, $\hat{K}(t) := K(t)/|K(t)|$.

We show in this chapter how the momentum diffusion may be obtained and that this analysis may be pushed beyond the time of the momentum diffusion, so that under certain assumptions concerning the mixing properties of H_1 in the spatial variable there exists $\alpha_0 > 0$ such that the process $\delta^{1+\alpha} X^\delta(t/\delta^{1+2\alpha})$ converges to the standard Brownian motion in $\mathbb{R}^d$ for all $\alpha \in (0, \alpha_0)$. The main difficulty of the proof is to obtain error estimates in the convergence of $K^\delta(\cdot)$ to the momentum diffusion. The error estimates allow us to push the analysis to times much longer than δ^{-1} where the momentum diffusion converges to the standard Brownian motion. The method of the proof is a modification of the cut-off technique used in [6] and [40].

2.2 The main result and preliminaries

2.2.1 The background Hamiltonian

We assume that the background Hamiltonian $H_0(k)$ is isotropic, that is, it depends only on $k = |k|$, and is uniform in space. Moreover, we assume that $H_0 : [0, +\infty) \to \mathbb{R}$ is a strictly increasing function satisfying $H_0(0) \geq 0$ and such that it is of C^3-class of regularity in $(0, +\infty)$ with $H_0'(k) > 0$ for all $k > 0$, and let

$$h^*(M) := \max_{k \in [M^{-1}, M]} (H_0'(k) + |H_0''(k)| + |H_0'''(k)|), \quad h_*(M) := \min_{k \in [M^{-1}, M]} H_0'(k). \tag{2.3}$$

Two examples of such Hamiltonians are the quantum Hamiltonian $H_0(k) = k^2/2$ and the acoustic wave Hamiltonian $H_0(k) = c_0 k$. The qualitative reason for the above assumptions on $H_0(k)$ is that we need the background dynamics 'to take the particle to various regions where it will sample the nearly independent random fluctuations. The overall effect will then lead to a Markovian limit. This makes the problem much simpler than a seemingly similar problem

$$\dot{X} = V(X), \tag{2.4}$$

with a mixing in space and time-independent random field $V(x)$. Unlike our problem, (2.4) lack any mechanism to move the particle around which makes it extremely difficult to obtain any rigorous, or even formal results for the particle behavior in (2.4).

2.2.2 The random medium

Let $(\Omega, \Sigma, \mathbb{P})$ be a probability space, and let $\mathbb{E}$ denote the expectation with respect to $\mathbb{P}$. We denote by $\|X\|_{L^p(\Omega)}$ the L^p-norm of a given random variable $X : \Omega \to \mathbb{R}$, $p \in [1, +\infty]$. Let $H_1 : \mathbb{R}^d \times [0, +\infty) \times \Omega \to \mathbb{R}$ be a random field that is measurable and strictly stationary in the first variable. This means that for any shift $x \in \mathbb{R}^d$, $k \in [0, +\infty)$, and a collection of points $x_1, \ldots, x_n \in \mathbb{R}^d$ the laws of $(H_1(x_1 + x, k), \ldots, H_1(x_n + x, k))$ and $(H_1(x_1, k), \ldots, H_1(x_n, k))$ are identical. In addition, we assume that $\mathbb{E}H_1(x, k) = 0$ for all $k \geq 0$, $x \in \mathbb{R}^d$, the realizations of $H_1(x, k)$ are $\mathbb{P}$–a.s. C^2-smooth in $(x, k) \in \mathbb{R}^d \times (0, +\infty)$ and they satisfy

$$D_{i,j}(M) := \max_{|\alpha|=i} \operatorname*{ess-sup}_{(x,k,\omega)\in\mathbb{R}^d\times[M^{-1},M]\times\Omega} |\partial_{\mathbf{x}}^{\alpha} \partial_k^j H_1(\mathbf{x}, k; \omega)| < +\infty, \quad i, j = 0, 1, 2. \tag{2.5}$$

We define $\tilde{D}(M) := \sum_{0\leq i+j\leq 2} D_{i,j}(M)$.

We suppose further that the random field is strongly mixing in the uniform sense. More precisely, for any $R > 0$ we let $\mathcal{C}_R^i$ and $\mathcal{C}_R^e$ be the σ–algebras generated by random variables $H_1(\mathbf{x}, k)$ with $k \in [0, +\infty)$, $\mathbf{x} \in \mathbb{B}_R$ and $\mathbf{x} \in \mathbb{B}_R^c$ respectively. The uniform mixing coefficient between the σ–algebras is

$$\phi(\rho) := \sup[\,|\mathbb{P}(B) - \mathbb{P}(B|A)| : \ R > 0,\ A \in \mathcal{C}_R^i,\ B \in \mathcal{C}_{R+\rho}^e\,],$$

for all $\rho > 0$. We suppose that $\phi(\rho)$ decays faster than any power: for each $p > 0$

$$h_p := \sup_{\rho\geq 0} \rho^p \phi(\rho) < +\infty. \tag{2.6}$$

The two-point spatial correlation function of the random field H_1 is

$$R(\mathbf{y}, k) := \mathbb{E}[H_1(\mathbf{y}, k) H_1(\mathbf{0}, k)].$$

Note that (2.6) implies that for each $p > 0$

$$h_p(M) := \sum_{i=0}^{4} \sum_{|\alpha|=i} \sup_{(\mathbf{y},k)\in\mathbb{R}^d\times[M^{-1},M]} (1 + |\mathbf{y}|^2)^{p/2} |\partial_{\mathbf{y}}^{\alpha} R(\mathbf{y}, k)| < +\infty, \quad M > 0. \tag{2.7}$$

We also assume that the correlation function $R(y, l)$ is of the C^∞-class for a fixed $l > 0$, is sufficiently smooth in l, and that for any fixed $l > 0$

$$\hat{R}(k, l) \text{ does not vanish identically on any hyperplane } H_p = \{k : \ (k \cdot p) = 0\}. \tag{2.8}$$

Here $\hat{R}(k, l) = \int R(x, l) \exp(-ik \cdot x) dx$ is the power spectrum of H_1.

The above assumptions are satisfied, for example, if $H_1(x, k) = c_1(x)h(k)$, where $c_1(x)$ is a stationary uniformly mixing random field with a smooth correlation function, and $h(k)$ is a smooth deterministic function.

2.2.3 The main results

Let the function $\phi_\delta(t, x, k)$ satisfy the Liouville equation

$$\begin{aligned} &\frac{\partial \phi^\delta}{\partial t} + \nabla_x H_\delta\,(x, k) \cdot \nabla_k \phi^\delta - \nabla_k H_\delta\,(x, k) \cdot \nabla_x \phi^\delta = 0, \\ &\phi^\delta(0, x, k) = \phi_0(\delta x, k). \end{aligned} \tag{2.9}$$

We assume that the initial data $\phi_0(x,k)$ is a compactly supported function four times differentiable in k, twice differentiable in x whose support is contained inside a spherical shell $\mathcal{A}(M) = \{(x,k) : M^{-1} < |k| < M\}$ for some positive $M > 0$.

Let us define the diffusion matrix D_{mn} by

$$D_{mn}(\hat{k},l) = -\frac{1}{2}\int_{-\infty}^{\infty} \frac{\partial^2 R(H_0'(l)s\hat{k},l)}{\partial x_n \partial x_m} ds = -\frac{1}{2H_0'(l)}\int_{-\infty}^{\infty} \frac{\partial^2 R(s\hat{k},l)}{\partial x_n \partial x_m} ds, \qquad m,n = 1,\dots,d. \tag{2.10}$$

Then we have the following result.

Theorem 2.2.1 *Let ϕ^δ be the solution of* (2.9) *and let $\bar{\phi}$ satisfy*

$$\begin{aligned} \frac{\partial \bar{\phi}}{\partial t} &= \sum_{m,n=1}^{d} \frac{\partial}{\partial k_m}\left(D_{mn}(\hat{k},k)\frac{\partial \bar{\phi}}{\partial k_n}\right) + H_0'(k)\,\hat{k}\cdot\nabla_x\bar{\phi} \\ \bar{\phi}(0,x,k) &= \phi_0(x,k). \end{aligned} \tag{2.11}$$

Suppose that $M \ge M_0 > 0$ and $T \ge T_0 > 0$. Then, there exist two constants C, $\alpha_0 > 0$ such that for all $T \ge T_0$

$$\sup_{(t,x,k)\in[0,T]\times K}\left|\mathbb{E}\phi^\delta\left(\frac{t}{\delta},\frac{x}{\delta},k\right) - \bar{\phi}(t,x,k)\right| \le CT(1+\|\phi_0\|_{1,4})\delta^{\alpha_0} \tag{2.12}$$

for all compact sets $K \subset \mathcal{A}(M)$.

Note that

$$\begin{aligned} \sum_{m=1}^{d} D_{nm}(\hat{k},k)\hat{k}_m &= -\sum_{m=1}^{d}\frac{1}{2H_0'(k)}\int_{-\infty}^{\infty}\frac{\partial^2 R(s\hat{k},k)}{\partial x_n \partial x_m}\hat{k}_m ds \\ &= -\sum_{m=1}^{d}\frac{1}{2H_0'(k)}\int_{-\infty}^{\infty}\frac{d}{ds}\left(\frac{\partial R(s\hat{k},k)}{\partial x_n}\right) ds = 0 \end{aligned}$$

and thus the K-process generated by (2.11) is indeed a diffusion process on a sphere $k = \text{const}$, or, equivalently, equations (2.11) for different values of k are decoupled. Assumption (2.8) implies the following.

Proposition 2.2.2 *The matrix $D(\hat{k},l)$ has rank $d-1$ for each $\hat{k}\in\mathbb{S}^{d-1}$ and each $l > 0$.*

We also show that solutions of (2.11) converge in the long time limit to the solutions of the spatial diffusion equation. More, precisely, we have the following result. Let $\bar{\phi}_\gamma(t,x,k) = \bar{\phi}(t/\gamma^2, x/\gamma, k)$, where $\bar{\phi}$ satisfies (2.11) with an initial data $\bar{\phi}_\gamma(0,t,x,k) = \phi_0(\gamma x, k)$. We also let $w(t,x,k)$ be the solution of the spatial diffusion equation:

$$\begin{aligned} \frac{\partial w}{\partial t} &= \sum_{m,n=1}^{d} a_{mn}(k)\frac{\partial^2 w}{\partial x_n \partial x_m}, \\ w(0,x,k) &= \bar{\phi}_0(x,k) \end{aligned} \tag{2.13}$$

with the averaged initial data

$$\bar{\phi}_0(x,k) = \frac{1}{\Gamma_{d-1}}\int_{\mathbb{S}^{d-1}} \phi_0(x,k)d\Omega(\hat{k}).$$

Here $d\Omega(\hat{k})$ is the surface measure on the unit sphere $\mathbb{S}^{d-1}$ and Γ_n is the area of an n-dimensional sphere. The diffusion matrix $A := [a_{nm}]$ in (2.13) is given explicitly as

$$a_{nm}(k) = \frac{1}{\Gamma_{d-1}} \int_{\mathbb{S}^{d-1}} H_0'(k)\hat{k}_n \chi_m(k) d\Omega(\hat{k}). \tag{2.14}$$

The functions χ_j appearing above are the mean-zero solutions of

$$\sum_{m,n=1}^{d} \frac{\partial}{\partial k_m} \left(D_{mn}(\hat{k}, k) \frac{\partial \chi_j}{\partial k_n} \right) = -H_0'(k)\hat{k}_j. \tag{2.15}$$

Note that equations (2.15) for χ_m are elliptic on each sphere $\{|k| = k\}$. This follows from the fact that the equations for each such sphere are all decoupled and Proposition 2.2.2. Also note that the matrix A is positive definite. Indeed, let $\mathbf{c} = (c_1, \ldots, c_d) \in \mathbb{R}^d$ be a fixed vector and let $\chi_{\mathbf{c}} := \sum_{m=1}^{d} c_m \chi_m$. Since the matrix D is non-negative we have

$$\begin{aligned}
(A\mathbf{c}, \mathbf{c})_{\mathbb{R}^d} &= -\frac{1}{\Gamma_{d-1}} \sum_{m,n=1}^{d} \int_{\mathbb{S}^{d-1}} \chi_{\mathbf{c}}(\hat{k}, l) \frac{\partial}{\partial k_m} \left(D_{mn}(\hat{k}, l) \frac{\partial \chi_{\mathbf{c}}(\hat{k}, l)}{\partial k_n} \right) d\Omega(\hat{k}) \qquad (2.16) \\
&= -\frac{1}{\Gamma_{d-1}} \sum_{m,n=1}^{d} \int_{\mathbb{R}^d} \chi_{\mathbf{c}}(\hat{k}, l) \frac{\partial}{\partial k_m} \left(D_{mn}(\hat{k}, l) \frac{\partial \chi_{\mathbf{c}}(\hat{k}, l)}{\partial k_n} \right) \delta(k - l) \frac{dk}{l^{d-1}} \\
&= \frac{1}{\Gamma_{d-1}} \int_{\mathbb{S}^{d-1}} (D(\hat{k}, l) \nabla \chi_{\mathbf{c}}(\hat{k}, l), \nabla \chi_{\mathbf{c}}(\hat{k}, l))_{\mathbb{R}^d} d\hat{\Omega}(\hat{k}) \geq 0.
\end{aligned}$$

The last equality holds after integration by parts because $D(\hat{k}, l)\hat{k} = 0$. Moreover, the inequality appearing in the last line of (2.16) is strict. This can be seen as follows. Since the null-space of the matrix $D(\hat{k}, l)$ is one-dimensional and consists of the vectors parallel to $\hat{k}$, in order for $(A\mathbf{c}, \mathbf{c})_{\mathbb{R}^d}$ to vanish one needs that the gradient $\nabla \chi_{\mathbf{c}}(\hat{k}, l)$ is parallel to $\hat{k}$ for all $\hat{k} \in \mathbb{S}^{d-1}$. This, however, together with (2.15) would imply that $\hat{k} \cdot \mathbf{c} = 0$ for all $\hat{k}$, which is impossible.

The following theorem holds.

Theorem 2.2.3 *For every pair of times $0 < T_* < T < +\infty$ the re-scaled solution $\bar{\phi}_\gamma(t, x, k) = \bar{\phi}(t/\gamma^2, x/\gamma, k)$ of (2.11) converges as $\gamma \to 0$ in $C([T_*, T]; L^\infty(\mathbb{R}^{2d}))$ to $w(t, x, k)$. Moreover, there exists a constant $C > 0$ so that we have*

$$\|w(t, \cdot) - \bar{\phi}_\gamma(t, \cdot)\|_{0,0} \leq C \left(\gamma T + \sqrt{\gamma} \right) \|\phi_0\|_{1,1} \tag{2.17}$$

for all $T_* \leq t \leq T$.

The proof of Theorem 2.2.3 is based on some classical asymptotic expansions and is quite straightforward. As an immediate corollary of Theorems 2.2.1 and 2.2.3 we obtain the following result, which is the main result of this chapter.

Theorem 2.2.4 *Let ϕ_δ be solution of (2.9) with the initial data $\phi_\delta(0, x, k) = \phi_0(\delta^{1+\alpha} x, k)$ and let $\bar{w}(t, x)$ be the solution of the diffusion equation (2.13) with the initial data $w(0, x, k) = \bar{\phi}_0(x, k)$. Then, there exists $\alpha_0 > 0$ and a constant $C > 0$ so that for all $0 \leq \alpha < \alpha_0$ and all $0 < T_* \leq T$ we have for all compact sets $K \subset \mathcal{A}(M)$:*

$$\sup_{(t,x,k) \in [T_*, T] \times K} \left| w(t, x, k) - \mathbb{E}\bar{\phi}_\delta(t, x, k) \right| \leq C T \delta^{\alpha_0 - \alpha}, \tag{2.18}$$

where $\bar{\phi}_\delta(t, x, k) := \phi_\delta \left(t/\delta^{1+2\alpha}, x/\delta^{1+\alpha}, k \right)$.

Theorem 2.2.4 shows that the movement of a particle in a weakly random quenched Hamiltonian is, indeed, approximated by a Brownian motion in the long time-large space limit, at least for times $T \ll \delta^{-\alpha_0}$. In fact, according to Remark **??** we can allow T_* to vanish as $\delta \to 0$ choosing $T_* = \delta^{3\alpha/2}$.

In the isotropic case when $R = R(|x|, k)$ we may simplify the above expressions for the diffusion matrices D_{mn} and a_{mn}. In that case we have

$$
\begin{aligned}
D_{mn}(\hat{k}, k) &= -\frac{1}{2}\int_{-\infty}^{\infty} \frac{\partial^2 R(H_0'(k)s\hat{k}, k)}{\partial x_n \partial x_m}\, ds \\
&= -\int_0^{\infty} \left[\frac{k_n k_m}{k^2} R''(H_0'(k)s, k) + \left(\delta_{nm} - \frac{k_n k_m}{k^2}\right) \frac{R'(H_0'(k)s, k)}{H_0'(k)s}\right] ds \\
&= -\frac{1}{H_0'(k)} \int_0^{\infty} \frac{R'(s,k)}{s}\, ds \left(\delta_{nm} - \frac{k_n k_m}{k^2}\right),
\end{aligned}
$$

so that the matrix $[D_{mn}(\hat{k}, k)]$ has the form

$$
D(\hat{k}, k) = D_0(k)\left(I - \hat{k} \otimes \hat{k}\right), \quad D_0(k) = -\frac{1}{H_0'(k)} \int_0^{\infty} \frac{R'(s,k)}{s} ds.
$$

The functions χ_j are given explicitly in this case by

$$
\chi_j(\hat{k}, k) = -\frac{|H_0'(k)|^2 |k|^2 \hat{k}_j}{(d-1)\bar{D}_0(k)}, \quad \bar{D}_0(k) = -\int_0^{\infty} \frac{R'(s,k)}{s} ds
$$

and

$$
a_{nm}(k) = \frac{|H_0'(k)|^3 |k|^2}{\Gamma_{d-1}(d-1)\bar{D}_0(k)} \int_{\mathbb{S}^{d-1}} \hat{k}_n \hat{k}_m d\Omega(\hat{k}) = \frac{|H_0'(k)|^3 |k|^2}{d(d-1)\bar{D}_0(k)} \delta_{nm}.
$$

2.2.4 A formal derivation of the momentum diffusion

We now recall how the diffusion operator in (2.11) can be derived in a quick formal way. We represent the solution of (2.9) as $\phi^\delta(t, x, k) = \psi^\delta(\delta t, \delta x, k)$ and write an asymptotic multiple scale expansion for ψ^δ

$$
\psi^\delta(t, x, k) = \bar{\phi}(t, x, k) + \sqrt{\delta}\phi_1\left(t, x, \frac{x}{\delta}, k\right) + \delta\phi_2\left(t, x, \frac{x}{\delta}, k\right) + \ldots \tag{2.19}
$$

We assume formally that the leading order term $\bar{\phi}$ is deterministic and independent of the fast variable $z = x/\delta$. We insert this expansion into (2.9) and obtain in the order $O\left(\delta^{-1/2}\right)$:

$$
\nabla_z H_1(z, k) \cdot \nabla_k \bar{\phi} - H_0'(k)\hat{k} \cdot \nabla_z \phi_1 = 0. \tag{2.20}
$$

Let $\theta \ll 1$ be a small positive regularization parameter that will be later sent to zero, and consider a regularized version of (2.20):

$$
\frac{1}{H_0'(k)} \nabla_z H_1(z, k) \cdot \nabla_k \bar{\phi} - \hat{k} \cdot \nabla_z \phi_1 + \theta\phi_1 = 0,
$$

Its solution is

$$
\phi_1(z, k) = -\frac{1}{H_0'(k)} \int_0^{\infty} \sum_{m=1}^{d} \frac{\partial H_1(z + s\hat{k}, k)}{\partial z_m} \frac{\partial \bar{\phi}(t, x, k)}{\partial k_m} e^{-\theta s} ds. \tag{2.21}
$$

The next order equation becomes upon averaging

$$\frac{\partial\bar\phi}{\partial t} = \mathbb{E}\left(\frac{\partial H_1(z,k)}{\partial k}\,\hat k\cdot\nabla_z\phi_1\right) - \mathbb{E}\left(\nabla_z H_1(z,k)\cdot\nabla_k\phi_1\right) + H_0'(k)\hat k\cdot\nabla_x\bar\phi. \tag{2.22}$$

The first two terms on the right hand side above may be computed explicitly using expression (2.21) for ϕ_1:

$$\begin{aligned}
&\mathbb{E}\left(\frac{\partial H_1(z,k)}{\partial k}\hat k\cdot\nabla_z\phi_1\right) - \mathbb{E}\left(\nabla_z H_1(z,k)\cdot\nabla_k\phi_1\right)\\
&= -\mathbb{E}\left[\sum_{m,n=1}^d \frac{\partial H_1(z,k)}{\partial k}\hat k_m\frac{\partial}{\partial z_m}\left(\frac{1}{H_0'(k)}\int_0^\infty \frac{\partial H_1(z+s\hat k,k)}{\partial z_n}\frac{\partial\bar\phi(t,x,k)}{\partial k_n}\,e^{-\theta s}ds\right)\right]\\
&+\mathbb{E}\left[\sum_{m,n=1}^d \frac{\partial H_1(z,k)}{\partial z_m}\frac{\partial}{\partial k_m}\left(\frac{1}{H_0'(k)}\int_0^\infty \frac{\partial H_1(z+s\hat k,k)}{\partial z_n}\frac{\partial\bar\phi(t,x,k)}{\partial k_n}\,e^{-\theta s}ds\right)\right].
\end{aligned}$$

Using spatial stationarity of $H_1(z,k)$ we may rewrite the above as

$$\begin{aligned}
&-\mathbb{E}\left[\sum_{m,n=1}^d \frac{\partial H_1(z,k)}{\partial k}\hat k_m\frac{\partial}{\partial z_m}\left(\frac{1}{H_0'(k)}\int_0^\infty \frac{\partial H_1(z+s\hat k,k)}{\partial z_n}\frac{\partial\bar\phi(t,x,k)}{\partial k_n}\,e^{-\theta s}ds\right)\right]\\
&-\mathbb{E}\left[\sum_{m,n=1}^d H_1(z,k)\frac{\partial}{\partial z_m}\frac{\partial}{\partial k_m}\left(\frac{1}{H_0'(k)}\int_0^\infty \frac{\partial H_1(z+s\hat k,k)}{\partial z_n}\frac{\partial\bar\phi(t,x,k)}{\partial k_n}\,e^{-\theta s}ds\right)\right]\\
&= -\sum_{m,n=1}^d \frac{\partial}{\partial k_m}\left[\frac{1}{H_0'(k)}\int_0^\infty \mathbb{E}\left(H_1(z,k)\frac{\partial^2 H_1(z+s\hat k,k)}{\partial z_n\partial z_m}\right)\frac{\partial\bar\phi(t,x,k)}{\partial k_n}\,e^{-\theta s}ds\right]\\
&= -\sum_{m,n=1}^d \frac{\partial}{\partial k_m}\left(\frac{1}{H_0'(k)}\int_0^\infty \frac{\partial^2 R(s\hat k,k)}{\partial x_n\partial x_m}\frac{\partial\bar\phi(t,x,k)}{\partial k_n}\,e^{-\theta s}ds\right)\\
&\to -\frac{1}{2}\sum_{m,n=1}^d \frac{\partial}{\partial k_m}\left(\frac{1}{H_0'(k)}\int_{-\infty}^\infty \frac{\partial^2 R(s\hat k,k)}{\partial x_n\partial x_m}\frac{\partial\bar\phi(t,x,k)}{\partial k_n}ds\right),\ \text{as } \theta\to 0^+.
\end{aligned}$$

We insert the above expression into (2.22) and obtain

$$\frac{\partial\bar\phi}{\partial t} = \sum_{m,n=1}^d \frac{\partial}{\partial k_n}\left(D_{nm}(\hat k,k)\frac{\partial\bar\phi}{\partial k_m}\right) + H_0'(k)\hat k\cdot\nabla_x\bar\phi \tag{2.23}$$

with the diffusion matrix $D(\hat k,k)$ as in (2.10). Observe that (2.23) is nothing but (2.11). However, the naive asymptotic expansion (2.19) may not be justified. The rigorous proof presented in the next section is based on a quite different method.

2.3 From the Liouville equation to the momentum diffusion. Estimation of the convergence rates: proof of Theorem 2.2.1

Outline of the proof

The basic idea of the proof of Theorem 2.2.1 is a modification of that of [6, 40]. We consider the trajectories corresponding to the Liouville equation (2.9) and introduce a stopping time, called τ_δ, that, among others, prevents near self-intersection of trajectories. This fact ensures that until the stopping time occurs the particle is "exploring a new territory" and, thanks to the strong mixing properties of the medium, "memory effects" are lost. Therefore, roughly speaking, until the stopping time the process is approximately characterized by the Markov property. Furthermore, since the amplitude of the random Hamiltonian is not strong enough to destroy the continuity of its path, it becomes a diffusion in the limit, as $\delta \to 0$. We introduce also an augmented process that follows the trajectories of the Hamiltonian flow until the stopping time τ_δ and becomes a diffusion after $t = \tau_\delta$. We show that the law of the augmented process is close to the law of a diffusion, see Proposition 2.3.3, with an explicit error bound. We also prove that the stopping time tends to infinity as $\delta \to 0$, once again with the error bound that is proved in Theorem 2.3.4. The combination of these two results allows us to estimate the difference between the solutions of the Liouville and the diffusion equations in a rather straightforward manner: they are close until the stopping time as the law of the diffusion is always close to that of the augmented process, while the latter coincides with the true process until τ_δ. On the other hand, the fact that $\tau_\delta \to \infty$ as $\delta \to 0$ shows that with a large probability the augmented process is close to the true process. This combination finishes the proof.

The random characteristics corresponding to (2.9)

Consider the motion of a particle governed by a Hamiltonian system of equations

$$\begin{cases} \frac{dz^{(\delta)}(t;\mathbf{x},\mathbf{k})}{dt} = (\nabla_{\mathbf{k}} H_\delta)\left(\frac{z^{(\delta)}(t;\mathbf{x},\mathbf{k})}{\delta}, \mathbf{m}^{(\delta)}(t;\mathbf{x},\mathbf{k})\right) \\ \frac{d\mathbf{m}^{(\delta)}(t;\mathbf{x},\mathbf{k})}{dt} = -\frac{1}{\sqrt{\delta}}(\nabla_z H_\delta)\left(\frac{z^{(\delta)}(t;\mathbf{x},\mathbf{k})}{\delta}, \mathbf{m}^{(\delta)}(t;\mathbf{x},\mathbf{k})\right) \\ z^{(\delta)}(0;\mathbf{x},\mathbf{k}) = \mathbf{x}, \quad \mathbf{m}^{(\delta)}(0;\mathbf{x},\mathbf{k}) = \mathbf{k}, \end{cases} \tag{2.24}$$

where the Hamiltonian $H_\delta(x,k) := H_0(k) + \sqrt{\delta} H_1(x,k)$, $k = |k|$. The trajectories of (2.24) are the characteristics of the Liouville equation (2.9). We denote by $Q^\delta_{s,\mathbf{x},\mathbf{k}}(\cdot)$ the law over $\mathcal{C}$ of the process corresponding to (2.24) starting at $t = s$ from $(\mathbf{x},\mathbf{k})$.

The stopping times

We now define the stopping time τ_δ, described in Section 2.3, that prevents the trajectories of (2.24) to have near self-intersections (recall that the intent of the stopping time is to prevent any "memory effects" of the trajectories). As we have already mentioned, we will later show that the probability of the event $[\,\tau_\delta < T\,]$ for a fixed $T > 0$ goes to zero, as $\delta \to 0$.

Let $0 < \epsilon_1 < \epsilon_2 < 1/2$, $\epsilon_3 \in (0, 1/2 - \epsilon_2)$, $\epsilon_4 \in (1/2, 1 - \epsilon_1 - \epsilon_2)$ be small positive constants that will be further determined later and set

$$N = [\delta^{-\epsilon_1}], \quad p = [\delta^{-\epsilon_2}], \quad q = p\,[\delta^{-\epsilon_3}], \quad N_1 = Np\,[\delta^{-\epsilon_4}]. \tag{2.25}$$

We will specify additional restrictions on the constants ϵ_j as the need for such constraints arises. However, the basic requirement is that ϵ_i, $i = 1,2,3$ should be sufficiently small and ϵ_4 is bigger than $1/2$, less than one and can be made as close to one as we would need it. It is important that $\epsilon_1 < \epsilon_2$ so that $N \ll p$ when $\delta \ll 1$. We introduce the following $(\mathcal{M}^t)_{t\geq 0}$– stopping times. Let $t_k^{(p)} := kp^{-1}$ be a mesh of times, and $\pi \in \mathcal{C}$ be a path. We define the "violent turn" stopping time

$$S_\delta(\pi) := \inf\left[t \ge 0 : \text{ for some } k \ge 0 \text{ we have } t \in \left[t_k^{(p)}, t_{k+1}^{(p)}\right) \text{ and } \right. \tag{2.26}$$
$$\left. \hat{K}(t_{k-1}^{(p)}) \cdot \hat{K}(t) \le 1 - \frac{1}{N}, \text{ or } \hat{K}\left(t_k^{(p)} - \frac{1}{N_1}\right) \cdot \hat{K}(t) \le 1 - \frac{1}{N}\right],$$

where by convention we set $\hat{K}(-1/p) := \hat{K}(0)$. Note that with the above choice of ϵ_4 we have $\hat{K}\left(t_k^{(p)} - 1/N_1\right) \cdot \hat{K}(t_k^{(p)}) > 1 - 1/N$, provided that $\delta \in (0, \delta_0]$ and δ_0 is sufficiently small. We adopt in (2.26) a customary convention that the infimum of an empty set equals $+\infty$. The stopping time S_δ is triggered when the trajectory performs a sudden turn – this is undesirable as the trajectory may then return back to the region it has already visited and create correlations with the past.

For each $t \ge 0$, we denote by $\mathfrak{X}_t(\pi) := \bigcup_{0 \le s \le t} X(s; \pi)$ the trace of the spatial component of the path π up to time t, and by $\mathfrak{X}_t(q; \pi) := [x : \text{dist}\,(x, \mathfrak{X}_t(\pi)) \le 1/q]$ a tubular region around the path. We introduce the stopping time

$$U_\delta(\pi) := \inf\left[t \ge 0 : \exists\, k \ge 1 \text{ and } t \in [t_k^{(p)}, t_{k+1}^{(p)}) \text{ for which } X(t) \in \mathfrak{X}_{t_{k-1}^{(p)}}(q)\right]. \tag{2.27}$$

It is associated with the return of the X component of the trajectory to the tube around its past – this is again an undesirable way to create correlations with the past. Finally, we set the stopping time

$$\tau_\delta(\pi) := S_\delta(\pi) \wedge U_\delta(\pi). \tag{2.28}$$

2.3.1 The cut-off functions and the corresponding dynamics

Let $M > 0$ be fixed and p, q, N, N_1 be the positive integers defined in Section 2.3. We define now several auxiliary functions that will be used to introduce the cut-offs in the dynamics. These cut-offs will ensure that the particle moving under the modified dynamics will avoid self-intersections, will have no violent turns and the changes of its momentum will be under control. In addition, up to the stopping time τ_δ the motion of the particle will coincide with the motion under the original Hamiltonian flow.

Let $a_1 = 2$ and $a_2 = 3/2$. The functions $\psi_j : \mathbb{R}^d \times \mathbb{S}_1^{d-1} \to [0, 1]$, $j = 1, 2$ are of C^∞ class and satisfy

$$\psi_j(\mathbf{k}, \mathbf{l}) = \begin{cases} 1, & \text{if } \quad \hat{\mathbf{k}} \cdot \mathbf{l} \ge 1 - 1/N \qquad \text{and} \qquad M_\delta^{-1} \le |\mathbf{k}| \le M_\delta \\ & \\ 0, & \text{if } \quad \hat{\mathbf{k}} \cdot \mathbf{l} \le 1 - a_j/N, \quad \text{or} \quad |\mathbf{k}| \le (2M_\delta)^{-1}, \quad \text{or} \quad |\mathbf{k}| \ge 2M_\delta. \end{cases} \tag{2.29}$$

One can construct ψ_j in such a way that for arbitrary nonnegative integers m, n it is possible to find a constant $C_{m,n}$ for which $\|\psi_j\|_{m,n} \le C_{m,n} N^{m+n}$. The cut-off function

$$\Psi(t, \mathbf{k}; \pi) := \begin{cases} \psi_1\left(\mathbf{k}, \hat{K}\left(t_{k-1}^{(p)}\right)\right) \psi_2\left(\mathbf{k}, \hat{K}\left(t_k^{(p)} - 1/N_1\right)\right) & \text{for } t \in [t_k^{(p)}, t_{k+1}^{(p)}) \text{ and } k \ge 1 \\ \psi_2(\mathbf{k}, \hat{K}(0)) & \text{for } t \in [0, t_1^{(p)}) \end{cases} \tag{2.30}$$

will allow us to control the direction of the particle motion over each interval of the partition as well as not to allow the trajectory to escape to the regions where the change of the size of the velocity can be uncontrollable.

Let $\phi : \mathbb{R}^d \times \mathbb{R}^d \to [0,1]$ be a function of the C^∞ class that satisfies $\phi(\mathbf{y},\mathbf{x}) = 1$, when $|\mathbf{y}-\mathbf{x}| \geq 3/q$ and $\phi(\mathbf{y},\mathbf{x}) = 0$, when $|\mathbf{y}-\mathbf{x}| \leq 2/q$. Again, in this case we can construct ϕ in such a way that $\|\phi\|_{m,n} \leq Cq^{m+n}$ for arbitrary integers m,n and a suitably chosen constant C. The function $\phi_k : \mathbb{R}^d \times \mathcal{C} \to [0,1]$ for a fixed path π is given by

$$\phi_k(\mathbf{y};\pi) = \prod_{0\leq l/q \leq t_{k-1}^{(p)}} \phi\left(\mathbf{y}, X\left(\frac{l}{q}\right)\right). \tag{2.31}$$

We set

$$\Phi(t,\mathbf{y};\pi) := \begin{cases} 1, & \text{if } 0 \leq t < t_1^{(p)} \\ \phi_k(\mathbf{y};\pi), & \text{if } t_k^{(p)} \leq t < t_{k+1}^{(p)}. \end{cases} \tag{2.32}$$

The function Φ shall be used to modify the dynamics of the particle in order to avoid a possibility of near self-intersections of its trajectory.

Finally, let us set

$$F_\delta(t,\mathbf{y},\mathbf{l};\pi,\omega) = \Theta(t,\delta\mathbf{y},\mathbf{l};\pi)\nabla_{\mathbf{y}} H_1(\mathbf{y},|\mathbf{l}|;\omega). \tag{2.33}$$

For a fixed $(\mathbf{x},\mathbf{k}) \in \mathbb{R}^{2d}_*$, $\delta > 0$ and $\omega \in \Omega$ we consider the modified particle dynamics with the cut-off that is described by the stochastic process $(y^{(\delta)}(t;\mathbf{x},\mathbf{k},\omega), \boldsymbol{l}^{(\delta)}(t;\mathbf{x},\mathbf{k},\omega))_{t\geq 0}$ whose paths are the solutions of the following equation

$$\begin{cases} \frac{dy^{(\delta)}(t;\mathbf{x},\mathbf{k})}{dt} = \left[H_0'(|\boldsymbol{l}^{(\delta)}(t;\mathbf{x},\mathbf{k})|) + \sqrt{\delta}\,\partial_l H_1\left(\frac{y^{(\delta)}(t;\mathbf{x},\mathbf{k})}{\delta}, |\boldsymbol{l}^{(\delta)}(t;\mathbf{x},\mathbf{k})|\right)\right]\hat{\boldsymbol{l}}^{(\delta)}(t;\mathbf{x},\mathbf{k},) \\ \frac{d\boldsymbol{l}^{(\delta)}(t;\mathbf{x},\mathbf{k})}{dt} = -\frac{1}{\sqrt{\delta}}\,F_\delta\left(t, \frac{y^{(\delta)}(t;\mathbf{x},\mathbf{k})}{\delta}, \boldsymbol{l}^{(\delta)}(t;\mathbf{x},\mathbf{k}); y^{(\delta)}(\cdot;\mathbf{x},\mathbf{k}), \boldsymbol{l}^{(\delta)}(\cdot;\mathbf{x},\mathbf{k})\right) \\ y^{(\delta)}(0;\mathbf{x},\mathbf{k}) = \mathbf{x}, \quad \boldsymbol{l}^{(\delta)}(0;\mathbf{x},\mathbf{k}) = \mathbf{k}. \end{cases} \tag{2.34}$$

We will denote by $\tilde{Q}^{(\delta)}_{\mathbf{x},\mathbf{k}}$ the law of the modified process $(y^{(\delta)}(\cdot;\mathbf{x},\mathbf{k}), \boldsymbol{l}^{(\delta)}(\cdot;\mathbf{x},\mathbf{k}))$ over $\mathcal{C}$ for a given $\delta > 0$ and by $\tilde{E}^{(\delta)}_{\mathbf{x},\mathbf{k}}$ the corresponding expectation. We assume that the initial momentum $\mathbf{k} \in A(M)$. From the construction of the cut-offs we immediately conclude that

$$\hat{\boldsymbol{l}}^{(\delta)}(t) \cdot \hat{\boldsymbol{l}}^{(\delta)}(t_{k-1}^{(p)}) \geq 1 - \frac{2}{N}, \quad t \in [t_{k-1}^{(p)}, t_{k+1}^{(p)}), \quad \forall\, k \geq 0. \tag{2.35}$$

2.3.2 Some consequences of the mixing assumption

For any $t \geq 0$ we denote by $\mathcal{F}_t$ the σ-algebra generated by $(y^{(\delta)}(s), \boldsymbol{l}^{(\delta)}(s))$, $s \leq t$. Here we suppress, for the sake of abbreviation, writing the initial data in the notation of the trajectory. In this section we assume that $M > 0$ is fixed, $X_1, X_2 : (\mathbb{R} \times \mathbb{R}^d \times \mathbb{R}^{d^2})^2 \to \mathbb{R}$ are certain continuous functions, Z is a random variable and g_1, g_2 are $\mathbb{R}^d \times [M^{-1}, M]$-valued random vectors. We suppose further that Z, g_1, g_2, are $\mathcal{F}_t$-measurable, while $\tilde{X}_1, \tilde{X}_2$ are random fields of the form

$$\tilde{X}_i(\mathbf{x},k) = X_i\left(\left(\partial_k^j H_1(\mathbf{x},k), \nabla_{\mathbf{x}}\partial_k^j H_1(\mathbf{x},k), \nabla^2_{\mathbf{x}}\partial_k^j H_1(\mathbf{x},k)\right)_{j=0,1}\right).$$

For $i = 1,2$ we denote $g_i := (g_i^{(1)}, g_i^{(2)})$ where $g_i^{(1)} \in \mathbb{R}^d$ and $g_i^{(2)} \in [M^{-1}, M]$. We also let

$$U(\theta_1,\theta_2) := \mathbb{E}\left[\tilde{X}_1(\theta_1)\tilde{X}_2(\theta_2)\right], \quad \theta_1,\theta_2 \in \mathbb{R}^d \times [M^{-1}, M]. \tag{2.36}$$

The following mixing lemma is useful in formalizing the "memory loss effect" and can be proved in the same way as Lemmas 5.2 and 5.3 of [6]. It is also similar in spirit to Lemma 1.2.2.

Lemma 2.3.1 *(i) Assume that $r, t \geq 0$ and*

$$\inf_{u \leq t} \left| g_i^{(1)} - \frac{y^{(\delta)}(u)}{\delta} \right| \geq \frac{r}{\delta}, \tag{2.37}$$

$\mathbb{P}$–a.s. on the set $Z \neq 0$ for $i = 1, 2$. Then, we have

$$\left| \mathbb{E} \left[\tilde{X}_1(g_1) \tilde{X}_2(g_2) Z \right] - \mathbb{E} \left[U(g_1, g_2) Z \right] \right| \leq 2\phi \left(\frac{r}{2\delta} \right) \|X_1\|_{L^\infty} \|X_2\|_{L^\infty} \|Z\|_{L^1(\Omega)}. \tag{2.38}$$

(ii) Let $\mathbb{E} X_1(\mathbf{0}, k) = 0$ for all $k \in [M^{-1}, M]$. Furthermore, we assume that g_2 satisfies (2.37),

$$\inf_{u \leq t} \left| g_1^{(1)} - \frac{y^{(\delta)}(u)}{\delta} \right| \geq \frac{r + r_1}{\delta} \tag{2.39}$$

and $|g_1^{(1)} - g_2^{(1)}| \geq r_1 \delta^{-1}$ for some $r_1 \geq 0$, $\mathbb{P}$-a.s. on the event $Z \neq 0$. Then, we have

$$\left| \mathbb{E} \left[\tilde{X}_1(g_1) \tilde{X}_2(g_2)\, Z \right] - \mathbb{E} \left[U(g_1, g_2) Z \right] \right| \leq C \phi^{1/2} \left(\frac{r}{2\delta} \right) \phi^{1/2} \left(\frac{r_1}{2\delta} \right) \|X_1\|_{L^\infty} \|X_2\|_{L^\infty} \|Z\|_{L^1(\Omega)} \tag{2.40}$$

for some absolute constant $C > 0$. Here the function U is given by (2.36).

2.3.3 The momentum diffusion

Let $\mathbf{k}(t)$ be a diffusion, starting at $k \in \mathbb{R}^d_*$ at $t = 0$, with the generator of the form

$$\begin{aligned} \mathcal{L}F(\mathbf{k}) &= \sum_{m,n=1}^{d} D_{mn}(\hat{\mathbf{k}}, |k|) \partial^2_{k_m, k_n} F(\mathbf{k}) + \sum_{m=1}^{d} E_m(\hat{\mathbf{k}}, |k|) \partial_{k_m} F(\mathbf{k}) \\ &= \sum_{m,n=1}^{d} \partial_{k_m} \left(D_{m,n}(\hat{\mathbf{k}}, |k|) \partial_{k_n} F(\mathbf{k}) \right), \quad F \in C_0^\infty(\mathbb{R}^d_*). \end{aligned} \tag{2.41}$$

Here the diffusion matrix is given by (2.10) and the drift vector is

$$E_m(\hat{\mathbf{k}}, l) = -\frac{1}{H_0'(l) l} \sum_{n=1}^{d} \int_0^{+\infty} s \frac{\partial^3 R(s\hat{\mathbf{k}}, l)}{\partial x_m \partial x_n^2}\, ds, \quad m = 1, \ldots, d.$$

Employing exactly the same argument as the one used in Section 4 of [6] it can be easily seen that this diffusion is supported on $\mathbb{S}^{d-1}_k$, where $k = |k|$. Moreover, it is non-degenerate on the sphere, for instance, under the assumption (2.8), cf. Proposition 4.3 of ibid.

Let $\mathfrak{Q}_{\mathbf{x},\mathbf{k}}$ be the law of the process $(\mathbf{x}(t), \mathbf{k}(t))$ that starts at $t = 0$ from $(\mathbf{x}, \mathbf{k})$ given by $\mathbf{x}(t) = x + \int_0^t H_0'(|\mathbf{k}(s)|) \hat{\mathbf{k}}(s) ds$, where $\mathbf{k}(t)$ is the diffusion described by (2.41). This process is a degenerate diffusion whose generator is given by

$$\tilde{\mathcal{L}} F(\mathbf{x}, \mathbf{k}) = \mathcal{L}_k F(\mathbf{x}, \mathbf{k}) + H_0'(|\mathbf{k}|)\, \hat{\mathbf{k}} \cdot \nabla_x F(\mathbf{x}, \mathbf{k}), \quad F \in C_0^\infty(\mathbb{R}^{2d}_*). \tag{2.42}$$

Here the notation $\mathcal{L}_k$ stresses that the operator $\mathcal{L}$ defined in (2.41) acts on the respective function in the k variable. We denote by $\mathfrak{M}_{x,k}$ the expectation corresponding to the path measure $\mathfrak{Q}_{\mathbf{x},\mathbf{k}}$.

2.3.4 The augmented process

The following construction of the augmentation of path measures has been carried out in Section 6.1 of [59]. Let $s \geq 0$ be fixed and $\pi \in \mathcal{C}$. Then, according to Lemma 6.1.1 of ibid. there exists a unique probability measure, that is denoted by $\delta_\pi \otimes_s \mathfrak{Q}_{X(s),K(s)}$, such that for any pair of events $A \in \mathcal{M}^s$, $B \in \mathcal{M}$ we have $\delta_\pi \otimes_s \mathfrak{Q}_{X(s),K(s)}[A] = \mathbf{1}_A(\pi)$ and $\delta_\pi \otimes_s \mathfrak{Q}_{X(s),K(s)}[\theta_s(B)] = \mathfrak{Q}_{X(s),K(s)}[B]$. The following result is a direct consequence of Theorem 6.2.1 of [59].

Proposition 2.3.2 *There exists a unique probability measure $R^{(\delta)}_{x,k}$ on $\mathcal{C}$ such that $R^{(\delta)}_{x,k}[A] := Q^{(\delta)}_{x,k}[A]$ for all $A \in \mathcal{M}^{\tau_\delta}$ and the regular conditional probability distribution of $R^{(\delta)}_{x,k}[\,\cdot\,|\mathcal{M}^{\tau_\delta}]$ is given by $\delta_\pi \otimes_{\tau_\delta(\pi)} \mathfrak{Q}_{X(\tau_\delta(\pi)),K(\tau_\delta(\pi))}$, $\pi \in \mathcal{C}$. This measure shall be also denoted by $Q^{(\delta)}_{x,k} \otimes_{\tau_\delta} \mathfrak{Q}_{X(\tau_\delta),K(\tau_\delta)}$.*

Note that for any $(\mathbf{x}, \mathbf{k}) \in \mathcal{A}(M)$ and $A \in \mathcal{M}^{\tau_\delta}$ we have

$$R^{(\delta)}_{\mathbf{x},\mathbf{k}}[A] = Q^{(\delta)}_{\mathbf{x},\mathbf{k}}[A] = \tilde{Q}^{(\delta)}_{\mathbf{x},\mathbf{k}}[A], \tag{2.43}$$

that is, the law of the augmented process coincides with that of the true process, and of the modified process with the cut-offs until the stopping time τ_δ. Hence, according to the uniqueness part of Proposition 2.3.2, in such a case $Q^{(\delta)}_{x,k} \otimes_{\tau_\delta} \mathfrak{Q}_{X(\tau_\delta),K(\tau_\delta)} = \tilde{Q}^{(\delta)}_{x,k} \otimes_{\tau_\delta} \mathfrak{Q}_{X(\tau_\delta),K(\tau_\delta)}$. We denote by $E^{(\delta)}_{x,k}$ the expectation with respect to the augmented measure described by the above proposition. Let also $R^{(\delta)}_{x,k,\pi}$, $E^{(\delta)}_{x,k,\pi}$ denote the respective conditional law and expectation obtained by conditioning $R^{(\delta)}_{x,k}$ on $\mathcal{M}^{\tau_\delta}$.

The following proposition is of crucial importance for us, as it shows that the law of the augmented process is close to that of the momentum diffusion as $\delta \to 0$. To abbreviate the notation we let

$$N_t(G) := G(t, X(t), K(t)) - G(0, X(0), K(0)) - \int_0^t (\partial_\varrho + \tilde{\mathcal{L}})G(\varrho, X(\varrho), K(\varrho)))\, d\varrho$$

for any $G \in C^{1,1,3}_b([0, +\infty) \times \mathbb{R}^{2d}_*)$ and $t \geq 0$.

Proposition 2.3.3 *Suppose that $(x, k) \in \mathcal{A}(M)$ and $\zeta \in C_b((\mathbb{R}^{2d}_*)^n)$ is nonnegative. Let $\gamma_0 \in (0, 1/2)$ and let $0 \leq t_1 < \cdots < t_n \leq T_* \leq t < v \leq T$. We assume further that $v - t \geq \delta^{\gamma_0}$. Then, there exist constants γ_1, C such that for any function $G \in C^{1,1,3}([T_*, T] \times \mathbb{R}^{2d}_*)$ we have*

$$\left| E^{(\delta)}_{x,k} \left\{ [N_v(G) - N_t(G)]\, \tilde{\zeta} \right\} \right| \leq C\delta^{\gamma_1}(v - t)\|G\|^{[T_*,T]}_{1,1,3} T^2 E^{(\delta)}_{x,k} \tilde{\zeta}. \tag{2.44}$$

Here $\tilde{\zeta}(\pi) := \zeta(X(t_1), K(t_1), \ldots, X(t_n), K(t_n))$, $\pi \in \mathcal{C}(T, \delta)$. The choice of the constants γ_1, C does not depend on (x, k), $\delta \in (0, 1]$, ζ, times $t_1, \ldots, t_n, T_*, T, v, t$, or the function G.

A very technical consequence of this proposition is an estimate of the stopping time:

Theorem 2.3.4 *Assume that the dimension $d \geq 3$. Then, one can choose $\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4$ in such a way that there exist constants $C, \gamma > 0$ for which*

$$R^{(\delta)}_{x,k}\, [\,\tau_\delta < T] \leq C\delta^\gamma T, \quad \forall\, \delta \in (0, 1],\, T \geq 1,\, (x, k) \in \mathcal{A}(M). \tag{2.45}$$

From the above two facts the proof of Theorem 2.2.1 is quite straightforward but we leave the technicalities out.

Chapter 3

The Wigner transform

3.1 The semiclassical limit of the Schrödinger equation

3.1.1 The unscaled Wigner transform

The Schrödinger equation

$$i\phi_t + \frac{1}{2}\Delta\phi - V(t,x)\phi = 0. \tag{3.1}$$

with a real potential $V(t,x)$ preserves the total energy of the solution (or the total number of particles depending on the point of view or physical application):

$$\mathcal{E}(t) = \int |\phi(t,x)|^2 dx = \mathcal{E}(0).$$

This may be verified by a straightforward time differentiation. However, often one is interested not only in the conservation of the total energy $\mathcal{E}(t)$ but also in its local spatial distribution – that is, where the energy is concentrated. This requires understanding of the local energy density $E(t,x) = |\phi(t,x)|^2$. Note that even if $\phi(t,x)$ is oscillatory the function $E(t,x)$ may vary slowly in space – this happens, for instance, in geometric optics. Unfortunately, while all the information about the "relatively simple" function $E(t,x)$ may be extracted from a "complicated" function $\phi(t,x)$, the energy density $E(t,x)$ itself does not satisfy a closed equation. Rather, its evolution is described as a conservation law

$$\frac{\partial E}{\partial t} + \nabla \cdot F = 0$$

with the flux

$$F(t,x) = \frac{1}{2i}\left(\bar{\phi}\nabla\phi - \phi\nabla\bar{\phi}\right).$$

A remedy for this lack of equation for $E(t,x)$ when the potential $V = 0$ was proposed by Wigner in his 1932 paper [84] (where he credits Szilard for this discovery). Wigner introduced the following object:

$$W(t,x,k) = \int \phi\left(t, x - \frac{y}{2}\right)\bar{\phi}\left(t, x + \frac{y}{2}\right) e^{ik\cdot y}\frac{dy}{(2\pi)^n}. \tag{3.2}$$

It is immediate to check that

$$\int W(t,x,k)dk = |\psi(t,x)|^2 = E(t,x), \tag{3.3}$$

so that in some sense $W(t,x,k)$ is "a local energy density resolved over momenta". In addition, the "average momentum" is

$$\begin{aligned}\int kW(t,x,k)dk &= \frac{1}{i}\int ik\phi\left(t,x-\frac{y}{2}\right)\bar{\phi}\left(t,x+\frac{y}{2}\right)e^{ik\cdot y}\frac{dydk}{(2\pi)^n}\\ &= -\frac{1}{i}\int \nabla_y\left[\phi\left(t,x-\frac{y}{2}\right)\bar{\phi}\left(t,x+\frac{y}{2}\right)\right]e^{ik\cdot y}\frac{dydk}{(2\pi)^n}\\ &= \frac{1}{2i}\left[\bar{\phi}(t,x)\nabla\phi(t,x)-\phi(t,x)\nabla\bar{\phi}(t,x)\right].\end{aligned}$$

Therefore, the flux can be expressed in terms of the Wigner transform as

$$F(t,x)=\int kW(t,x,k)dk,$$

re-enforcing the interpretation of $W(t,x,k)$ as a phase space energy density. It is also immediate to observe that $W(t,x,k)$ is real-valued.

The function $W(t,x,k)$ satisfies an evolution equation:

$$W_t + k\cdot\nabla_x W = 0. \tag{3.4}$$

Therefore, one may describe energy density evolution for the Schrödinger equation with zero potential as follows: compute the initial data $W(0,x,k)$, solve the kinetic equation (3.4) and find $|\phi(t,x)|^2$ using (3.3).

However, there is one drawback in the interpretation of $W(t,x,k)$ as electron energy density resolved over positions and momenta – there is no reason for $W(t,x,k)$ to be non-negative! Moreover, the same analysis for the Schrödinger equation (3.1) with a potential leads to the following evolution equation for $W(t,x,k)$:

$$\frac{\partial W}{\partial t}+k\cdot\nabla_x W=\frac{1}{i}\int e^{ip\cdot x}\hat{V}(p)\left[W\left(k-\frac{p}{2}\right)-W\left(k-\frac{p}{2}\right)\right]\frac{dp}{(2\pi)^n}. \tag{3.5}$$

While the uniform kinetic equation (3.4) posseses some nice properties – in particular, it preserves positivity of the initial data and has a particle interpretation: it describes density evolution of particles moving along the trajectories $\dot{X}=K$, $\dot{K}=0$, the Wigner equation (3.5) has very few attractions. In particular, it does not preserve positivity of the initial data. Probably, for that reason the Wigner transform ideas did not evolve mathematically (at least the did not spread widely) until the work of P. Gérard and L. Tartar in the late eighties. They have realized that the Wigner transforms become a useful tool in the analysis of the semiclassical asymptotics, that is, in the study of the oscillatory solutions of the Schrödinger equation (as well as in other oscilaltory problems).

3.1.2 The semiclassical Wigner transform

The definition of the Wigner transform for oscillatory functionns has to be modified: to see this consider a simple oscillating plane wave $\phi_\varepsilon(x)=e^{ik_0\cdot x/\varepsilon}$ with a fixed $k_0\in\mathbb{R}^n$. Then its Wigner transform as defined by (3.2) is

$$W(x,k)=\int e^{ik\cdot y}e^{ik_0\cdot(x-y/2)/\varepsilon-ik_0\cdot(x+y/2)/\varepsilon}\frac{dy}{(2\pi)^n}=\delta\left(k-\frac{k_0}{\varepsilon}\right).$$

We see that $W(x,k)$ does not have a nice limit as $\varepsilon\to 0$ – on the other hand its rescaled version $W_\varepsilon(x,k)=\varepsilon^{-d}W(x,k/\varepsilon)$ does converge to $\delta(k-k_0)$. This motivates the following defininition of the (rescaled) Wigner transform of a family of functions $\phi_\varepsilon(x)$:

$$W_\varepsilon(x,k)=\frac{1}{\varepsilon^d}\int\phi_\varepsilon\left(x-\frac{y}{2}\right)\bar{\phi}_\varepsilon\left(x+\frac{y}{2}\right)e^{ik\cdot y/\varepsilon}\frac{dy}{(2\pi)^n}$$

that may be more conveniently re-written as

Definition 3.1.1 *The Wigner transform (or the Wigner distribution) of a family of functions $\phi_\varepsilon(x)$ is a distribution $W_\varepsilon(x,k) \in \mathcal{S}'(\mathbb{R}^n \times \mathbb{R}^n)$ defined by*

$$W_\varepsilon(t,x,k) = \int \phi_\varepsilon\left(x - \frac{\varepsilon y}{2}\right) \bar{\phi}_\varepsilon\left(x + \frac{\varepsilon y}{2}\right) e^{ik\cdot y} \frac{dy}{(2\pi)^n}. \tag{3.6}$$

Expression (3.6) shows that $W_\varepsilon(x,k)$ is well suited to study functions oscillalting on the scale $\varepsilon \ll 1$ – in that case the difference of the arguments εy is chosen so that the function ϕ_ε changes by $O(1)$.

We will be mostly using the Wigner transform for families of solutions of non-dissipative evolution equations that conserve the L^2-norm (or a weighted L^2-norm). The scaling in (3.6) is particularly well suited for families of functions $\phi_\varepsilon(x)$ that are uniformly (in $\varepsilon \in (0,1)$) bounded in $L^2(\mathbb{R}^n)$. Let us define the space of test functions

$$\mathcal{A} = \left\{ \lambda(x,k) \in \mathcal{S}(\mathbb{R}^n \times \mathbb{R}^n) : \int \sup_x \left[\left| \tilde{\lambda}(x,y) \right| \right] dy < +\infty \right\}$$

with the norm

$$\|\lambda\|_{\mathcal{A}} = \int \sup_x \left[\left| \tilde{\lambda}(x,y) \right| \right] dy.$$

We have the following proposition.

Proposition 3.1.2 *Let the family of functions $\phi_\varepsilon(x)$ be uniformly bounded in $L^2(\mathbb{R}^n)$. Then the corresponding family of Wigner transforms $W_\varepsilon(x,k)$ is uniformly bounded in $\mathcal{A}'(\mathbb{R}^n \times \mathbb{R}^n)$.*

The following is an immediate corollary of the above proposition and Banach-Alaoglu theorem.

Corollary 3.1.3 *Let the family of functions $\psi_\varepsilon(x)$ be uniformly bounded in $L^2(\mathbb{R}^n)$. Then the corresponding family of Wigner transforms $W_\varepsilon(x,k)$ has a weak-$\star$ converging subsequence in the space $\mathcal{A}'(\mathbb{R}^n \times \mathbb{R}^n)$.*

The limit is a non-negative measure of a bounded total mass.

Proposition 3.1.4 *Let $\phi_\varepsilon(x)$ be a uniformly bounded family of functions in $L^2(\mathbb{R}^n)$, and let $W(x,k) \in \mathcal{S}'(\mathbb{R}^n \times \mathbb{R}^n)$ be a limit point of the corresponding family $W_\varepsilon(x,k)$. Then we have $W(x,k) \geq 0$ and the total mass $\int_{\mathbb{R}^{2n}} W(dxdk) < +\infty$.*

We summarize Corollary 3.1.3 and Proposition 3.1.4 into the following theorem.

Theorem 3.1.5 *Let the family ϕ_ε be uniformly bounded in $L^2(\mathbb{R}^n)$. Then the Wigner transform W_ε converges weakly along a subsequence $\varepsilon_k \to 0$ to a distribution $W(x,k) \in \mathcal{S}'(\mathbb{R}^n \times \mathbb{R}^n)$. Any such limit point $W(x,k)$ is a non-negative measure of bounded total mass.*

Can the weak convergence of the Wigner transforms become strong? This is possible in principle – for instance, the Wigner transforms of $\psi_\varepsilon(x) = e^{ik_0\cdot x/\varepsilon}$ is independent of ε – $W_\varepsilon(x,k) = \delta(k - k_0)$. However, this is impossible in $L^2(\mathbb{R}^n \times \mathbb{R}^n)$ as the L^2-norm of W_ε is unbounded unless $\phi_\varepsilon(x)$ converges strongly to zero:

$$\begin{aligned}
&\int |W_\varepsilon(x,k)|^2 dxdk \\
&= \int e^{ik\cdot y - ik\cdot y'} \phi_\varepsilon\left(x - \frac{\varepsilon y}{2}\right) \bar{\phi}_\varepsilon\left(x + \frac{\varepsilon y}{2}\right) \bar{\phi}_\varepsilon\left(x - \frac{\varepsilon y'}{2}\right) \phi_\varepsilon\left(x + \frac{\varepsilon y'}{2}\right) \frac{dydy'dxdk}{(2\pi)^{2n}} \\
&= \int \left| \phi_\varepsilon\left(x - \frac{\varepsilon y}{2}\right) \phi_\varepsilon\left(x + \frac{\varepsilon y}{2}\right) \right|^2 \frac{dydx}{(2\pi)^n} = \frac{1}{(2\pi\varepsilon)^n} \|\phi_\varepsilon\|^4_{L^2(\mathbb{R}^n)}.
\end{aligned}$$

Therefore, it is impossible to expect even weak convergence of W_ε in $L^2(\mathbb{R}^n \times \mathbb{R}^n)$ unless the family ϕ_ε converges strongly to zero. In that case, however, $W_\varepsilon = 0$, which is not a very interesting case.

3.1.3 Examples of the Wigner measures

We now present some examples of the Wigner measures.

A strongly converging sequence. Let $\phi_\varepsilon(x)$ converge strongly in $L^2(\mathbb{R}^n)$ to a limit $\phi(x)$. Then the limit Wigner measure is $W(x,k) = |\phi(x)|^2\delta(k)$. To see this we take a test function $a(x,k)$ and write

$$\langle a, W_\varepsilon\rangle = (a(x,\varepsilon D)\phi_\varepsilon, \phi_\varepsilon) = (a(x,\varepsilon D)[\phi_\varepsilon - \phi], \phi_\varepsilon) + (a(x,\varepsilon D)\phi, [\phi_\varepsilon - \phi]) + (a(x,\varepsilon D)\phi, \phi).$$

The first two terms above tend to zero as $\varepsilon \to 0$ as $\|\phi_\varepsilon - \phi\|_{L^2} \to 0$. Moreover, we also have

$$a(x,\varepsilon D)\phi \to a(x,0)\phi(x) \text{ in } L^2(\mathbb{R}^n)$$

as $\varepsilon \to 0$. It follows that

$$\langle a, W_\varepsilon\rangle \to \int a(x,0)|\phi(x)|^2 dx,$$

and thus the limit Wigner measure is indeed $W(x,k) = |\phi(x)|^2\delta(k)$. This means that unless we have some oscillations the limit Wigner measure is supported at $k = 0$.

The localized case. The Wigner transform of the family $f_\varepsilon(x) = \varepsilon^{-n/2}\phi(x/\varepsilon)$ with a compactly supported function $\phi(x)$ is given by $W(x,k) = (2\pi)^{-n}|\hat{\phi}(k)|^2\delta(x)$. This is verified as follows:

$$\begin{aligned}
\langle a, W_\varepsilon\rangle &= \int a(x,k)\phi\left(\frac{x}{\varepsilon} - \frac{y}{2}\right)\bar{\phi}\left(\frac{x}{\varepsilon} + \frac{y}{2}\right)e^{ik\cdot y}\frac{dydxdk}{(2\pi\varepsilon)^n} \\
&= \int a(\varepsilon x,k)\phi\left(x - \frac{y}{2}\right)\bar{\phi}\left(x + \frac{y}{2}\right)e^{ik\cdot y}\frac{dydxdk}{(2\pi)^n} \to \int a(0,k)\phi(x)\bar{\phi}(z)e^{ik\cdot(z-x)}\frac{dzdxdk}{(2\pi)^n} \\
&= \int\int a(0,k)|\hat{\phi}(k)|^2\frac{dk}{(2\pi)^n}.
\end{aligned}$$

The WKB case. The Wigner measure of the family $\phi_\varepsilon(x) = A(x)\exp\{iS(x)/\varepsilon\}$ with a smooth amplitude $A(x)$ and phase function $S(x)$, is $W(x,k) = |A(x)|^2\delta(k - \nabla S(x))$ since

$$\begin{aligned}
W^\varepsilon(x,k) &= \int_{\mathbb{R}^d} e^{ik\cdot y}e^{iS(x-\frac{\varepsilon y}{2})/\varepsilon}A(x - \frac{\varepsilon y}{2})e^{-iS(x+\frac{\varepsilon y}{2})/\varepsilon}\bar{A}(x + \frac{\varepsilon y}{2})\frac{dy}{(2\pi)^n} \\
&= \int_{\mathbb{R}^d} e^{ik\cdot y}e^{-i\nabla S(x)\cdot y}|A(x)|^2\frac{dy}{(2\pi)^n} + O(\varepsilon) = |A(x)|^2\delta(k - \nabla S) + O(\varepsilon).
\end{aligned}$$

Coherent states. The WKB and concentrated cases can be combined – this is a coherent state

$$\phi_\varepsilon(x) = \frac{1}{\varepsilon^{n/2}}\phi\left(\frac{x - x_0}{\varepsilon}\right)e^{ik_0\cdot x}.$$

The Wigner measure of this family is

$$W(x,k) = \frac{1}{(2\pi)^n}\delta(x - x_0)|\hat{\phi}(k - k_0)|^2.$$

Scale mismatch. The Wigner transform captures oscillations on a scale ε but not on a different scale. To see this consider a WKB family $\phi_\varepsilon(x) = A(x)e^{ik_0\cdot x/\varepsilon^\alpha}$ – we have treated the case $\alpha = 1$ but now we look at $0 \le \alpha < 1$ or $\alpha > 1$. First, if $\alpha \in (0, 1)$ then we have

$$W^\varepsilon(x,k) = \int_{\mathbb{R}^d} e^{ik\cdot y} e^{ik_0\cdot(x-\frac{\varepsilon y}{2})/\varepsilon^\alpha} A(x - \frac{\varepsilon y}{2}) e^{-ik_0\cdot(x+\frac{\varepsilon y}{2})/\varepsilon^\alpha} \bar{A}(x + \frac{\varepsilon y}{2})\frac{dy}{(2\pi)^n}$$
$$= \int_{\mathbb{R}^d} e^{i(k-\varepsilon^{1-\alpha}k_0)\cdot y}|A(x)|^2 \frac{dy}{(2\pi)^n} + O(\varepsilon) = |A(x)|^2\delta(k) + o(1).$$

Therefore, if $0 \le \alpha < 1$ then W_ε has the limit $W(x,k) = |A(x)|^2\delta(k)$ as in the case $\alpha = 0$ – the limit does not capture the oscillations at all. On the other hand, if $\alpha > 1$ then

$$\langle a, W_\varepsilon\rangle = \int e^{ik\cdot y} e^{ik_0\cdot(x-\frac{\varepsilon y}{2})/\varepsilon^\alpha} a(x,k) A(x - \frac{\varepsilon y}{2}) e^{-ik_0\cdot(x+\frac{\varepsilon y}{2})/\varepsilon^\alpha} \bar{A}(x + \frac{\varepsilon y}{2})\frac{dydxdk}{(2\pi)^n}$$
$$= \int e^{-ik_0\cdot y/\varepsilon^{1-\alpha}} \tilde{a}(x,y) A(x - \frac{\varepsilon y}{2})\bar{A}(x + \frac{\varepsilon y}{2})\frac{dxdy}{(2\pi)^n} \to 0$$

as $\varepsilon \to 0$. We see that when the family oscillates on a scale much smaller than ε the limit Wigner measure computed with respect to a "too large" scale ε vanishes and does not capture the oscillations correctly. This is a mixed blessing of the Wigner measures – they are very useful but only as long they are computed with respect to a correct scale. We will make this statement precise in the next section.

3.1.4 Basic properties of the Wigner measures

An important fact is that the Wigner measure is a local notion in space. We say that a family of functions $\phi_\varepsilon(x)$ is pure if the Wigner transforms W_ε converge as $\varepsilon \to 0$ to the limit $W(x,k)$ – that is, we do not need to pass to a subsequence $\varepsilon_k \to 0$ and the limit is unique.

Lemma 3.1.6 (Localization) *Let $\phi_\varepsilon(x)$ be a pure family of uniformly bounded functions in L^2 and let $\mu(x,k)$ be the unique limit Wigner measure of this family. Let $\theta(x)$ be a smooth function. Then the family $\psi_\varepsilon(x) = \theta(x)\phi_\varepsilon(x)$ is also pure, and the Wigner transforms $W_\varepsilon[\psi_\varepsilon]$ of the family $\psi_\varepsilon(x)$ converge to $|\theta(x)|^2\mu(x,k)$ as $\varepsilon \to 0$. Moreover, let ϕ_ε be a uniformly bounded pure family of L^2 functions, and let ψ_ε coincide with ϕ_ε in an open neighbourhood of a point x_0. Then the the limit Wigner measures $\mu[\phi]$ and $\mu[\psi]$ coincide in this neighborhood.*

Another useful and intuitively clear property is that the Wigner measure of waves going in different directions is the sum of the individual Wigner measures.

Lemma 3.1.7 (Orthogonality) *Let ϕ_ε, ψ_ε be two pure families of functions with Wigner measures μ and ν, respectively,which are mutually singular. Then the Wigner measure of the sum $\phi_\varepsilon + \psi_\varepsilon$ is $\mu + \nu$.*

The above properties: positivity, orthogonality and localization show that the Wigner measure may be indeed reasonably interpreted as the phase space energy density. However, the following pair of examples shows that the limit may not capture the energy correctly. The first "bad" example is the family

$$\phi_\varepsilon(x) = A(x)e^{ik\cdot x/\varepsilon^2}.$$

Then the limit Wigner transform is $W = 0$ while the spatial energy density $E(_\varepsilon(x) = |\phi_\varepsilon(x)|^2 \equiv |A(x)|^2$ does not vanish in the limit $\varepsilon \to 0$. The second "misbehavior" can be seen on the family

$$\phi_\varepsilon(x) = \theta\left(x - \frac{1}{\varepsilon}\right) \tag{3.7}$$

with $\theta(x) \in C_c^\infty(\mathbb{R}^n)$. Then the limit Wigner measure $W(x,k) = 0$ and the local energy density $|\phi_\varepsilon(x)|^2$ converges weakly to zero as well. However, the total mass $\|\phi_\varepsilon\|_{L^2} \equiv \|\theta\|_{L^2}$ is not captured correctly by the limit.

It turns out that the above two examples exhaust the possibilities for the Wigner measure to fail to capture the energy correctly and it is well suited for families of functions that depend on a small parameter in an oscillatory manner, the ε-oscillatory families of [69]. The ε-oscillatory property guarantees that the functions ϕ_ε oscillate on a scale which is not smaller than $O(\varepsilon)$, and is conveniently characterized by the following definition.

Definition 3.1.8 *A family of functions ϕ_ε that is bounded in L^2_{loc} is said to be ε-oscillatory if for every smooth and compactly supported function $\theta(x)$*

$$\limsup_{\varepsilon\to 0} \int_{|\xi|\geq R/\varepsilon} |\widehat{\theta\phi_\varepsilon}(\xi)|^2 d\xi \to 0 \quad \text{as} \quad R \to +\infty. \tag{3.8}$$

A simple and intuitive sufficient condition for (3.8) is that there exist a positive integer j and a constant C independent of ε such that

$$\varepsilon^j \left\| \frac{\partial^j f_\varepsilon}{\partial x^j} \right\|_{L^2_{loc}} \leq C. \tag{3.9}$$

Indeed, if (3.9) is satisfied then

$$\int_{\mathbb{R}^n} |\xi|^j |\widehat{(\theta f_\varepsilon)}|^2 d\xi \leq \frac{C}{\varepsilon^j}$$

and therefore

$$\int_{|\xi|\geq R/\varepsilon} |\widehat{\theta\phi_\varepsilon}(\xi)|^2 d\xi \leq \left(\frac{\varepsilon}{R}\right)^j \int_{|\xi|\geq R/\varepsilon} |\xi|^j |\widehat{\theta\phi_\varepsilon}(\xi)|^2 d\xi \leq \frac{C}{\varepsilon^j}\left(\frac{\varepsilon}{R}\right)^j = \frac{C}{R^j} \to 0 \text{ as } R \to +\infty$$

so that (3.8) holds. Condition (3.9) is satisfied, for instance, for high frequency plane waves $\phi_\varepsilon(x) = Ae^{i\xi\cdot x/\varepsilon}$ with wave vector ξ/ε, $\xi \in \mathbb{R}^n$ but not by a similar family with a wave vector ξ/ε^2: $\psi_\varepsilon(x) = Ae^{i\xi\cdot x/\varepsilon^2}$. Another natural example of ε-oscillatory functions is $g_\varepsilon(x) = g(x/\varepsilon)$, where $g(x)$ is a periodic function with a bounded gradient.

In order to curtail the ability of a family of functions to "run away to infinity" (as happens with the family (3.7)) we introduce the following definition.

Definition 3.1.9 *A bounded family $\phi_\varepsilon(x) \in L^2(\mathbb{R}^n)$ is said to be compact at infinity if*

$$\limsup_{\varepsilon\to 0} \int_{|x|\geq R} |\phi_\varepsilon(x)|^2 dx \to 0 \text{ as } R \to +\infty. \tag{3.10}$$

The main reason for introducing ε-oscillatory and compact at infinity families of functions is the following theorem concerning weak convergence of energy, i.e. of the integral of the square of the wave function.

Theorem 3.1.10 *Let ϕ_ε be a pure, uniformly bounded family in L^2_{loc} with the limit Wigner measure $\mu(x,k)$. Then, if $|\phi_\varepsilon(x)|^2$ converges to a measure ν on $\mathbb{R}^n$, we have*

$$\int_{\mathbb{R}^n} \mu(\cdot, dk) \leq \nu \tag{3.11}$$

with equality if and only if ϕ_ε is an ε-oscillatory family. Moreover, we also have

$$\int_{\mathbb{R}^n\times\mathbb{R}^n} \mu(dx,dk) \leq \limsup_{\varepsilon\to 0} \int_{\mathbb{R}^n} |\phi_\varepsilon(x)|^2 dx \tag{3.12}$$

with equality holding if and only if ϕ_ε is ε-oscillatory and compact at infinity. In this case lim sup *can be replaced by* lim *on the right side of (3.12).*

With this theorem and the positivity property we can interpret $\mu(x,k)$ as the limit phase space energy density of the family ϕ_ε, that is, energy density resolved over directions and wavenumbers.

3.1.5 The evolution of the Wigner transform

We will now derive the evolution equation for the Wigner measure of a family of functions $\phi_\varepsilon(t,x)$ that satisfy the semiclassical Schrödinger equation

$$i\varepsilon\frac{\partial\phi_\varepsilon}{\partial t}+\frac{\varepsilon^2}{2}\Delta\phi_\varepsilon-V(x)\phi_\varepsilon(x)=0 \tag{3.13}$$

with a smooth potential $V(x)$. The initial data $\phi_\varepsilon(0,x)=\phi_\varepsilon^0(x)$ forms an ε-oscillatory and compact at infinity family of functions uniformly bounded in $L^2(\mathbb{R}^n)$. As (3.13) preserves the L^2-norm of solutions, the family $\phi_\varepsilon(t,x)$ is bounded in $L^2(\mathbb{R}^n)$ for each $t\geq 0$ and it makes sense to define the Wigner transform

$$W_\varepsilon(t,x,k)=\int\psi_\varepsilon\left(t,x-\frac{\varepsilon y}{2}\right)\bar{\psi}_\varepsilon\left(t,x+\frac{\varepsilon y}{2}\right)e^{ik\cdot y}\frac{dy}{(2\pi)^n}. \tag{3.14}$$

We first obtain the equation for the limit Wigner transform directly "by hand". Differentiating (3.14) with respect to time, using (3.13) we arrive at the following equation for the Wigner transform

$$W_t^\varepsilon+k\cdot\nabla_x W^\varepsilon=\frac{i}{\varepsilon}\int_{\mathbb{R}^n}e^{ip\cdot x}\hat{V}(p)\left[W^\varepsilon(x,k-\frac{\varepsilon p}{2})-W^\varepsilon(x,k+\frac{\varepsilon p}{2})\right]\frac{dp}{(2\pi)^n}. \tag{3.15}$$

The limit Wigner measure $W(t,x,k)$ satisfies the Liouville equation in phase space

$$W_t+k\cdot\nabla_x W-\nabla V\cdot\nabla_k W=0 \tag{3.16}$$

with the initial condition $W(0,x,k)=W_0(x,k)$. We have the following proposition.

Proposition 3.1.11 *Let the family $\phi_\varepsilon^0(x)$ be uniformly bounded in $L^2(\mathbb{R}^n)$ and pure and let $W_0(x,k)$ be its Wigner measure. Then the Wigner transforms $W_\varepsilon(t,x,k)$ converge uniformly on finite time intervals in $\mathcal{S}'$ to the solution of (3.16) with the initial data $W(0,x,k)=W_0(x,k)$.*

Let us now compare the information one may obtain from the Liouville equation (3.16) to the standard geometric optics. First, we derive the eikonal and transport equations for the semiclassical Schrödinger equation (3.13). We consider initial data of the form

$$\phi^\varepsilon(0,x)=e^{iS_0(x)/\varepsilon}A_0(x) \tag{3.17}$$

with a smooth, real valued initial phase function $S_0(x)$ and a smooth compactly supported complex valued initial amplitude $A_0(x)$. We then look for an asymptotic solution of (3.13) in the same form as the initial data (3.17), with an evolved phase and amplitude

$$\phi^\varepsilon(t,x)=e^{iS(t,x)/\varepsilon}(A(t,x)+\varepsilon A_1(t,x)+\dots). \tag{3.18}$$

Inserting this form into (3.13) and equating the powers of ε we get evolution equations for the phase and amplitude

$$S_t+\frac{1}{2}|\nabla S|^2+V(x)=0,\qquad S(0,x)=S_0(x) \tag{3.19}$$

and

$$(|A|^2)_t + \nabla \cdot (|A|^2 \nabla S) = 0, \qquad |A(0,x)|^2 = |A_0(x)|^2. \tag{3.20}$$

The phase equation (3.19) is called the eikonal and the amplitude equation (3.20) the transport equation. The eikonal equation that evolves the phase is nonlinear and, in general, it will have a solution only up to some finite time t^* that depends on the initial phase.

How are the eikonal and transport equations related to the Liouville equation (3.16)? As we have computed before, for the WKB initial data (3.17) the initial Wigner distribution has the form

$$W_0(x,k) = |A_0(x)|^2 \delta(k - \nabla S_0(x)). \tag{3.21}$$

As long as the geometric optics approximation (3.18) remains valid we expect the solution of the Liouville equation (3.16) to have the same form:

$$W(t,x,k) = |A(t,x)|^2 \delta(k - \nabla S(t,x)). \tag{3.22}$$

We insert this ansatz into (3.16) :

$$\left(\frac{\partial}{\partial t} + k \cdot \nabla_x - \nabla V \cdot \nabla_k\right)\left(|A(t,x)|^2 \delta(k - \nabla S(t,x))\right) = 0. \tag{3.23}$$

or, equivalently,

$$\begin{aligned} &\delta(k - \nabla S)\left(\frac{\partial}{\partial t} + k \cdot \nabla_x - \nabla V \cdot \nabla_k\right)(|A(t,x)|^2) \\ &+|A(t,x)|^2 \sum_{m,p=1}^{n} \left(\frac{\partial^2 S}{\partial t \partial x_m} + k_p \frac{\partial^2 S}{\partial x_p \partial x_m} - \frac{\partial V}{\partial x_m}\right) D_m = 0, \end{aligned} \tag{3.24}$$

where

$$D_m = \delta(k_1 - S_{x_1}) \ldots \delta(k_{m-1} - S_{x_{m-1}}) \delta'(k_m - S_{x_m}) \delta(k_{m+1} - S_{x_{m+1}}) \ldots \delta(k_n - S_{x_n}).$$

Equating similar terms in (3.24) we obtain the transport equation (3.20) from the term in the first line, while the coefficient at D_m gives the eikonal equation (3.19) differentiated with respect to x_m. Expression (3.22) holds of course only until the time when the solution of the eikonal equation stops being smooth.

Let us see what happens with the Wigner measure when a caustic forms. Consider the Schrödinger equation (3.13) with $V = 0$ – the corresponding Liouville equation is

$$W_t + k \cdot \nabla_x W = 0, \quad W(0,x,k) = W_0(x,k). \tag{3.25}$$

Its solution is $W(t,x,k) = W_0(x - kt, k)$ and clearly exists for all time. If the initial phase $S_0(x) = -x^2/2$ with a smooth initial amplitude $A_0(x)$ then the Wigner transform at $t = 0$ is $W_0(x,k) = |A_0(x)|^2 \delta(k + x)$ so that solution of (3.25) is $W(t,x,k) = |A_0(x - kt)|^2 \delta(k + x - kt)$. This means that at the time $t = 1$ the Wigner measure $W(t = 1, x, k) = |A_0(x - k)|^2 \delta(x)$is no longer singular in wave vectors k but rather in space being concentrated at $x = 0$. This is the caustic point. On the other hand, solution of the eikonal equation (3.19) with the same initial phase and $V = 0$ is given by $S(t,x) = -x^2/(2(1 - t))$ – we see that the same caustic appears at $t = 1$. The transport equation becomes

$$(|A|^2)_t - \frac{x}{1-t} \cdot \nabla(|A|^2)_t - \frac{n}{1-t}|A|^2.$$

The corresponding trajectories satisfy

$$\dot{X} = -\frac{X}{1-t}, \quad X(0) = x$$

and are given by $X(t) = x(1-t)$ – hence they all arrive to the point $x = 0$ at the time $t = 1$. At this time the geometric optics approximation breaks down and is no longer valid while the solution of the Liouville equation exists beyond this time.

We see that from the Wigner distribution we can recover the information contained in the leading order of the standard high frequency approximation. In addition, it provides flexibility to deal with initial data that is not of the form (3.21).

3.1.6 Wigner transforms of mixtures of states

We have noted before that the $L^2(\mathbb{R}^n \times \mathbb{R}^n)$-norm of the Wigner transform blows up in the limit $\varepsilon \to 0$ unless the underlying family of functions ϕ_ε converges strongly to zero in $L^2(\mathbb{R}^n)$. On the other hand, the L^2-norm of the Wigner transforms for each $\varepsilon > 0$ is preserved – it just so happens that it blows up in the limit. The L^2-norm is often much more convenient to use than the norm in $\mathcal{A}'$ and its conservation is typically an easy consequence of the evolution equation for the Wigner transform. For example, if ϕ_ε satisfy the Schrödinger equation

$$i\varepsilon\frac{\partial \phi_\varepsilon}{\partial t} + \frac{\varepsilon^2}{2}\Delta\phi_\varepsilon - V(x)\phi_\varepsilon = 0, \tag{3.26}$$

then the Wigner transform W_ε satisfies

$$\frac{\partial W_\varepsilon}{\partial t} + k \cdot \nabla_x W_\varepsilon = \frac{1}{i\varepsilon}\int e^{ip\cdot x}\hat{V}(p)\left[W_\varepsilon\left(k - \frac{\varepsilon p}{2}\right) - W_\varepsilon\left(k + \frac{\varepsilon p}{2}\right)\right]\frac{dp}{(2\pi)^n}. \tag{3.27}$$

It is immediate to verify that (3.27) preserves the L^2-norm:

$$\frac{d}{dt}\int |W_\varepsilon(t,x,k)|^2 dxdk = 0.$$

It is much more difficult to verify that the $\mathcal{A}'$-norm of solutions does not grow. Therefore, it would be convenient to have a tool of working with the L^2-norm of the Wigner transform. This is what mixtures of state do. They arise, either naturally or artifically when families of solutions are cosnidered rather than one solution. That is, we consider a measure $P(d\omega)$ on a state space Ω (which can be a probability space but needs not be) and introduce a family of initial data $\psi_0^\varepsilon(x,\omega)$ for the Schrödinger equation parametrized by $\omega \in \Omega$. Accordingly we may define a mixture of states (the terminology comes from the quantum mechanics)

$$\bar{W}_\varepsilon(t,x,k) = \int_\Omega W_\varepsilon(t,x,k,\omega)P(d\omega)$$

with

$$W_\varepsilon(t,x,k,\omega) = \int e^{ik\cdot y}\phi_\varepsilon\left(t, x - \frac{\varepsilon y}{2}, \omega\right)\bar{\phi}_\varepsilon\left(t, x - \frac{\varepsilon y}{2}, \omega\right)\frac{dy}{(2\pi)^n}.$$

The point is that while the L^2-norm of $W_\varepsilon(t,x,k,\omega)$ blows up for each fixed state $\omega \in \Omega$, the L^2-norm of the average Wigner transform $\bar{W}_\varepsilon(t,x,k)$ may remain bounded. In paticular, in the case of the Schrödinger equation, as $\bar{W}_\varepsilon$ satisfies (3.27), its L^2-norm is bounded as long as the L^2-norm of the initial data $\bar{W}_\varepsilon(0,x,k)$ is uniformly bounded. Let us give a couple of examples when this might happen. The first one arises when the initial data is random, and the second comes from the analysis of the time-reversal experiments that we will study in some detail later.

Statistical averaging: take the initial data for the Schrödinger equation of the form $\phi_0^\varepsilon(x;\omega) = \psi(x)V(x/\varepsilon;\omega)$, where $V(y;\omega)$ is a mean zero, scalar spatially homogeneous random process with a rapidly decaying two-point correlation function $R(z)$:

$$E\left\{V(y)V(y+z)\right\} = \int V(y;\zeta)V(y+z;\zeta)dP(\omega) = R(z) \in \mathcal{S}(\mathbb{R}^n),$$

and $\psi(x) \in C_c^\infty(\mathbb{R}^n)$. The "average" Wigner transform is then

$$\begin{aligned}
\bar{W}_\varepsilon(x,k) &= \int_\Omega \left(\int e^{ik\cdot y} \phi_\varepsilon \left(x - \frac{\varepsilon y}{2}, \omega\right) \bar{\phi}_\varepsilon \left(x - \frac{\varepsilon y}{2}, \omega\right) \frac{dy}{(2\pi)^n} \right) dP(\omega) \\
&= \int_\Omega \left(\int e^{ik\cdot y} \psi \left(x - \frac{\varepsilon y}{2}\right) \bar{\psi} \left(x - \frac{\varepsilon y}{2}\right) V\left(\frac{x}{\varepsilon} - \frac{y}{2}, \omega\right) V\left(\frac{x}{\varepsilon} + \frac{y}{2}, \omega\right) \frac{dy}{(2\pi)^n} \right) dP(\omega) \\
&= \int e^{ik\cdot y} R(y) \psi \left(x - \frac{\varepsilon y}{2}\right) \bar{\psi} \left(x - \frac{\varepsilon y}{2}\right) \frac{dy}{(2\pi)^n} \to |\psi(x)|^2 \tilde{R}(k).
\end{aligned}$$

Hence the limit Wigner distribution is given by $W(x,k) = |\psi(x)|^2\tilde{R}(k)$, where $\tilde{R}(k)$ is the inverse Fourier transform of $R(y)$. In addition, convergence is strong in $L^2(\mathbb{R}^n \times \mathbb{R}^n)$:

$$\|\bar{W}_\varepsilon - W\|_{L^2}^2 = \int |R(y)|^2 \left(\psi \left(x - \frac{\varepsilon y}{2}\right) \bar{\psi} \left(x - \frac{\varepsilon y}{2}\right) - |\psi(x)|^2 \right)^2 \frac{dxdy}{(2\pi)^n} = \int I_\varepsilon(y)|R(y)|^2 \frac{dy}{(2\pi)^n}$$

with

$$I_\varepsilon(y) = \int \left(\psi \left(x - \frac{\varepsilon y}{2}\right) \bar{\psi} \left(x - \frac{\varepsilon y}{2}\right) - |\psi(x)|^2 \right)^2 dx.$$

However, we have $|I_\varepsilon(y)| \le 4\|\psi\|_{L^4}^4$ and

$$I_\varepsilon(y) = \int \left(\psi(x - \frac{\varepsilon y}{2})\psi^*(x + \frac{\varepsilon y}{2}) - |\psi(x)|^2 \right)^2 dx \to 0$$

as $\varepsilon \to 0$ since $\psi \in C_c(\mathbb{R}^d)$, pointwise in y. Therefore $\|\bar{W}_\varepsilon - W\|_2 \to 0$ by the Lebesgue dominated convergence theorem.

Smoothing of oscillations: the initial data is of the form $\phi_0^\varepsilon(x;\zeta) = \psi(x)e^{i\zeta\cdot x/\varepsilon}$, where $\psi(x) \in C_c(\mathbb{R}^d)$. The state space $S = \mathbb{R}^n$, and the measure P is $P(d\omega) = g(\omega)d\omega$, $\omega \in \mathbb{R}^n$, and $g \in \mathcal{S}(\mathbb{R}^n)$. Then the limit Wigner distribution is $W(x,k) = |\psi(x)|^2 g(k)$ and convergence of $\bar{W}_\varepsilon(x,k)$ to the limit is strong in $L^2(\mathbb{R}^n \times \mathbb{R}^n)$. This is verified exactly in the same way as in the previous example.

3.2 The high frequency limit for symmetric hyperbolic systems

3.2.1 Matrix-valued Wigner transform

The definition of the Wigner transform may be generalized in a straightforward manner for families of vector-valued functions $u_\varepsilon(x) \in L^2(\mathbb{R}^n;\mathbb{C}^m)$. The Wigner transform is then an $m \times m$ matrix

$$W_\varepsilon(x,k) = \int e^{ik\cdot y} u_\varepsilon \left(x - \frac{\varepsilon y}{2}\right) u_\varepsilon^* \left(x + \frac{\varepsilon y}{2}\right) \frac{dy}{(2\pi)^n}. \tag{3.28}$$

Here we denote by u^* the conjugate-transpose of the vector u. The basic properties of the scalar Wigner transform can be immediately generalized to the matrix case. In particular, $W_\varepsilon(x,k)$ is a self-adjoint matrix, and we have the following:

Theorem 3.2.1 *Let the family of vector-valued functions $u_\varepsilon(x)$ be uniformly bounded in $L^2(\mathbb{R}^n;\mathbb{C}^m)$. Then the matrix-valued Wigner transform W_ε converges weakly along a subsequence $\varepsilon_k \to 0$ to a matrix-valued distribution $W(x,k) \in \mathcal{S}'(\mathbb{R}^n \times \mathbb{R}^n; \mathbb{C}^m \times \mathbb{C}^m)$. Any such limit point $W(x,k)$ is a non-negative matrix for each (x,k).*

The localization Lemma 3.1.6, orthogonality Lemma 3.1.7 as well as "energy capturing" Theorem 3.1.10 also hold.

3.2.2 The evolution of the Wigner transform: constant coefficients

We now consider the evolution of the Wigner transform for general equations other than the linear Schrödinger equation. We begin with systems of equations with constant coefficients of the form

$$\begin{aligned} &\varepsilon \frac{\partial u^\varepsilon}{\partial t} + P(\varepsilon D)u^\varepsilon = 0 \\ &u^\varepsilon(t=0) = u_0^\varepsilon \end{aligned} \tag{3.29}$$

with u^ε being a $\mathbb{C}^m$-valued vector function. A typical example we have in mind is a symmetric hyperbolic system

$$\frac{\partial u}{\partial t} + D^j \frac{\partial u}{\partial x_j} = 0$$

with symmetric matrices D^j, $j = 1, \ldots, n$ – in that case $P(k) = ik_j D^j$. In general, the operator $P(\varepsilon D)$ is associated with a multiplier $P(k)$. We assume that $P \in C^\infty(\mathbb{R}^n \backslash \{0\})$ and $P^*(k) = -P(k)$. It follows that the total energy is conserved:

$$N(t) = \int n^\varepsilon(t,x)dx = \int n_0^\varepsilon(x)dx = N(0).$$

Here $n_\varepsilon(t,x) = |u^\varepsilon(t,x)|^2$ is the energy density and $n_0^\varepsilon(x)$ its initial value. Therefore, it makes sense to consider the Wigner transform of solutions and their weak limits.

We impose the following conditions on the symbol: all eigenvalues $\omega_\alpha(k)$ of the self-adjoint matrix $iP(k)$ may be ordered as

$$\omega_1(k) < \cdots < \omega_p(k)$$

with the multiplicities r_α independent of k. We denote by $\Pi_\alpha(k)$ the orthogonal projection onto the eigenspace corresponding to $\omega_\alpha(k)$ and assume that $\omega_\alpha(k)$ and $\Pi_\alpha(k)$ are smooth functions of k away from $k = 0$.

Theorem 3.2.2 *Let the initial data $u_0^\varepsilon(x)$ for (3.29) be a pure family, uniformly bounded in $L^2(\mathbb{R}^n)$, ε-oscillatory and compact at infinity with the unique limit Wigner matrix measure $W_0(x,k)$. Assume that $\hat{u}_0^\varepsilon(k)$ vanishes for $|k| \le r$ for some $r > 0$. Then the Wigner transform $W_\varepsilon(t,x,k)$ converges weakly in $\mathcal{S}'(\mathbb{R}_+ \times \mathbb{R}^n \times \mathbb{R}^n)$ to*

$$W(t,x,k) = \sum_{\alpha=1}^{p} W_\alpha(t,x,k).$$

The matrices $W_\alpha(t,x,k)$ satisfy the Liouville equations

$$\frac{\partial W_\alpha}{\partial t} + \nabla_k \omega_\alpha(k) \cdot \nabla_x W_\alpha = 0, \quad W_\alpha(0,x,k) = \Pi_\alpha(k) W_0(x,k) \Pi_\alpha(k). \tag{3.30}$$

Energy propagation for solutions of (3.29) is described by the following theorem.

Theorem 3.2.3 *Under the same assumptions the energy density $n^\varepsilon(t,x)$ converges weakly (for each time $t \geq 0$) to the measure $n^0(t,x)$ given by*

$$n^0(t,x) = \sum_{\alpha=1}^{p} \int w_\alpha^0(x - t\nabla\omega_\alpha(k), dk). \tag{3.31}$$

Here $w_\alpha^0(x,k) = Tr(\Pi_\alpha W \Pi_\alpha)(x,k)$. Moreover, convergence is uniform on finite time intervals.

The reason why we do not have uniform in time convergence of the matrix Wigner transform but do have it for the energy density lies in the cross-mode terms $\Pi_\alpha W_\varepsilon \Pi_\beta$ with $\alpha \neq \beta$ – they fats have temporal oscillations but do not go to zero uniformly in time. For example, consider a special solution of (3.29) which is a sum of two plane waves with the same wave vector:

$$u_\varepsilon(x) = A_\alpha b_\alpha(k_0) e^{ik_0\cdot x/\varepsilon - i\omega_\alpha(k_0)t/\varepsilon} + A_\beta b_\beta(k_0) e^{ik_0\cdot x/\varepsilon - i\omega_\beta(k_0)t/\varepsilon}$$

with $\omega_\alpha(k_0) \neq \omega_\beta(k_0)$. Then the matrix Wigner transform is

$$\begin{aligned} W_\varepsilon(t,x,k) = \Big[&|A_\alpha|^2 ab_\alpha(k_0) ab_\alpha^*(k_0) + |A_\beta|^2 ab_\beta(k_0) ab_\beta^*(k_0) \\ &+ A_\alpha \bar{A}_\beta b_\beta(k_0) ab_\alpha^*(k_0) e^{i(\omega_\beta(k_0)-\omega_\alpha(k_0))t/\varepsilon} + \bar{A}_\alpha A_\beta b_\alpha(k_0) ab_\beta^*(k_0) e^{i(\omega_\alpha(k_0)-\omega_\beta(k_0))t/\varepsilon}\Big] \delta(k-k_0). \end{aligned}$$

The cross-terms are oscillating rapidly in time – hence they vanish as $\varepsilon \to 0$ but only in the weak sense. On the other hand, these terms have zero energy – their trace vanishes. Therefore, the energy does not have these temporaly oscillating terms – this simple example captures the basic phenomenon that the cross-mode terms are oscillatory in time but carry no energy.

3.2.3 The evolution of the Wigner transform: slowly varying coefficients

We now consider the Wigner transforms of solutions of symmetric hyperbolic systems of the form

$$\frac{\partial u_\varepsilon}{\partial t} + B(x) D^j \frac{\partial}{\partial x_j} (B(x) u_\varepsilon) = 0. \tag{3.32}$$

The matrix $B(x)$ is positive-definite and the constant matrices D^j are symmetric and independent of t and x. The total energy

$$\mathcal{E}(t) = \int |u_\varepsilon(t,x)|^2 dx = \mathcal{E}(0)$$

is conserved:

$$\frac{\partial E}{\partial t} + \nabla \cdot F = 0$$

with the energy density $E(t,x) = |u(t,x)|^2$ and the flux $F_j(t,x) = (D^j Bu, Bu)$. We will assume in this section, as usually, that away from $k = 0$ the dispersion matrix $L(x,k) = B(x) k_j D^j B(x)$ has eigenvalues $\omega_\alpha(x,k)$ with constant multiplicity r_α independent of x and $k \neq 0$, and both ω_α and the corresponding eigenvectors b_α^i, $i = 1, \dots, r_\alpha$ are smooth functions of $x \in \mathbb{R}^n$ and $k \in \mathbb{R}^n \backslash \{0\}$.

Energy conservation allows us to talk about the matrix Wigner transforms of the solutions and study their limits. As in the constant coefficient case, the matrix $W(x,k)$ satisfies

$$L(x,k) W(t,x,k) = W(t,x,k) L(x,k), \quad L(x,k) = \frac{1}{i} B(x) P(x,k) B(x), \tag{3.33}$$

It follows that $\Pi_\alpha(x,k)W(t,x,k)\Pi_\beta(t,x,k) = 0$ for $\alpha \neq \beta$ – here $\Pi_\alpha(x,k)$ is the projection matrix on the eigenspace of the matrix $L(x,k)$ corresponding to an eigenvalue $\omega_\alpha(x,k)$. Thus, the limit Wigner matrix has a representation

$$W(t,x,k) = \sum_\alpha \Pi_\alpha(x,k)W(t,x,k)\Pi_\alpha(x,k). \tag{3.34}$$

We may also write it in a more explicit form as

$$W(t,x,k) = \sum_\alpha \sum_{i,j=1}^{r_\alpha} w_\alpha^{ij}(t,x,k)b_\alpha^i(x,k)b_\alpha^{j*}(x,k). \tag{3.35}$$

The vectors b_α^i form the orthonormal basis of the eigenspace corresponding to the eigenvalue ω_α. The limit energy density is simply

$$E(t,x) = \sum_\alpha \int \mathrm{Tr} w_\alpha(t,x,k)dk$$

for ε-oscillatory and compact at infinity families of solutions – we will see that this property is preserved by evolution. The limit flux under the same assumption is

$$F_j(t,x) = \sum_\alpha \int \frac{\partial \omega_\alpha}{\partial k_j} \mathrm{Tr} w_\alpha(t,x,k)dk. \tag{3.36}$$

Let us define the matrices

$$\bar{N}_\alpha^{ni} = \frac{1}{2}\left[((B\nabla_k P \cdot \nabla_x B)b_\alpha^i, b_\alpha^n) - (b_\alpha^i, (B\nabla_k P \cdot \nabla_x B)b_\alpha^n)\right]. \tag{3.37}$$

The matrix $\bar{N}^\alpha$ is skew-symmetric and hence vanishes when the eigenvalue ω_α is simple. Then the $r_\alpha \times r_\alpha$ coherence matrice $w^\alpha(t,x,k)$ satisfy the matrix Liouville equations

$$\frac{\partial w_\alpha}{\partial t} + \nabla_k \omega_\alpha \cdot \nabla_x w_\alpha - \nabla_x \omega_\alpha \cdot \nabla_k w_\alpha + [\bar{N}^\alpha, w^\alpha] = 0. \tag{3.38}$$

This system of equation is the main result of this section. We have now proved the following theorem.

Theorem 3.2.4 *Let $u_\varepsilon(t,x)$ be the solution of the initial value problem*

$$\frac{\partial u_\varepsilon}{\partial t} + B(x)D^j \frac{\partial}{\partial x_j}(B(x)u_\varepsilon) = 0 \tag{3.39}$$

with an ε-oscillatory and compact at infinity pure family of initial data $u_\varepsilon(0,x) = u_\varepsilon^0(x)$. The coefficient matrices $B(x)$ are symmetric positive-definite and D^j are independent of t and x. Then the Wigner transforms $W_\varepsilon(t,x,k)$ converge weakly in $\mathcal{S}'(\mathbb{R}_+ \times \mathbb{R}^n \times \mathbb{R}^n)$ to the matrix distribution

$$W(t,x,k) = \sum_{\alpha=1}^{p} \sum_{i,j=1}^{r_\alpha} w_\alpha^{ij}(t,x,k)b_\alpha^i(x,k)b_\alpha^j(x,k).$$

The coherence matrices w_α satisfy the matrix Liouville equations (3.38) with the initial data $w_\alpha^{mn}(0,x,k) = Tr[W_0(x,k)b_\alpha^n(x,k)b_\alpha^{m*}(x,k)]$. Here $W_0(x,k)$ is the Wigner transform of the family $u_\varepsilon^0(x)$.

A few comments on the matrix Liouville equations (3.38) are in order. First of all, the coupling matrix N^α vanishes if the coefficient matrix B is independent of x – this is seen from its explicit form. Furthermore, as in the constant coefficients case equations for various modes are all decoupled. This means that slow variations (relative to the wave length) of the background material properties do not induce mode coupling in the leading order. They do, however, suffice to couple various polarizations corresponding to the same mode if the mode is polarized. Still the "coupling" commutator term in the Liouville equations may be eliminated by an appropriate choice of the basis. Let us write $w_\alpha = U\bar{w}_\alpha U^*$ with the matrix U to be determined. Then we have

$$\frac{\partial U}{\partial t}\bar{w}_\alpha U + U\frac{\partial \bar{w}_\alpha}{\partial t}U^* + U\bar{w}_\alpha\frac{\partial U^*}{\partial t} + U\{\omega_\alpha, \bar{w}_\alpha\}U^* + U\bar{w}_\alpha\{\omega_\alpha, U^*\} + \{\omega_\alpha, U\}\bar{w}_\alpha U^*$$
$$+\bar{N}^\alpha U\bar{w}_\alpha U^* - U\bar{w}_\alpha U^*\bar{N}^\alpha = 0.$$

Now if choose U to be the solution of the evolution equation

$$\frac{\partial U}{\partial t} + \{\omega_\alpha, U\} + \bar{N}^\alpha U = 0, \quad U(0,x,k) = I,$$

then the matrix $\bar{w}_\alpha$ satisfies a Liouville equation without the commutator term

$$\frac{\partial \bar{w}_\alpha}{\partial t} + \nabla_k\omega_\alpha \cdot \nabla_x\bar{w}_\alpha - \nabla_x\omega_\alpha \cdot \nabla_k\bar{w}_\alpha = 0, \quad \bar{w}_\alpha(0,x,k) = w^0_\alpha(x,k). \tag{3.40}$$

This means that the matrix $U(t,x,k)$ describes the rotation (recall that the matrix N^α is skew-symmetric) of the polarization vector along the bicharacteristics.

As in the case of constant coefficients, the non-uniform in time convergence of the matrix Wigner transform to the limit in Theorem 3.2.4 is not an artifact of the proof. However, the phase space energy density, that is, the trace of the Wigner matrix converges to its limit $\bar{E}(t,x) = \sum_\alpha \int \mathrm{Tr} w^\alpha(t,x,k)dk$ uniformly in time (and weakly in space). This is because the time derivative $\partial W_\varepsilon/\partial t$ is uniformly bounded in time.

The limit Liouville equations preserve the total energy $\bar{E}(t,x)$ defined above. Therefore, as long as the initial data is ε-oscillatory and compact at infinity, convergence of the trace of the Wigner matrix is tight for all $t \geq 0$. As a consequence, using Theorem 3.1.10 we conclude that the family of solutions of (3.32) remain ε-oscillatory and compact at infinity.

3.3 High frequency Wigner limits: examples

3.3.1 High Frequency Approximation for Acoustic Waves

We will now apply the results of the previous section to acoustic waves. We will also review the usual form of the high frequency approximation and make explicit the relation between the phase space form of the high frequency approximation and the usual one.

The acoustic equations for the velocity and pressure disturbances u and p are

$$\begin{aligned} \rho\frac{\partial u}{\partial t} + \nabla p &= 0 \\ \kappa\frac{\partial p}{\partial t} + \mathrm{div} u &= 0. \end{aligned} \tag{3.41}$$

Here $\rho = \rho(x)$ is the medium density and $\kappa = \kappa(x)$ is its compressibility. Equations (3.41) can be re-written in terms of $v(t,x) = \sqrt{\rho(x)}u(t,x)$ and $q(t,x) = \sqrt{\kappa(x)}p(t,x)$ as

$$\begin{aligned} \frac{\partial v}{\partial t} + \frac{1}{\sqrt{\rho}} \nabla \left[\frac{1}{\sqrt{\kappa}} q \right] &= 0 \\ \frac{\partial q}{\partial t} + \frac{1}{\sqrt{\kappa(x)}} \mathrm{div} \left[\frac{1}{\sqrt{\rho}} v \right] &= 0. \end{aligned} \tag{3.42}$$

The energy density and flux for acoustic waves are given by

$$\mathcal{E}(t,x) = \frac{1}{2}|v(t,x)|^2 + \frac{1}{2}q^2(t,x), \quad \mathcal{F}(t,x) = c(x)q(t,x)v(t,x). \tag{3.43}$$

Equations (3.42) have the form (3.32) with the matrix

$$B(x) = \mathrm{diag}\left[\frac{1}{\sqrt{\rho(x)}}, \frac{1}{\sqrt{\rho(x)}}, \frac{1}{\sqrt{\rho(x)}}, \frac{1}{\sqrt{\kappa(x)}}\right]$$

while each of the matrices $D^i = e_1 e_4^* + e_4 e_1^*$ has all zero entries except for D^i_{i4} and D^i_{4i} which are equal to one. For instance, the matrix D^1 is

$$D^1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

Then the dispersion matrix $L(x,k)$ has the form

$$L = v(x) \begin{pmatrix} 0 & 0 & 0 & k_1 \\ 0 & 0 & 0 & k_2 \\ 0 & 0 & 0 & k_3 \\ k_1 & k_2 & k_3 & 0 \end{pmatrix} \tag{3.44}$$

with the sound speed $c(x) = 1/\sqrt{\kappa(x)\rho(x)}$. It has one double eigenvalue $\omega_1 = \omega_2 = 0$ and two simple eigenvalues $\omega_\pm = \pm c(x)|k|$. The corresponding orthonormal basis of eigenvectors is

$$b^1 = (z^{(1)}(k), 0), \quad b^2 = (z^{(2)}(k), 0), \quad b^\pm = \left(\frac{\hat{k}}{\sqrt{2}}, \pm \frac{1}{\sqrt{2}} \right), \tag{3.45}$$

with the vectors $\hat{k}$, $z^{(1)}(k)$ and $z^{(2)}(k)$, which form an orthonormal triplet:

$$\hat{k} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}, z^{(1)} = \begin{pmatrix} \cos\theta\cos\phi \\ \cos\theta\sin\phi \\ -\sin\theta \end{pmatrix}, z^{(2)} = \begin{pmatrix} -\sin\phi \\ \cos\phi \\ 0 \end{pmatrix}. \tag{3.46}$$

The limit Wigner matrix of the family $\mathbf{v}_\varepsilon = (v_\varepsilon, q_\varepsilon)$, according to (3.35) can be represented as

$$W(t,x,k) = \sum_{i,j=1}^{2} w_0^{ij}(t,x,k) b^i(k) b^{j*}(k) + w_+(t,x,k) b^+(k) b^{+*}(k) + w_-(t,x,k) b^-(k) b^{-*}(k). \tag{3.47}$$

In order to understand better the physical meaning of these modes let us write the vector $v_\varepsilon(x)$ as a sum $v_\varepsilon(t,x) = v_{in}^\varepsilon(t,x) + v_{irr}^\varepsilon$ with an incompressible field $v_{in}^\varepsilon(t,x)$: $\nabla \cdot v_{in}^\varepsilon = 0$ and an irrotational component v_{irr}^ε: $\nabla \times v_{irr}^\varepsilon = 0$. The limit Wigner matrices W_{in} and W_{irr} of the families $v_{in}^\varepsilon(t,x)$ and $v_{irr}^\varepsilon(t,x)$ satisfy $W_{in}(t,x,k)k = 0$ and $W_{irr}(t,x,k)z = 0$ for any vector z orthogonal to k. Decomposition (3.47) tells us that $W = W_{irr} + W_{in}$ with

$$W_{in} = \sum_{i,j=1}^{2} w_0^{ij}(t,x,k) b^i(k) b^{j*}(k), \quad W_{irr} = w_+(t,x,k) b^+(k) b^{+*}(k) + w_-(t,x,k) b^-(k) b^{-*}(k).$$

Therefore, the eigenvectors $b^1(k)$ and $b^2(k)$ correspond to transverse advection modes, orthogonal to the direction of propagation. These modes do not propagate because $\omega_{1,2} = 0$: equation (3.38) for the coherence matrix w_0 is of the form $\dfrac{\partial w_0}{\partial t} = 0$ – hence $w_0(t,x,k) = 0$ if it is zero initially. This is the case when the initial data is irrotational. The eigenvectors $b^+(k)$ and $b^-(k)$ represent acoustic waves, which are longitudinal, and which propagate with the sound speed $c(x)$: the scalar amplitudes $w_\pm(t,x,k)$ satisfy the scalar Liouville equations

$$\frac{\partial w_\pm}{\partial t} \pm c(x)\hat{k} \cdot \nabla_x w_\pm \mp |k| \nabla_x c(x) \cdot \nabla_k w_\pm = 0. \tag{3.48}$$

Next, as we did for the Schrödinger equation, we establish the connection with the usual high frequency approximation for acoustic waves. We consider acoustic equations (3.42) with initial data of the form

$$\mathbf{v}(0,x) = \mathbf{v}_0(x) e^{iS_0(x)/\varepsilon}, \quad \mathbf{v} = (v,q) \tag{3.49}$$

where S_0 is the real valued initial phase function. We look for a solution in the form

$$\mathbf{v}(t,x) = (\underline{A}_0(t,x) + \varepsilon \underline{A}_1 + \dots) e^{iS(t,x)/\varepsilon}, \tag{3.50}$$

where $\underline{A}_0 = (v_0, q_0)$. We insert (3.50) into (3.42) to get in the leading order in ε

$$\begin{pmatrix} S_t & c(x)\nabla S \\ c(x)\nabla S \cdot & S_t \end{pmatrix} \begin{pmatrix} v_0 \\ q_0 \end{pmatrix} = 0. \tag{3.51}$$

The next term in the expansion yields

$$-i \begin{pmatrix} S_t & c(x)\nabla S \\ c(x)\nabla S \cdot & S_t \end{pmatrix} \begin{pmatrix} v_1 \\ q_1 \end{pmatrix} = \begin{pmatrix} \partial_t v_0 + \dfrac{1}{\sqrt{\rho}} \nabla \left[\dfrac{1}{\sqrt{\kappa}} q_0 \right] \\ \partial_t q_0 + \dfrac{1}{\sqrt{\kappa}} \nabla \left[\dfrac{1}{\sqrt{\rho}} \cdot v_0 \right] \end{pmatrix}. \tag{3.52}$$

Equation (3.51) gives the eiconal equation for the phase S

$$S_t^2 - c^2(x)(\nabla S)^2 = 0. \tag{3.53}$$

Then assuming that $S_t = +c(x)|\nabla S|$ we have

$$\begin{pmatrix} v_0 \\ q_0 \end{pmatrix} = \mathcal{A}(x) b^+(\nabla S(t,x)), \tag{3.54}$$

where b^+ is given by (3.45). The amplitude $\mathcal{A}(t,x)$ is determined by the solvability condition for (3.52), which gives the transport equation

$$\frac{\partial}{\partial t}|\mathcal{A}|^2 + \nabla\cdot\left(|\mathcal{A}|^2 c(x)\frac{\nabla S}{|\nabla S|}\right) = 0. \tag{3.55}$$

The eiconal and transport equations (3.53) and (3.55) can also be derived from the Liouville equation (3.48) as we did for the Schrödinger equation. In the high frequency limit, initial conditions of the form (3.49) imply that

$$w_+(0,x,k) = |\mathcal{A}_0(x)|^2\delta(k - \nabla S_0(x)). \tag{3.56}$$

Let the functions $S(t,x)$ and $|\mathcal{A}(t,x)|^2$ be the solutions of the eiconal and transport equations (3.53) and (3.55), respectively, with the initial conditions $S(0,x) = S_0(x)$ and $|\mathcal{A}(0,x)|^2 = |\mathcal{A}_0(x)|^2$. Then the solution of equation (3.48) is

$$w_+(t,x,k) = |\mathcal{A}(t,x)|^2\delta(k - \nabla S(t,x)). \tag{3.57}$$

Conversely, given initial conditions of the form (3.56) for (3.48) and w_+ given by (3.57), then S and $\mathcal{A}$ must satisfy the eiconal and transport equations (3.53) and (3.55), respectively. This is because the eiconal equation follows by integrating (3.48) with respect to k while the transport equation follows by multiplying it by k and then integrating with respect to k. This shows that we can recover from the Liouville equation (3.48) the leading order term of the usual high frequency approximation.

3.3.2 Phase space geometric optics for electromagnetic waves

Maxwell's equations in an isotropic medium and in suitable units are

$$\begin{aligned}\frac{\partial E}{\partial t} &= \frac{1}{\epsilon}\mathrm{curl}H \\ \frac{\partial H}{\partial t} &= -\frac{1}{\mu}\mathrm{curl}E\end{aligned} \tag{3.58}$$

where the dielectric permittivity is $\epsilon(x)$ and the relative magnetic permeability is $\mu(x)$. In this section as well as in other instances when we consider electromagnetic waves ϵ denotes the dielectric permittivity while the small parameter is denoted by ε. It follows from Maxwell's equations that if at the initial time we have

$$\mathrm{div}(\epsilon E) = \mathrm{div}(\mu H) = 0 \tag{3.59}$$

then these conditions hold for all time. We will always assume that (3.59) holds.

As a symmetric hyperbolic system Maxwell's equations can be written as

$$\frac{\partial}{\partial t}\begin{pmatrix}\bar{E}\\ \bar{H}\end{pmatrix} + \begin{pmatrix}\frac{1}{\sqrt{\epsilon}} & 0 & \\ 0 & \frac{1}{\sqrt{\mu}} & 0\end{pmatrix}\begin{pmatrix}0 & -\nabla\times\\ \nabla\times & 0\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{\epsilon}} & 0\\ 0 & \frac{1}{\sqrt{\mu}}\end{pmatrix}\begin{pmatrix}\bar{E}\\ \bar{H}\end{pmatrix} = 0 \tag{3.60}$$

with $\bar{E} = \sqrt{\epsilon}E$ and $\bar{H} = \sqrt{\mu}H$. The 6×6 dispersion matrix L is

$$L = -c(x) \begin{pmatrix} 0 & 0 & 0 & 0 & -k_3 & k_2 \\ 0 & 0 & 0 & k_3 & 0 & -k_1 \\ 0 & 0 & 0 & -k_2 & k_1 & 0 \\ 0 & k_3 & -k_2 & 0 & 0 & 0 \\ -k_3 & 0 & k_1 & 0 & 0 & 0 \\ k_2 & -k_1 & 0 & 0 & 0 & 0 \end{pmatrix} = c(x) \begin{pmatrix} 0 & -T \\ T & 0 \end{pmatrix} \tag{3.61}$$

with the speed of light $c(x) = 1/\sqrt{\epsilon(x)\mu(x)}$ and the matrix $T(k)$ defined by $T(k)p = k \times p$ or

$$T(k) = \begin{pmatrix} 0 & -k_3 & k_2 \\ k_3 & 0 & -k_1 \\ -k_2 & k_1 & 0 \end{pmatrix}. \tag{3.62}$$

The dispersion matrix L has three eigenvalues, each with multiplicity two. They are $\omega_0 = 0$, $\omega_+ = c|k|$, $\omega_- = -c|k|$. The basis formed by the corresponding eigenvectors is

$$\begin{aligned} & b^{(01)} = (\hat{k}, 0),\ b^{(02)} = (0, \hat{k}), \\ & b^{(+,1)} = (\frac{z^{(1)}}{\sqrt{2}}, \frac{z^{(2)}}{\sqrt{2}}),\ b^{(+,2)} = (\frac{z^2}{\sqrt{2}}, -\frac{z^{(1)}}{\sqrt{2}}), \\ & b^{(-,1)} = (\frac{z^{(1)}}{\sqrt{2}}, -\frac{z^{(2)}}{\sqrt{2}}),\ b^{(-,2)} = (\frac{z^{(2)}}{\sqrt{2}}, \frac{z^{(1)}}{\sqrt{2}}), \end{aligned} \tag{3.63}$$

where the vectors k, $z^{(1)}(k)$ and $z^{(2)}(k)$ form an orthonormal triplet (3.46). The coherence matrix w_0 corresponding to the mode $\omega_0 = 0$ vanishes if (3.59) holds – this is checked in the same way as the absence of the vortical modes for the acoustic waves. The other eigenvectors correspond to transverse modes propagating with the speed $c(x)$. As in the acoustic case, we need only consider the eigenspace corresponding to ω_+. The 2×2 coherence matrices $w_\pm$ satisfy the Liouville equations (3.38), for instance, the evolution equation for $w = W_+$ is

$$\frac{\partial w}{\partial t} + c(x)\hat{k} \cdot \nabla_x w - |k| \nabla_x c(x) \cdot \nabla_k w + \bar{N} w - w \bar{N} = 0. \tag{3.64}$$

The 2×2 skew symmetric coupling matrix $N_+(x,k)$ is determined by its non-zero element

$$\bar{N}_+^{12} = \frac{1}{2} \left[((B \nabla_k P \cdot \nabla_x B) b^{+,2}, b^{+,1}) - (b^{+,2}, (B \nabla_k P \cdot \nabla_x B) b^{+,1}) \right]. \tag{3.65}$$

The coherence matrix $W^+(t,x,k)$ is related to the four Stokes parameters [65, 66], which are commonly used for the description of polarized light because they are directly measurable. Let l and r be two directions orthogonal to the direction of propagation and let $I = I_l + I_r$ be the the total intensity of light, with I_l and I_r denoting the intensities in the directions l and r, respectively. Let $Q = I_l - I_r$ be the difference between the two intensities. Also let $U = 2 < E_l E_r \cos\delta >$ and $V = 2 < E_l E_r \sin\delta >$ denote the intensity coherence, with fixed phase shift δ, between the amplitude of light in the directions l and r, respectively. Light is unpolarized if $U = V = Q = 0$. If the directions l and r are chosen to be $z^{(1)}(k)$ and $z^{(2)}(k)$, given by (3.46), then the coherence matrix $w^+(t,x,k)$ is related to the Stokes parameters (I,Q,U,V) by

$$w^+(t,x,k) = \frac{1}{2}\begin{pmatrix} I+Q & U+iV \\ U-iV & I-Q \end{pmatrix}. \tag{3.66}$$

When light is unpolarized, then the coherence matrix w^+ is proportional to the 2×2 identity matrix I. We will later see that in a random medium after a long propagation time, indeed, w^+ becomes nearly proportional to identity.

3.4 Quantum waves in a periodic structure

3.4.1 The Wigner equation

We consider now the phase space energy behavior for oscillatory solutions of the Schrödinger equation in a periodic potential with a period that is comparable to the wave length of the initial data. The starting point is the Schrödinger equation

$$i\frac{\partial\phi}{\partial t} + \frac{1}{2}\Delta\phi - V(x)\,\phi = 0, \tag{3.67}$$

with a periodic potential $V(x)$. We are interested in the behavior of solutions on the scales much larger than the period $V(x)$. Accordingly we rescale time and space variables $t = t'/\varepsilon$, $x = x'/\varepsilon$ (and drop the primes):

$$\begin{aligned} &i\varepsilon\frac{\partial\phi_\varepsilon}{\partial t} + \frac{\varepsilon^2}{2}\Delta\phi_\varepsilon - V\left(\frac{x}{\varepsilon}\right)\phi_\varepsilon = 0 \\ &\phi_\varepsilon(0,x) = \phi_\varepsilon^0(x). \end{aligned} \tag{3.68}$$

The initial data $\phi_\varepsilon^0(x)$ is uniformly bounded in $L^2(\mathbb{R}^n)$, ε-oscillatory and compact at inifnity. These assumptions are natural as the initial data for the unscaled equation (3.67) vary on the scale $O(1)$, that is, comparable to the period of the potential. Since the potential and the initial data in (3.68) oscillate on the same scale we do not expect a semiclassical behavior in the limit $\varepsilon \to 0$. It turns out that energy density of solutions does not, indeed, behave in a classical manner but nevertheless can be described precisely in the limit. In particular we will see that the strong inhomogeneities modify the dispersion relation. Nevertheless the end result truns out to be a family of Liouville equations for the limit Wigner transforms albeit with a modified dispersion relation.

The potential $V(z)$ is periodic: $V(z+\nu) = V(z)$. Here the period vector ν belongs to the period lattice L:

$$L = \left\{\sum_{j=1}^{n} n_j e_j |\ n_j \in \mathbb{Z}\right\}, \tag{3.69}$$

and $e_1,\ldots,e_n$ form a basis of $\mathbb{R}^n$ with the dual basis e^j defined by $(e_j\cdot e^k) = 2\pi\delta_{jk}$ and the dual lattice L^* defined by (3.69) with e_j replaced by e^j. We denote by C the basic period cell of L and by B the Brillouin zone:

$$B = \{k\in\mathbb{R}^n |\ k \text{ is closer to } \mu = 0 \text{ than any other point } \mu\in L^*\}.$$

It is convenient in this problem to consider the Wigner transform defined relative to the standard quantization:

$$W_\varepsilon(t,x,k) = \int_{\mathbb{R}^n} e^{ik\cdot y}\phi_\varepsilon(t,x-\varepsilon y)\bar{\phi}_\varepsilon(t,x)\frac{dy}{(2\pi)^n}. \tag{3.70}$$

We deduce from (3.68) and (3.70) the following evolution equation for $W_\varepsilon(t,x,k)$:

$$\frac{\partial W_\varepsilon}{\partial t} + k\cdot\nabla_x W_\varepsilon + \frac{i\varepsilon}{2}\Delta_x W_\varepsilon = \frac{1}{i\varepsilon}\sum_{\mu\in L^*} e^{i\mu\cdot x/\varepsilon}\hat{V}(\mu)\left[W_\varepsilon(x,k-\mu) - W_\varepsilon(x,k)\right]. \tag{3.71}$$

Here $\hat{V}(\mu)$ are the periodic Fourier coefficients of $V(y)$:

$$\hat{V}(\mu) = \frac{1}{|C|}\int_C e^{-i\mu\cdot y}V(y)dy, \quad V(y) = \sum_{\mu\in L^*} e^{i\mu\cdot y}\hat{V}(\mu). \tag{3.72}$$

We will also need the Parseval summation formula

$$\frac{1}{|C|}\sum_{\mu\in L^*} e^{i\mu\cdot z} = \sum_{\nu\in L}\delta(z-\nu). \tag{3.73}$$

The Wigner equation (3.71) is analogous to the evolution equation (3.15) obtained in the case of slowly varying coefficients. The Laplacian on the left side in (3.71) appears because we have chosen to define the Wigner transform in the standard rather than in the Weyl quantization. It goes to zero weakly after multiplication by ε. However, (3.71) has an important difference compared to the Wigner equation (3.15) that arises when potential is slowly-varying: there is a rapid phase in the complex exponential on the right side.

We will follow in this section an approach based on formal asymptotic expansions. This is an effective and convenient tool to obtain an answer which is especially useful in a random medium. At the end we will explain how it may be made rigorous in the present periodic problem. To deal with the fast oscillatory term we introduce a formal multiple scales expansion for W_ε:

$$W_\varepsilon(t,x,k) = W_0\left(t,x,\frac{x}{\varepsilon},k\right) + \varepsilon W_1(t,x,\frac{x}{\varepsilon},k) + \dots \tag{3.74}$$

Each term in this expansion is a periodic function of the fast variable $z = x/\varepsilon$ modulated by a slow dependence on the slow variable x. To account for the dependence on z we have to replace

$$\nabla_x \to \nabla_x + \frac{1}{\varepsilon}\nabla_z$$

in (3.71) and rewrite it as

$$\begin{aligned}\frac{\partial W_\varepsilon}{\partial t} + k\cdot\left[\nabla_x + \frac{1}{\varepsilon}\nabla_z\right]W_\varepsilon + \frac{i\varepsilon}{2}(\nabla_x + \frac{1}{\varepsilon}\nabla_z)\cdot(\nabla_x + \frac{1}{\varepsilon}\nabla_z)W_\varepsilon \\ = \frac{1}{i\varepsilon}\sum_{\mu\in L^*} e^{i\mu\cdot z}\hat{V}(\mu)\left[W_\varepsilon(k-\mu) - W_\varepsilon(k)\right].\end{aligned} \tag{3.75}$$

We insert the asymptotic expansion (3.74) into (3.75) and get in the order ε^{-1}:

$$\mathcal{L}W_0 = 0, \tag{3.76}$$

where the skew symmetric operator $\mathcal{L}$ is given by

$$\mathcal{L}f(z,k) = k\cdot\nabla_z f + \frac{i}{2}\Delta_z f - \frac{1}{i}\sum_{\mu\in L^*} e^{i\mu\cdot z}\hat{V}(\mu)\left[f(z,k-\mu)-f(z,k)\right].$$

This equation is the analog of (3.33) in the case of slowly varying coefficients – they both require the Wigner transform to live in the kernel of an operator which (as we will see below) defines the dispersion relations. However, while the operator that appears in (3.33) algebraic, (3.76) involves a partial differential operator and the construction of its eigenvectors is more involved.

Equation $\mathcal{L}f = 0$, that is,

$$k\cdot\nabla_z f + \frac{i}{2}\Delta_z f - \frac{1}{i}\sum_{\mu\in L^*} e^{i\mu\cdot z}\hat{V}(\mu)\left[f(z,k-\mu)-f(z,k)\right] = 0$$

is (at least formally) nothing but the equation for unscaled Wigner transform of solutions of the Schrödinger equation

$$i\frac{\partial\phi}{\partial t} + \frac{1}{2}\Delta_z\phi - V(z)\phi = 0 \tag{3.77}$$

but without the time derivative $\partial f/\partial t$. How can the time derivative disappear in the Wigner equation? The simplest situation is when solutions of the Schrödinger equation itself are steady:

$$\frac{1}{2}\Delta_z\phi - V(z)\phi = 0.$$

More generally, if solutions of (3.77) have one frequency in time: $\psi(t,z) = e^{i\omega t}\phi(z;\omega)$ then their Wigner transform is time-independent. The function $\phi(z;\omega)$ solves the eigenvalue problem:

$$\frac{1}{2}\Delta_z\phi - V(z)\phi = \omega\phi. \tag{3.78}$$

In the next section we discuss such eigenvalue problems in some detail.

3.4.2 The Bloch eigenfunctions

The Bloch eigenfunctions. The eigenfunctions of the operator $\mathcal{L}$ are constructed as follows. Given a vector $p\in\mathbb{R}^n$ consider the eigenvalue problem on the period cell C:

$$-\frac{1}{2}\Delta_z\Psi(z,p) + V(z)\Psi(z,p) = E(p)\Psi(z,p) \tag{3.79}$$
$$\Psi(z+\nu,p) = e^{ip\cdot\nu}\Psi(z,p),\ \text{for all } \nu\in L$$
$$\frac{\partial\Psi}{\partial z_j}(z+\nu,p) = e^{ip\cdot\nu}\frac{\partial\Psi}{\partial z_j}(z),\ \text{for all } \nu\in L.$$

This problem has a complete orthonormal basis of eigenfunctions $\Psi_m^\alpha(z,p)$ in $L^2(C)$:

$$(\Psi_m^\alpha,\Psi_j^\beta) = \int_C \Psi_m^\alpha(z,p)\bar{\Psi}_j^\beta(z,p)\frac{dz}{|C|} = \delta_{mj}\delta_{\alpha\beta}. \tag{3.80}$$

They are called the Bloch eigenfunctions, corresponding to the real eigenvalues $E_m(p)$ of multiplicity r_m. Here $\alpha = 1,\dots,r_m$ labels eigenfunctions inside the eigenspace. The eigenvalues $E_m(p)$ are L^*-periodic in p and have constant finite multiplicity outside a closed subset F_m of $p\in\mathbb{R}^n$ of measure zero. They may be arranged $E_1(p) < E_2(p) < \cdots < E_j(p) < \dots$ with $E_j(p)\to\infty$ as $j\to\infty$, uniformly in p [83]. We consider momenta p outside the set F_m.

The Bloch transform. The Bloch transform of a function $\phi(x) \in L^2(\mathbb{R}^n)$ is defined by

$$\tilde{\phi}_m^\alpha(p) = \int_{\mathbb{R}^n} \phi(z)\bar{\Psi}_m^\alpha(z,p)dz, \quad p \in B.$$

The inverse Bloch transform is given by

$$\phi(x) = \frac{1}{|B|}\sum_{m=1}^{\infty}\sum_{\alpha=1}^{r_m}\int_B \tilde{\phi}_m^\alpha(p)\Psi_m^\alpha(x,p)dp, \quad x \in \mathbb{R}^n.$$

Let $\phi(x), \eta(x) \in L^2(R^d)$, then the Plancherel formula holds:

$$\int_{\mathbb{R}^n} \phi(x)\bar{\eta}(x)dx = \frac{1}{|B|}\sum_{m,\alpha}\int_B \tilde{\phi}_m^\alpha(p)\overline{\tilde{\eta}_m^\alpha(p)}dp.$$

The mapping $\phi \to \tilde{\phi}$ is one-to-one and onto, from $L^2(\mathbb{R}^n) \to \oplus_{m,\alpha}L^2(B)$. We deduce from these properties the orthogonality relations:

$$\delta(y-x) = \frac{1}{|B|}\sum_{m,\alpha}\int_B dp\Psi_m^\alpha(x,p)\bar{\Psi}_m^\alpha(y,p)$$

and

$$\delta_{jm}\delta_{\alpha\beta}\delta_{per}(p-q) = \frac{1}{|B|}\int_{\mathbb{R}^n} \Psi_j^\alpha(x,p)\bar{\Psi}_m^\beta(x,q)dx. \tag{3.81}$$

The periodic delta function δ_{per} in (3.81) is understood as follows: for any periodic test function $\phi(p) \in C^\infty(B)$

$$\phi(p) = \int_B \phi(q)\delta_{per}(p-q)dq.$$

The eigenfunctions of the operator $\mathcal{L}$. Given any vector $k \in \mathbb{R}^n$ we may decompose it uniquely as

$$k = p_k + \mu_k \tag{3.82}$$

with $p_k \in B$ and $\mu_k \in L^*$. We then define the z-periodic functions $\tilde{Q}_{mn}^{\alpha\beta}(z,\mu,p)$, $\mu \in L^*$, $p \in B$ by

$$\tilde{Q}_{mn}^{\alpha\beta}(z,\mu,p) = \int_C e^{i(p+\mu)\cdot y}\Psi_m^\alpha(z-y,p)\bar{\Psi}_n^\beta(z,p)\frac{dy}{|C|} = \int_C e^{i\mu\cdot y}\Phi_m^\alpha(z-y,p)\bar{\Phi}_n^\beta(z,p)\frac{dy}{|C|} \tag{3.83}$$

and set $Q_{mn}^{\alpha\beta}(z,\mu,p) = \tilde{Q}_{mn}^{\alpha\beta}(z,\mu_k,p_k)$. The functions $Q_{mn}^{\alpha\beta}(z,k)$ are eigenfunctions of the operator $\mathcal{L}$:

$$\mathcal{L}Q_{mn}^{\alpha\beta}(z,k) = i(E_m(k) - E_n(k))Q_{mn}^{\alpha\beta}(z,k) \tag{3.84}$$

since $E_m(k) = E_m(p)$ as Bloch eigenvalues are periodic with respect to the dual lattice L^*. These eigenfunctions are orthonormal in the following sense: for each fixed $p \in B$ we have

$$\sum_{\mu\in L^*}\int_C \tilde{Q}_m^{\alpha'\beta'}(z,\mu,p)\overline{\tilde{Q}_j}\alpha\beta(z,\mu,p)\frac{dz}{|C|} \tag{3.85}$$

$$= \sum_{\mu\in L^*}\int_{C^3} e^{i\mu\cdot y - i\mu\cdot y'}\Phi_m^{\alpha'}(z-y,p)\bar{\Phi}_m^{\beta'}(z,p)\bar{\Phi}_j^\alpha(z-y,p)\Phi_j^\beta(z,p)\frac{dydy'dz}{|C|^2}$$

$$= \int_{C\times C}\Phi_m^{\alpha'}(z,p)\bar{\Phi}_m^{\beta'}(y,p)\bar{\Phi}_j^\alpha(z,p)\Phi_j^\beta(y,p)\frac{dydz}{|C|^2} = \delta_{mj}\delta_{\alpha\alpha'}\delta_{\beta\beta'}. \tag{3.86}$$

It follows, of course that the following orthogonality relation holds

$$\int_{C\times\mathbb{R}^n} Q_m^{\alpha'\beta'}(z,k)\bar{Q}_j^{\alpha\beta}(z,k)\frac{dzdk}{|C|} = \delta_{mj}\delta_{\alpha\alpha'}\delta_{\beta\beta'}. \tag{3.87}$$

3.4.3 The Liouville equations

We go back to the derivation of the Liuoville equations for the Wigner transform. First, (3.84) implies that, for any p, the kernel of the operator $\mathcal{L}$ is spanned by the functions $Q^{\alpha\beta}_{mm}$, which we denote by $Q^{\alpha\beta}_{m}$ (to indicate that there is no summation over m). Then condition (3.76) implies that the leading term $W_0(t,x,z,k)$ may be written as

$$W_0(t,x,z,k) = W_0(t,x,z,p+\mu) = \sum_{m,\alpha,\beta} \sigma^{\alpha\beta}_m(t,x,p) Q^{\alpha\beta}_m(z,\mu,p), \quad p \in B, \ \mu \in L^* \qquad (3.88)$$

with $\mu = \mu_k$, $p = p_k$. This defines $\sigma_m(t,x,p)$, which is scalar if the eigenvalue $E_m(p)$ is simple, and is a matrix of size $r_m \times r_m$ if $E_m(p)$ has multiplicity $r_m > 1$. We call σ_m the coherence matrices in analogy to the non-periodic case. They are defined inside the Brillouin zone $p \in B$ but it is convenient to extend them as functions in $\mathbb{R}^n$, L^*-periodic in p.

Next we look at ε^0 terms in (3.75). We get an equation

$$\frac{\partial W_0}{\partial t} + k \cdot \nabla_x W_0 + i \nabla_x \cdot \nabla_z W_0 = -\mathcal{L} W_1. \qquad (3.89)$$

The operator $\mathcal{L}$ is skew-symmetric on $L^2(C \times \mathbb{R}^n)$. Therefore for (3.89) to be solvable for W_1, its right side should be orthogonal to the kernel of $\mathcal{L}$. This solvability condition after some intermediate computations lead to the Liouville equations for the coherence matrices σ_m:

$$\frac{\partial \sigma_m}{\partial t} + \nabla_p E_m \cdot \nabla_x \sigma_m = 0. \qquad (3.90)$$

The approach we have taken above with the formal perturbation expansion is formal and does not produce a mathematical proof in itself. However, it is not very difficult in this particular case to turn it into a proof since we already know a priori bounds for $W_\varepsilon(t,x,k)$. A more elegant approach to this problem is via the Wigner band series [96]. The Wigner transform approach we took is more convenient in the formal analysis when random perturbations of the potential are introduced but very little is known in this directions rigorously.

Chapter 4

The radiative transport limit

4.1 The radiative transport limit in a deterministic setting

This material is based on [55].

The weak limit $\bar{W}(t,x,k)$ of the Wigner transform of the solution of the Schrödinger equation in the weak coupling limit

$$i\varepsilon\frac{\partial\psi_\varepsilon}{\partial t} + \varepsilon^2\Delta\psi_\varepsilon + \sqrt{\varepsilon}V\big(\frac{x}{\varepsilon}\big)\psi_\varepsilon = 0 \tag{4.1}$$

with a random potential V satisfies the radiative transport equation

$$\frac{\partial\bar{W}}{\partial t} + k\cdot\nabla_x\bar{W} = \int_{\mathbb{R}^d}|\alpha(p-k)|^2[\bar{W}(p)-\bar{W}(k)]\delta\left(\frac{k^2-p^2}{2}\right)dp. \tag{4.2}$$

Here $x\in\mathbb{R}^d$ is the physical space coordinate and $k\in\mathbb{R}^d$ is the wave vector. The passage from (4.1) to (4.2) with a spatially homogeneous random potential V has been first proved in [102, 97] for a short time interval and later extended to a global in time result in [94]. The scattering cross-section $|\alpha(p)|^2$ in (4.2) turns out to be the power spectrum of the random potential V.

The proofs in [102, 97, 94] are based on the intricate analysis of the individual contributions of various terms in the Duhamel expansion of (4.1) and are highly technical. The difficulties are intrinsic to the problem as the limit is only weak and the oscillatory terms are not small in the strong norms. The problem becomes much simpler if the random potential is random in time as well [86, 87, 95, 100] – this introduces an additional mixing that allows to obtain L^2 estimates based on the perturbed test function method.

Here we consider a deterministic model where the kinetic limit can be obtained in a straightforward manner. It turns out that this may be achieved by introducing a high-frequency damping in the Wigner equation, replacing the exact equation for the Wigner transform with

$$\frac{\partial W_\varepsilon}{\partial t}+k\cdot\nabla_x W_\varepsilon+\frac{\theta}{\varepsilon}\left(W_\varepsilon-\chi_\varepsilon\star W_\varepsilon\right)=\frac{1}{i\sqrt{\varepsilon}}\int e^{ip\cdot x/\varepsilon}\left[W_\varepsilon(x,k-\frac{p}{2})-W_\varepsilon(x,k+\frac{p}{2})\right]\hat{V}(p)\frac{dp}{(2\pi)^d}, \tag{4.3}$$

with a positive function $\chi_\varepsilon=\varepsilon^{-d}\chi(x/\varepsilon)$ such that $\int\chi(x)dx=1$. The regularization parameter $\theta\ll 1$ is small. Heuristically, the last term on the left side of (4.3) is absorbing for the high frequency component as $\chi_\varepsilon\star W_\varepsilon^{hf}\approx 0$ while it is not damping the low frequencies of W_ε, since $\chi_\varepsilon\star W_\varepsilon^{lf}\approx W_\varepsilon^{lf}$ for the low frequency part of W_ε. This is also reflected in the energy balance

$$\frac{1}{2}\frac{d}{dt}\int|W(t,x,k)|^2dxdk=-\frac{\theta}{\varepsilon}\int(1-\hat{\chi}(\varepsilon p))|\hat{W}(t,p,k)|^2dpdk\le 0. \tag{4.4}$$

Hence, the purpose of the weak high frequency damping is to capture correctly only the low frequency behavior while getting rid of the high frequency oscillations. This leads to the strong L^2-convergence of the solution of (4.3) to the solution of a kinetic equation as the high frequency oscillations are absent in the limit.

The potential V in (4.3) is not required to be random or periodic: the only requirement is that its Fourier transform has a non-trivial singular part: see (4.8) below. This is another interesting aspect of the current set-up: the regularized Wigner equation may be homogenized in a very general setting with almost no underlying small-scale structure, such as periodicity or statistical homogeneity, assumed.

On the other hand, the derivation of a scattering equation from the true Wigner equation with a given potential is certainly impossible in a general deterministic framework. Introduction of a regularization allows us to get forward with several steps which are based on three different limits. Firstly the homogenization parameter ε vanishes, secondly the potential pseudo period lattice, denoted by δ below vanishes and thirdly the regularization parameter θ vanishes. We note that the final result of the three sequential limits is exactly the same kinetic equation (4.2) with an appropriately defined function $\alpha(p)$. Two comments are in order: first, the final kinetic equation is completely independent of the choice of the regularization function $\chi(x)$. Second, only the singular part of the measure-valued Fourier transform $\hat{V}(p)$ contributes to the scattering cross-section.

We note that the result we prove below, the strong convergence to the homogenized limit, is certainly impossible for the unregularized Wigner equation because it preserves the L^2 norm of the solution, while the scattering equation does not.

Our formalism allows us to use different methods that rely on the homogenization methods as presented in [88, 93] for instance, that is, building a multi-scale expansion

$$W_\varepsilon = \bar{W} + \sqrt{\varepsilon} W_1(t, x, \frac{x}{\varepsilon}, k) + \varepsilon W_2(t, x, \frac{x}{\varepsilon}, k) + \dots$$

Here again the regularized equation allows us to make sense of the expansion. The specific difficulty is that the corrector equation for W_1, W_2 is ill-posed without regularization in our framework.

We consider a regularized Wigner equation

$$\frac{\partial W_\varepsilon}{\partial t} + k \cdot \nabla_x W_\varepsilon + \frac{\theta}{\varepsilon}\left(W_\varepsilon - \chi_\varepsilon \star W_\varepsilon\right) = \mathcal{L}_\varepsilon W_\varepsilon, \qquad t \geq 0,\ x \in \mathbb{R}^d,\ k \in \mathbb{R}^d, \tag{4.5}$$

$$\mathcal{L}_\varepsilon f(x,k) = \frac{1}{i\sqrt{\varepsilon}} \int e^{ip\cdot x/\varepsilon} \left[f(x, k - \frac{p}{2}) - f(x, k + \frac{p}{2}) \right] \hat{V}(p) \frac{dp}{(2\pi)^d}. \tag{4.6}$$

The function $\chi_\varepsilon(x) = \frac{1}{\varepsilon^d} \chi\left(\frac{x}{\varepsilon}\right)$ in (4.5) with $\chi \in \mathcal{S}(\mathbb{R}^d)$ (the Schwartz space) and $\chi(x) = \chi(|x|) \geq 0$ radially symmetric, and normalized so that

$$\int_{\mathbb{R}^d} \chi(x) dx = 1.$$

Henceforth, $\hat{\chi} \in \mathcal{S}(\mathbb{R}^d)$ satisfies

$$\hat{\chi} \in \mathbb{R}, \qquad |\hat{\chi}(p)| < 1 \ \text{ for } p \neq 0, \qquad \hat{\chi}(0) = 1.$$

The parameter θ is small but fixed – we may allow θ to depend on ε so that $\theta \gg \varepsilon$ but we do not pursue this issue here for the sake of clarity of presentation. The last term on the left side of (4.5) is regularizing in L^2, that is:

$$\frac{1}{2}\frac{d}{dt} \int |W_\varepsilon(t,x,k)|^2 dx dk = -\frac{\theta}{\varepsilon} \int |1 - \hat{\chi}(\varepsilon p)|^2 \, |\hat{W}_\varepsilon(p,k)|^2 \frac{dp dk}{(2\pi)^d}. \tag{4.7}$$

The energy balance (4.7) shows that the effect of the regularization is damping of the high frequencies. This allows us to show the strong convergence of the solution of (4.5) to the solution of a kinetic equation in the limit $\varepsilon \to 0$. The regularization allows us to make the formal asymptotic expansions rigorous and circumvent dealing with the weak convergence.

We assume that the Fourier transform of the potential $V(x)$ has the form

$$\hat{V}(p) = \sum_{j=1}^{\infty} \alpha_j[\delta(p - p_j) + \delta(p + p_j)] + \hat{\Phi}(p) \tag{4.8}$$

with the real Fourier coefficients $\alpha_j \in \mathbb{R}$ and $\hat{\Phi}(p)$ that is smooth, sufficiently rapidly decaying and with $\hat{\Phi}(0) = 0$. We also assume that the sequence α_j satisfies the following conditions:

$$\sum_{j=1}^{\infty} \frac{|\alpha_j|}{|1 - \hat{\chi}(p_j)|} < +\infty \tag{4.9}$$

and

$$\sum_{j,l=1}^{\infty} \frac{|\alpha_j||\alpha_l|}{|1 - \hat{\chi}(p_l)||1 - \hat{\chi}(p_j + p_l)|} + \sum_{j \neq l} \frac{|\alpha_j||\alpha_l|}{|1 - \hat{\chi}(p_l)||1 - \hat{\chi}(p_j - p_l))|} < +\infty. \tag{4.10}$$

Recall that $\hat{\chi}(0) = 1$ so that (4.9) means that $\hat{V}(p)$ is not singular at $p = 0$: oscillations are not concentrated at the zero wave number.

These conditions are satisfied if, for instance, $\alpha_j \in l^1$ and the wave vectors p_j are non-resonant: there exists $\omega_0 > 0$ so that

$$|p_j| \geq \omega_0 > 0, \quad |p_j \pm p_l| \geq \omega_0 \text{ for } j \neq l. \tag{4.11}$$

On the other hand, (4.9) implies that $\alpha_j \in l^1$ and thus the potential $V(x))$ satisfies

$$|V(x)| \leq \int |\hat{V}(p)| dp < +\infty.$$

It follows that the operator $\mathcal{L}_\varepsilon$ is uniformly bounded from $L^2(\mathbb{R}^d \times \mathbb{R}^d)$ into itself and the existence theory for (4.5)–(4.6) is thus standard.

We define the scattering kernel

$$K_\theta(k,p) = \frac{1}{(2\pi)^d} \frac{2\theta(1 - \hat{\chi}(p))}{\theta^2(1 - \hat{\chi}(p))^2 + ((k + \frac{p}{2}) \cdot p)^2}, \tag{4.12}$$

and use the convention that for $j \leq -1$, $p_j = -p_{-j}$. Then we have the following theorem which shows that only the singular (oscillatory) component of the potential affects the limit.

Theorem 4.1.1 *Let the initial data $W_\varepsilon(0,x,k) = W_0(x,k)$ for (4.5) belong to $L^2(\mathbb{R}^d \times \mathbb{R}^d)$ and assume (4.8), (4.9) and (4.10) on the potential $V(x)$ and the regularization function $\chi(x)$. Then the operator $\mathcal{L}_\varepsilon$ is uniformly bounded on $L^2(\mathbb{R}^d \times \mathbb{R}^d)$ and the solution of (4.5) converges in $C\big([0,T]; L^2(\mathbb{R}^d \times \mathbb{R}^d)\big)$ to the solution of the kinetic equation*

$$\frac{\partial \bar{W}}{\partial t} + k \cdot \nabla_x \bar{W} = \sum_{j \in \mathbb{Z}^*} |\alpha_j|^2 K_\theta(k,p_j)[\bar{W}(k + p_j) - \bar{W}(k)] \tag{4.13}$$

with the initial data $\bar{W}(0,x,k) = W_0(x,k)$.

Note that the scattering kernel $K_\theta(k,p_j)$ is positive and (4.13) is a kinetic equation that may be given a probabilistic interpretation. Physically, the scattering cross-section depends only on the singular part of the potential because a weak $O(\sqrt{\varepsilon})$ localized potential due to $\hat{\Phi}(p)$ in (4.8) does not affect the wave energy propagation over long distances, as opposed to the potential due to the singular part of the spectrum that is "present everywhere".

Let us now assume that we are given a family of potentials $V^\delta(x)$ of the form (4.8), parametrized by a parameter $\delta > 0$, such that, uniformly,

$$\sum_{j=1}^{\infty} |\alpha_j^\delta|^2 \, \frac{1}{1-\hat{\chi}(p_j^\delta)} < \infty. \tag{4.14}$$

For instance the wave vectors p_j^δ may be picked so that there is exactly one p_j in each cube of a cubic lattice in $\mathbb{R}^d_+ = \{q = (q_1,\ldots,q_d) \in \mathbb{R}^d : \ q_1 > 0\}$ with the cube side $\delta \ll 1$, while the amplitudes are scaled so that $\alpha_j^\delta = \delta^{d/2}\alpha(p_j^\delta)$ for a smooth function $\alpha(p)$. Then the scattering term on the right side of (4.13) has the form

$$\mathcal{K}_\theta^\delta \bar{W}(k) = \delta^d \sum_{j\in\mathbb{Z}^*} |\alpha(p_j^\delta)|^2 K_\theta(k,p_j^\delta)[\bar{W}(k+p_j^\delta) - \bar{W}(k)]$$

that is a Riemann sum of

$$\int |\alpha(p)|^2 K_\theta(k,p)[\bar{W}(k+p) - \bar{W}(k)]dp = \int |\alpha(p-k)|^2 K_\theta(k,p-k)[\bar{W}(p) - \bar{W}(k)]dp,$$

with

$$\int |\alpha(p)|^2 \, \frac{1}{1-\hat{\chi}(p)} dp < \infty. \tag{4.15}$$

We have the following convergence result.

Theorem 4.1.2 *Let the initial data $W_0(x,k)$ for (4.13) belong to $L^2(\mathbb{R}^d \times \mathbb{R}^d)$ and make the above assumptions (4.14), (4.15) on the distribution of the points p_j^δ and amplitudes α_j^δ. Then, the operator $\mathcal{K}_\theta^\delta$ is uniformly bounded in $L^2(\mathbb{R}^d)$ as δ vanishes and the solution $\bar{W}_\theta^\delta$ of (4.13) converges in $C\big([0,T];L^2(\mathbb{R}^d\times\mathbb{R}^d)\big)$ to the solution of the kinetic equation*

$$\frac{\partial \bar{U}}{\partial t} + k\cdot\nabla_x \bar{U} = \int_{\mathbb{R}^d} |\alpha(p-k)|^2 K_\theta(k,p-k)[\bar{U}(p) - \bar{U}(k)]dp \tag{4.16}$$

with the initial data $\bar{U}(0,x,k) = W_0(x,k)$.

Equation (4.16) is now a continuous scattering equation but it allows interaction of waves with different frequencies $\omega = k^2/2$, unlike the kinetic equation (4.2) which preserves the energy sphere. The final observation is that the scattering kernel $K_\theta(k,p-k)$ converges as $\theta \to 0$:

$$\begin{aligned} P_\theta(k,p) &= |\alpha(p-k)|^2 K_\theta(k,p-k) \\ &= |\alpha(p-k)|^2 2\theta(1-\hat{\chi}(p-k)) \left\{ \theta^2\,(1-\hat{\chi}(p-k))^2 + \left(\frac{p^2-k^2}{2}\right)^2 \right\}^{-1} \\ &\to \frac{2\pi|\alpha(p-k)|^2}{1-\hat{\chi}(p-k)}\,\delta\left(\frac{p^2-k^2}{2(1-\hat{\chi}(p-k))}\right) = 2\pi|\alpha(p-k)|^2\,\delta\left(\frac{p^2-k^2}{2}\right). \end{aligned} \tag{4.17}$$

This calculation requires an extra assumption in order to manipulate the operator

$$\mathcal{P}_\theta U(k) = \int |\alpha(p-k)|^2 K_\theta(k,p-k)[U(p) - U(k)]dp,$$

namely

$$M_\alpha := \int_{S^{d-1}} \sup_{r>0} r^{d-2} |\alpha(r\omega)|^2 \, d\omega < \infty. \tag{4.18}$$

This implies our last result.

Theorem 4.1.3 *Let the initial data $W_0(x,k)$ for (4.16) belong to $L^2(\mathbb{R}^d \times \mathbb{R}^d)$ and assume (4.18) on the scattering function $\alpha(p)$ and the bound of Lemma* **??** *on χ. Then, the operator $\mathcal{P}_\theta$ is uniformly bounded in $L^2(\mathbb{R}^d)$ and the solution $\bar{U}_\theta$ of (4.16) converges in $C\big([0,T]; L^2(\mathbb{R}^d \times \mathbb{R}^d)\big)$, as $\theta \to 0$, to the solution of the kinetic equation*

$$\frac{\partial \bar{Z}}{\partial t} + k \cdot \nabla_x \bar{Z} = \int_{\mathbb{R}^d} |\alpha(p-k)|^2 [\bar{Z}(p) - \bar{Z}(k)] \delta\left(\frac{k^2 - p^2}{2}\right) dp \tag{4.19}$$

with the initial data $\bar{W}(0,x,k) = W_0(x,k)$.

Note that the final equation (4.19) is independent from the regularization function $\chi(p)$ and is nothing but the transport equation (4.2) with an appropriately defined scattering cross-section $\alpha(\cdot)$.

Chapter 5

Application of the transport theory to the time reversal experiments

5.1 Time-reversal experiments

In time reversal experiments, acoustic waves are emitted from a localized source, recorded in time by an array of receivers-transducers, time reversed, and re-transmitted into the medium, so that the signals recorded first are re-emitted last and vice versa [20, 21, 28, 35, 42, 46]: a schematic description of the time reversal procedure is depicted in Fig. 5.1.

Figure 5.1: The Time Reversal Procedure. Top: Propagation of signal and measurements in time. Bottom: Time reversal of recorded signals and back-propagation into the medium.

Early experiments in time reversal acoustics are described in [20]; see also the more recent papers [26, 27, 28] – this list is by no means exhaustive and the literature on the subject is by now vast. The re-transmitted signal refocuses at the location of the original source with a modified shape that depends on the array of receivers. The salient feature of these time reversal experiments is that refocusing is much better when wave propagation occurs in complicated environments than in homogeneous media. Time reversal techniques with improved refocusing in heterogeneous medium have found important applications in medicine, non-destructive testing, underwater acoustics, and wireless communications (see the above references). It has been also applied to imaging in weakly random media [10, 14, 28] and led to a recent concept of coherent interferometric imaging (CINT) of Borcea, Papanicolaou and Tsogka [15, 16, 17].

A very qualitative explanation for the better refocusing observed in heterogeneous media is based on *multipathing*. Since waves can scatter off a larger number of heterogeneities, more paths coming from the source reach the recording array, thus more is known about the source by the transducers than in a homogeneous medium. The heterogeneous medium plays the role of a lens that widens the aperture through which the array of receivers sees the source. Refocusing is also qualitatively justified by ray theory (geometrical optics). The phase shift caused by multiple scattering is exactly compensated when the time reversed signal follows the same path back to the source location. This phase cancellation happens only at the source location. The phase shift along paths leading to other points in space is essentially random. The interference of multiple paths will thus be constructive at the source location and destructive anywhere else. This explains why refocusing at the source location is improved when the number of scatterers is large.

As convincing as they are, the above explanations remain qualitative and do not allow us to quantify how the refocused signal is modified by the time reversal procedure. Quantitative justifications require to analyze wave propagation more carefully. The first quantitative description of time reversal was obtained in [18] in the framework of one-dimensional random media. That paper provides the first mathematical explanation of two of the most prominent features of time reversal: heterogeneities improve refocusing and refocusing occurs for almost every realization of the random medium. Various extensions and generalizations to the three-dimensional layered case, including nonlinear effects, have been done in the work by Garnier, Fouque, Nachbin, Papanicolaou and Solna, and are described in detail in the recent excellent book [30]. The first multi-dimensional quantitative description of time reversal was obtained in [13] for the parabolic approximation, i.e., for waves that propagate in a privileged direction with no backscattering (see also [54] for further analysis of time reversal in this regime). That paper shows that the random medium indeed plays the role of a lens. The back-propagated signal behaves as if the initial array were replaced by another one with a much bigger effective aperture. In a slightly different context, time reversal in ergodic cavities was analyzed in [8]. There, wave mixing is created by reflection at the boundary of a chaotic cavity, which plays a similar role to the heterogeneities in a heterogeneous medium.

In this chapter we consider the theory of time-reversal experiments for general classical waves propagating in weakly fluctuating random media. It is convenient to understand refocusing in time reversal experiments in the following three-step general framework:

(i) A signal propagating from a localized source is recorded at a single time $T > 0$ by an array of receivers.

(ii) The recorded signal is processed at the array location.

(iii) The processed signal is emitted from the array and propagates in the *same* medium during the same amount of time T.

As we will see, this formulation allows us to reduce the mathematical problem of the description of the refocused signal to the question of the passage from the wave equations to the kinetic models. While the latter problem is also difficult, we may apply whatever is known in that area to the time-reversal problems. Accordingly, the mathematical rigor of our statements on time-reversal experiments below depends on the regime of consideration – for instance, they are mostly formal in the radiative transfer regime but are rigorous in the random geometric optics regime (see [6] for the precise statements). To keep the presentation uniform we will concentrate here solely on the transport regime.

The first main result of this chapter is that the repropagated signal will refocus at the location of the original source for a large class of waves and a large class of processings. The experiments described above correspond to the specific processing of acoustic waves in which pressure is kept unchanged and the sign of the velocity field is reversed.

The second main result is a quantitative description of the re-transmitted signal. We show that the re-propagated signal $\mathbf{u}^B(\xi)$ at a point ξ near the source location can be written in the high frequency limit as the following convolution of the original source $\mathbf{S}$

$$\mathbf{u}^B(\xi) = (F * \mathbf{S})(\xi). \tag{5.1}$$

The kernel F depends on the location of the recording array and on the signal processing. The quality of the refocusing depends on the spatial decay of F. It turns out that it can be expressed in terms of the Wigner transform [101] of two wave fields. The decay properties of

F depend on the smoothness of the Wigner transform in the phase space and it is here that the kinetic theories becomes useful. Here we consider the high frequency regime when the wavelength of the initial signal is small compared to the distance of propagation. In addition we assume that the wavelength is comparable to the correlation length of the medium. This is the radiative transport regime. It has been extensively studied mathematically for the Schrödinger equation [23, 102] and formally using perturbation expansions for the classical waves [7, 101]. In this regime the Wigner transform satisfies a radiative transport equation, which is used to describe the evolution of the energy density of waves in random media [36, 101, 56, 102]. The transport equations possess a smoothing effect so that the Wigner distribution becomes less singular in random media, which implies a stronger decay of the convolution kernel F and a better refocusing. The diffusion approximation to the radiative transport equations provides simple reconstruction formulas that can be used to quantify the refocusing quality of the back-propagated signal. This construction applies to a large class of classical waves: acoustic, electromagnetic, elastic, and others, and allows for a large class of signal processings at the recording array.

5.2 Classical Time Reversal and One-Step Time Reversal

Propagation of acoustic waves is described by a system of equations for the pressure $p(t,x)$ and acoustic velocity $\mathbf{v}(t,x)$:

$$\begin{aligned} \rho(x)\frac{\partial \mathbf{v}}{\partial t} + \nabla p = 0 \\ \kappa(x)\frac{\partial p}{\partial t} + \nabla\cdot\mathbf{v} = 0, \end{aligned} \tag{5.2}$$

with suitable initial conditions and where $\rho(x)$ and $\kappa(x)$ are density and compressibility of the underlying medium, respectively. These equations can be recast as the following linear hyperbolic system

$$A(x)\frac{\partial \mathbf{u}}{\partial t} + D^j\frac{\partial \mathbf{u}}{\partial x^j} = 0, \quad x \in \mathbb{R}^3 \tag{5.3}$$

with the vector $\mathbf{u} = (\mathbf{v}, p) \in \mathbb{C}^4$. The matrix $A = \mathrm{Diag}(\rho,\rho,\rho,\kappa)$ is positive definite. The 4×4 matrices D^j, $j = 1,2,3$, are symmetric and given by $D^j_{mn} = \delta_{m4}\delta_{nj} + \delta_{n4}\delta_{mj}$. We use the Einstein convention of summation over repeated indices.

The time reversal experiments in [20] consist of two steps. First, the direct problem

$$\begin{aligned} & A(x)\frac{\partial \mathbf{u}}{\partial t} + D^j\frac{\partial \mathbf{u}}{\partial x^j} = 0,\ 0 \le t \le T \\ & \mathbf{u}(0,x) = \mathbf{S}(x) \end{aligned} \tag{5.4}$$

with a localized source $\mathbf{S}$ centered at a point x_0 is solved. The signal is recorded during the period of time $0 \le t \le T$ by an array of receivers located at $\Omega \subset \mathbb{R}^3$. Second, the signal is time reversed and re-emitted into the medium. Time reversal is described by multiplying $\mathbf{u} = (\mathbf{v}, p)$ by the matrix $\Gamma = \mathrm{Diag}(-1,-1,-1,1)$. The back-propagated signal solves

$$\begin{aligned} & \frac{\partial \mathbf{u}}{\partial t} + A^{-1}(x)D^j\frac{\partial \mathbf{u}}{\partial x^j} = \frac{1}{T}\mathbf{R}(2T-t,x),\ T \le t \le 2T \\ & \mathbf{u}(T,x) = 0 \end{aligned} \tag{5.5}$$

with the source term

$$\mathbf{R}(t,x) = \Gamma\mathbf{u}(t,x)\chi(x). \tag{5.6}$$

The function $\chi(x)$ is either the characteristic function of the set where the recording array is located, or some other function that allows for possibly space-dependent amplification of the re-transmitted signal.

The back-propagated signal is then given by $\mathbf{u}(2T, x)$. We can decompose it as

$$\mathbf{u}(2T, x) = \frac{1}{T}\int_0^T ds\ \mathbf{w}(s, x; s), \tag{5.7}$$

where the vector-valued function $\mathbf{w}(t, x; s)$ solves the initial value problem

$$\begin{aligned} &A(x)\frac{\partial \mathbf{w}(t, x; s)}{\partial t} + D^j \frac{\partial \mathbf{w}(t, x; s)}{\partial x^j} = 0, \quad 0 \le t \le s \\ &\mathbf{w}(0, x; s) = \mathbf{R}(s, x). \end{aligned}$$

We deduce from (5.7) that it is sufficient to analyze the refocusing properties of $\mathbf{w}(s, x; s)$ for $0 \le s \le T$ to obtain those of $\mathbf{u}(2T, x)$. For a fixed value of s, we call the construction of $\mathbf{w}(s, x; s)$ one-step time reversal.

We define one-step time reversal more generally as follows. The direct problem (5.4) is solved until time $t = T$ to yield $\mathbf{u}(T^-, x)$. At time T, the signal is recorded and processed. The processing is modeled by an amplification function $\chi(x)$, a blurring kernel $f(x)$, and a (possibly spatially varying) time reversal matrix Γ. After processing, we have

$$\mathbf{u}(T^+, x) = \Gamma(f * (\chi\mathbf{u}))(T^-, x)\chi(x). \tag{5.8}$$

The processed signal then propagates for the same amount of time T:

$$\begin{aligned} &A(x)\frac{\partial \mathbf{u}}{\partial t} + D^j \frac{\partial \mathbf{u}}{\partial x^j} = 0, \ T \le t \le 2T \\ &\mathbf{u}(T^+, x) = \Gamma(f * (\chi\mathbf{u}))(T^-, x)\chi(x). \end{aligned} \tag{5.9}$$

The main question is whether $\mathbf{u}(2T, x)$ refocuses at the location of the original source $\mathbf{S}(x)$ and how the original signal has been modified by the time reversal procedure. Notice that in the case of full ($\Omega = \mathbb{R}^3$) and exact ($f(x) = \delta(x)$) measurements with $\Gamma = \mathrm{Diag}(-1, -1, -1, 1)$, the time-reversibility of first-order hyperbolic systems implies that $\mathbf{u}(2T, x) = \Gamma\mathbf{S}(x)$, which corresponds to exact refocusing. When only partial measurements are available we shall see in the following sections that $\mathbf{u}(2T, x)$ is closer to $\Gamma\mathbf{S}(x)$ when propagation occurs in a heterogeneous medium than in a homogeneous medium.

The pressure field $p(t, x)$ satisfies the following scalar wave equation

$$\frac{\partial^2 p}{\partial t^2} - \frac{1}{\kappa(x)}\nabla \cdot \left(\frac{1}{\rho(x)}\nabla p\right) = 0. \tag{5.10}$$

A schematic description of the one-step procedure for the wave equation is presented in Fig. 5.2. A numerical experiment for the one-step time reversal procedure is shown in Fig. 5.3. In the

Figure 5.2: The One-Step Time Reversal Procedure. Here, p_t denotes $\dfrac{\partial p}{\partial t}$.

numerical simulations, there is no blurring, $f(x) = \delta(x)$, and the array of receivers is the domain $\Omega = (-1/6, 1/6)^2$ ($\chi(x)$ is the characteristic function of Ω). Note that the truncated signal does not retain any information about the ballistic part of the original wave (the part

Figure 5.3: Numerical experiment using the one-step time reversal procedure. Top Left: initial condition $p(0,x)$, a peaked Gaussian of maximal amplitude equal to 1. Top Right: forward solution $p(T^-,x)$, of maximal amplitude 0.04. Bottom Right: recorded solution $p(T^+,x)$, of maximal amplitude 0.015 on the domain $\Omega = (-1/6,1/6)^2$. Bottom Left: back-propagated solution $p(2T,x)$, of maximal amplitude 0.07.

that propagates without scattering with the underlying medium). In a homogeneous medium, the truncated signal would then be nearly identically zero (not quite zero since the numerics are done in two dimensions) and no refocusing would be observed. The interesting aspect of time reversal is that a coherent signal emerges at time $2T$ out of a signal at time T^+ that seems to have no useful information.

5.3 Theory of Time Reversal in Random Media

Our objective is now to present a theory that explains in a quantitative manner the refocusing properties described in the preceding sections. We consider here the one-step time reversal for acoustic wave. Generalizations to other types of waves and more general processings in (5.9) are given in Section 5.4.

5.3.1 Refocused Signal

We recall that the one-step time reversal procedure consists of letting an initial pulse $\mathbf{S}(x)$ propagate according to (5.4) until time T,

$$\mathbf{u}(T^-,x) = \int_{\mathbb{R}^3} G(T,x;z)\mathbf{S}(z)dz,$$

where $G(T,x;z)$ is the Green's matrix solution of

$$\begin{aligned} &A(x)\frac{\partial G(t,x;y)}{\partial t} + D^j\frac{\partial G(t,x;y)}{\partial x^j} = 0,\ \ 0 \le t \le T \\ &G(0,x;y) = I\delta(x-y). \end{aligned} \tag{5.11}$$

At time T, the "intelligent" array reverses the signal. For acoustic pulses, this means keeping pressure unchanged and reversing the sign of the velocity field. The array of receivers is located in $\Omega \subset \mathbb{R}^3$. The amplification function $\chi(x)$ is an arbitrary bounded function supported in Ω, such as its characteristic function ($\chi(x) = 1$ for $x \in \Omega$ and $\chi(x) = 0$ otherwise) when all transducers have the same amplification factor. We also allow for some blurring of the recorded data modeled by a convolution with a function $f(x)$. The case $f(x) = \delta(x)$ corresponds to exact measurements. Finally, the signal is time reversed, that is, the direction of the acoustic velocity is reversed. Here, the operator Γ in (5.8) is simply multiplication by the matrix

$$\Gamma = \mathrm{Diag}(-1,-1,-1,1). \tag{5.12}$$

The signal at time T^+ after time reversal takes then the form

$$\mathbf{u}(T^+,x) = \int_{\mathbb{R}^6} \Gamma G(T,y';z)\chi(x)\chi(y')f(x-y')\mathbf{S}(z)dzdy'. \tag{5.13}$$

The last step (5.9) consists of letting the time reversed field propagate through the random medium until time $2T$. To compare this signal with the initial pulse $\mathbf{S}$, we need to reverse the acoustic velocity once again, and define

$$\mathbf{u}^B(x) = \Gamma\mathbf{u}(2T, x) = \int_{\mathbb{R}^9} \Gamma G(T, x; y)\Gamma G(T, y'; z)\chi(y)\chi(y')f(y-y')\mathbf{S}(z)dydy'dz. \tag{5.14}$$

The time reversibility of first-order hyperbolic systems implies that $\mathbf{u}^B(x) = \mathbf{S}(x)$ when $\Omega = \mathbb{R}^d$, $\chi \equiv 1$, and $f(x) = \delta(x)$, that is, when full and non-distorted measurements are available. It remains to understand which features of $\mathbf{S}$ are retained by $\mathbf{u}^B(x)$ when only partial measurement is available.

5.3.2 Localized Source and Scaling

We consider an asymptotic solution of the time reversal problem (5.4), (5.9) when the support λ of the initial pulse $\mathbf{S}(x)$ is much smaller than the distance L of propagation between the source and the recording array: $\varepsilon = \lambda/L \ll 1$. We also take the size a of the array comparable to L: $a/L = O(1)$. We assume that the time T between the emission of the original signal and recording is of order L/c_0, where c_0 is a typical speed of propagation of the acoustic wave. We consequently consider the initial pulse to be of the form

$$\mathbf{u}(0, x) = \mathbf{S}(\frac{x - x_0}{\varepsilon})$$

in non-dimensionalized variables $x' = x/L$ and $t' = t/(L/c_0)$. We drop primes to simplify notation. Here x_0 is the location of the source. The transducers obviously have to be capable of capturing signals of frequency ε^{-1} and blurring should happen on the scale of the source, so we replace $f(x)$ by $\varepsilon^{-d}f(\varepsilon^{-1}x)$. Finally, we are interested in the refocusing properties of $\mathbf{u}^B(x)$ in the vicinity of x_0. We therefore introduce the scaling $x = x_0 + \varepsilon\xi$. With these changes of variables, expression (5.14) is recast as

$$\begin{aligned}\mathbf{u}^B(\xi; x_0) &= \Gamma\mathbf{u}(2T, x_0 + \varepsilon\xi) \\ &= \int_{\mathbb{R}^9} \Gamma G(T, x_0 + \varepsilon\xi; y)\Gamma G(T, y'; x_0 + \varepsilon z)\chi(y, y')\mathbf{S}(z)dydy'dz,\end{aligned} \tag{5.15}$$

where

$$\chi(y, y') = \chi(y)\chi(y')f(\frac{y - y'}{\varepsilon}). \tag{5.16}$$

In the sequel we will also allow the medium to vary on a scale comparable to the source scale ε. Thus the Green's function G and the matrix A depend on ε. We do not make this dependence explicit to simplify notation. We are interested in the limit of $\mathbf{u}^B(\xi; x_0)$ as $\varepsilon \to 0$.

5.3.3 Adjoint Green's Function

The analysis of the re-propagated signal relies on the study of the two point correlation at nearby points of the Green's matrix in (5.15). There are two undesirable features in (5.15). First, the two nearby points $x_0+\varepsilon\xi$ and $x_0+\varepsilon z$ are terminal and initial points in their respective Green's matrices. Second, one would like the matrix Γ between the two Green's matrices to be outside of their product. However, Γ and G do not commute. For these reasons, we introduce the *adjoint* Green's matrix, solution of

$$\begin{aligned}&\frac{\partial G_*(t, x; y)}{\partial t}A(x) + \frac{\partial G_*(t, x; y)}{\partial x^j}D^j = 0 \\ &G_*(0, x; y) = A^{-1}(x)\delta(x - y).\end{aligned} \tag{5.17}$$

We now prove that

$$G_*(t,x;y) = \Gamma G(t,y;x)A^{-1}(x)\Gamma. \tag{5.18}$$

Note that for all initial data $\mathbf{S}(x)$, the solution $\mathbf{u}(t,x)$ of (5.4) satisfies

$$\mathbf{u}(t,x) = \int_{\mathbb{R}^d} G(t-s,x;y)\mathbf{u}(s,y)dy$$

for all $0 \le s \le t \le T$ since the coefficients in (5.4) are time-independent. Differentiating the above with respect to s and using (5.4) yields

$$0 = \int_{\mathbb{R}^d} \Big(-\frac{\partial G(t-s,x;y)}{\partial t}\mathbf{u}(s,y) - G(t-s,x;y)A^{-1}(y)D^j \frac{\partial \mathbf{u}(s,y)}{\partial y^j}\Big) dy$$

Upon integrating by parts and letting $s=0$, we get

$$0 = \int_{\mathbb{R}^d} \Big(-\frac{\partial G(t,x;y)}{\partial t} + \frac{\partial}{\partial y^j}\left[G(t,x;y)A^{-1}(y)D^j\right] \Big)\mathbf{S}(y)dy.$$

Since the above relation holds for all test functions $\mathbf{S}(y)$, we deduce that

$$\frac{\partial G(t,x;y)}{\partial t} - \frac{\partial}{\partial y^j}\left[G(t,x;y)A^{-1}(y)D^j\right] = 0. \tag{5.19}$$

Interchanging x and y in the above equation and multiplying it on the left and the right by Γ, we obtain that

$$\frac{\partial}{\partial t}\left[\Gamma G(t,y;x)A^{-1}(x)\right]A(x)\Gamma - \frac{\partial}{\partial x^j}\left[\Gamma G(t,y;x)A^{-1}(x)\right]D^j\Gamma = 0. \tag{5.20}$$

We remark that

$$\Gamma D^j = -D^j\Gamma \qquad \text{and} \qquad \Gamma A(x) = A(x)\Gamma, \tag{5.21}$$

so that

$$\frac{\partial}{\partial t}\left[\Gamma G(t,y;x)A^{-1}(x)\Gamma\right]A(x) + \frac{\partial}{\partial x^j}\left[\Gamma G(t,y;x)A^{-1}(x)\Gamma\right]D^j = 0$$

with $\Gamma G(0,y;x)A^{-1}(x)\Gamma = A^{-1}(x)\delta(x-y)$. Thus (5.18) follows from the uniqueness of the solution to the above hyperbolic system with given initial conditions. We can now recast (5.15) as

$$\begin{aligned} \mathbf{u}^B(\xi;x_0) \ = \ & \int_{\mathbb{R}^9} \Gamma G(T,x_0+\varepsilon\xi;y)G_*(T,x_0+\varepsilon z;y')\Gamma \\ & \qquad \times\chi(y)\chi(y')f(\frac{y-y'}{\varepsilon})A(x_0+\varepsilon z)\mathbf{S}(z)dydy'dz. \end{aligned} \tag{5.22}$$

One may further simplify (5.22) with the help of the auxiliary matrix-valued functions $Q(t,x;q)$ and $Q_*(t,x,q)$ defined by

$$\begin{aligned} Q(T,x;q) &= \int_{\mathbb{R}^d} G(T,x;y)\chi(y)e^{iq\cdot y/\varepsilon}dy, \\ Q_*(T,x;q) &= \int_{\mathbb{R}^3} G_*(T,x;y)\chi(y)e^{-iq\cdot y/\varepsilon}dy. \end{aligned} \tag{5.23}$$

They solve the hyperbolic systems of equations (5.4) and (5.17) with initial conditions given by $Q(0,x;q) = \chi(x)e^{iq\cdot x/\varepsilon}I$ and $Q_*(0,x;q) = A^{-1}(x)\chi(x)e^{-iq\cdot x/\varepsilon}$, respectively. Thus (5.22) becomes

$$\mathbf{u}^B(\xi;x_0) = \int_{\mathbb{R}^6} \Gamma Q(T,x_0+\varepsilon\xi;q)Q_*(T,x_0+\varepsilon z;q)\Gamma A(x_0+\varepsilon z)\mathbf{S}(z)\hat{f}(q)\frac{dqdz}{(2\pi)^3}, \tag{5.24}$$

where $\hat{f}(q) = \int_{\mathbb{R}^d} e^{-iq\cdot x}f(x)dx$ is the Fourier transform of $f(x)$.

5.3.4 Wigner Transform

The back-propagated signal in (5.24) now has the suitable form to be analyzed in the Wigner transform formalism [96, 101]. We define

$$W_\varepsilon(t,x,k) = \int_{\mathbb{R}^d} \hat{f}(q) U_\varepsilon(t,x,k;q)dq, \tag{5.25}$$

where

$$U_\varepsilon(t,x,k;q) = \int_{\mathbb{R}^d} e^{ik\cdot y} Q(t,x-\frac{\varepsilon y}{2};q) Q_*(t,x+\frac{\varepsilon y}{2};q)\frac{dy}{(2\pi)^3}. \tag{5.26}$$

Taking the inverse Fourier transform we verify that

$$Q(t,x;q)Q_*(t,y;q) = \int_{\mathbb{R}^3} e^{-ik\cdot(y-x)/\varepsilon} U_\varepsilon(t,\frac{x+y}{2},k;q)dk,$$

hence

$$\mathbf{u}^B(\xi;x_0) = \int_{\mathbb{R}^6} e^{ik\cdot(\xi-z)} \Gamma W_\varepsilon(T,x_0+\varepsilon\frac{z+\xi}{2},k)\Gamma A(x_0+\varepsilon z)\mathbf{S}(z)\frac{dzdk}{(2\pi)^3}. \tag{5.27}$$

We have thus reduced the analysis of $\mathbf{u}(\xi;x_0)$ as $\varepsilon \to 0$ to that of the asymptotic properties of the Wigner transform W_ε. The Wigner transform has been used extensively in the study of wave propagation in random media, especially in the derivation of radiative transport equations modeling the propagation of high frequency waves. We refer to [96, 98, 101]. Note that in the usual definition of the Wigner transform, one has the adjoint matrix Q^* in place of Q_* in (5.26). This difference is not essential since Q_* and Q^* satisfy the same evolution equation, though with different initial data.

The main reason for using the Wigner transform in (5.27) is that W_ε has a weak limit W as $\varepsilon \to 0$. Its existence follows from simple a priori bounds for $W_\varepsilon(t,x,k)$. Let us introduce the space $\mathcal{A}$ of matrix-valued functions $\phi(x,k)$ bounded in the norm $\|\cdot\|_{\mathcal{A}}$ defined by

$$\|\phi\|_{\mathcal{A}} = \int_{\mathbb{R}^3} \sup_x \|\tilde{\phi}(x,y)\|dy, \qquad \text{where} \quad \tilde{\phi}(x,y) = \int_{\mathbb{R}^3} e^{-ik\cdot y}\phi(x,k)dk.$$

We denote by $\mathcal{A}'$ its dual space, which is a space of distributions large enough to contain matrix-valued bounded measures, for instance. We then have the following result:

Lemma 5.3.1 *Let $\chi(x) \in L^2(\mathbb{R}^3)$ and $\hat{f}(q) \in L^1(\mathbb{R}^3)$. Then there is a constant $C > 0$ independent of $\varepsilon > 0$ and $t \in [0,\infty)$ such that for all $t \in [0,\infty)$, we have $\|W_\varepsilon(t,x,k)\|_{\mathcal{A}'} < C$.*

The proof of this lemma is essentially contained in [96, 98], see also [4]. One may actually get L^2-bounds for W_ε in our setting because of the regularizing effect of $\hat{f}$ in (5.25) but this is not essential for the purposes of this chapter as we are working on a formal level. However, this setting is one example when the mixture of states arises naturally. This is also crucial for trhe rigorous justification of the analog of the results of this chapter in the geometic optics regime in [6].

We therefore obtain the existence of a subsequence $\varepsilon_k \to 0$ such that W_{ε_k} converges weakly to a distribution $W \in \mathcal{A}'$. Moreover, an easy calculation shows that at time $t = 0$, we have

$$W(0,x_0,k) = |\chi(x_0)|^2 A_0^{-1}(x_0)\hat{f}(k). \tag{5.28}$$

Here, $A_0 = A$ when A is independent of ε, and $A_0 = \lim\limits_{\varepsilon\to 0} A_\varepsilon$ if we assume that the family of matrices $A_\varepsilon(x)$ is uniformly bounded and continuous with the limit A_0 in $\mathcal{C}(\mathbb{R}^d)$. These assumptions on A_ε are sufficient to deal with the radiative transport regime we will consider in section 5.3.7. Under the same assumptions on A_ε, we have the following result.

Proposition 5.3.2 *The back-propagated signal* $\mathbf{u}^B(\xi;x_0)$ *given by (5.27) converges weakly in* $\mathcal{S}'(\mathbb{R}^3\times\mathbb{R}^3)$ *as* $\varepsilon\to 0$ *to the limit*

$$\mathbf{u}^B(\xi;x_0)=\int_{\mathbb{R}^6}e^{ik\cdot(\xi-z)}\Gamma W(T,x_0,k)\Gamma A_0(x_0)\mathbf{S}(z)\frac{dzdk}{(2\pi)^3}. \tag{5.29}$$

The proof of this proposition is based on taking the duality product of $\mathbf{u}^B(\xi;x_0)$ with a vector-valued test function $\boldsymbol{\phi}(\xi;x_0)$ in $\mathcal{S}(\mathbb{R}^3\times\mathbb{R}^3)$. After a change of variables we obtain $\langle\mathbf{u}^B,\boldsymbol{\phi}\rangle=\langle W_\varepsilon,Z_\varepsilon\rangle$. Here the duality product for matrices is given by the trace $\langle A,B\rangle=\sum_{i,k}\langle A_{ik},B_{ik}\rangle$, and

$$Z_\varepsilon(x_0,k)=\int_{\mathbb{R}^6}e^{ik\cdot(z-\xi)}\Gamma\boldsymbol{\phi}(\xi,x_0-\varepsilon\frac{z+\xi}{2})\mathbf{S}^*(z)A_\varepsilon(x_0+\varepsilon\frac{z-\xi}{2})\Gamma\frac{dzd\xi}{(2\pi)^3}. \tag{5.30}$$

Defining Z as the limit of Z_ε as $\varepsilon\to 0$ by replacing formally ε by 0 in the above expression, (5.29) follows from showing that $\|Z_\varepsilon-Z\|_{\mathcal{A}}\to 0$ as $\varepsilon\to 0$. This is straightforward and we omit the details.

The above proposition tells us how to reconstruct the back-propagated solution in the high frequency limit from the limit Wigner matrix W. Notice that we have made almost no assumptions on the medium described by the matrix $A_\varepsilon(x)$. At this level, the medium can be either homogeneous or heterogeneous, and the particular scale of oscillations is not important as long as $A_\varepsilon(x)$ strongly converge to A_0. Without any further assumptions, we can also obtain some information about the matrix W. Let us define the dispersion matrix for the system (5.4) as [101]

$$L(x,k)=A_0^{-1}(x)k_jD^j. \tag{5.31}$$

It is given explicitly by

$$L(x,k)=\begin{pmatrix}0&0&0&k_1/\rho(x)\\0&0&0&k_2/\rho(x)\\0&0&0&k_3/\rho(x)\\k_1/\kappa(x)&k_2/\kappa(x)&k_3/\kappa(x)&0\end{pmatrix}.$$

The matrix L has a double eigenvalue $\omega_0=0$ and two simple eigenvalues $\omega_\pm(x,k)=\pm c(x)|k|$, where $c(x)=1/\sqrt{\rho(x)\kappa(x)}$ is the speed of sound. The eigenvalues $\omega_\pm$ are associated with eigenvectors $\mathbf{b}_\pm(x,k)$ and the eigenvalue $\omega_0=0$ is associated with the eigenvectors $\mathbf{b}_j(x,k)$, $j=1,2$. They are given by

$$\mathbf{b}_\pm(x,k)=\begin{pmatrix}\pm\dfrac{\hat{k}}{\sqrt{2\rho(x)}}\\ \dfrac{1}{\sqrt{2\kappa(x)}}\end{pmatrix},\qquad \mathbf{b}_j(x,k)=\begin{pmatrix}\dfrac{\mathbf{z}^j(k)}{\sqrt{\rho(x)}}\\ 0\end{pmatrix}, \tag{5.32}$$

where $\hat{k}=k/|k|$ and $z^1(k)$ and $z^2(k)$ are chosen so that the triple $(\hat{k},z^1(k),z^2(k))$ forms an orthonormal basis. The eigenvectors are normalized so that

$$(A_0(x)\mathbf{b}_j(x,k)\cdot\mathbf{b}_k(x,k))=\delta_{jk}, \tag{5.33}$$

for all $j,k\in J=\{+,-,1,2\}$. The space of 4×4 matrices is clearly spanned by the basis $\mathbf{b}_j\otimes\mathbf{b}_k$. We then have the following result:

Proposition 5.3.3 *There exist scalar distributions $a_\pm$ and a_0^{mn}, $m,n=1,2$ so that the limit Wigner distribution matrix can be decomposed as*

$$W(t,x,k) = \sum_{j,m=1}^{2} a_0^{jm}(t,x,k)\mathbf{b}_j(x,k)\otimes\mathbf{b}_m(x,k) \qquad (5.34)$$
$$+\, a_+(t,x,k)\mathbf{b}_+(x,k)\otimes\mathbf{b}_+(x,k) + a_-(t,x,k)\mathbf{b}_-(x,k)\otimes\mathbf{b}_-(x,k).$$

The main result of this proposition is that the cross terms $\mathbf{b}_j\otimes\mathbf{b}_k$ with $\omega_j\neq\omega_k$ do not contribute to the limit W. The proof of this proposition can be found in [96] and a formal derivation in [101].

The initial conditions for the amplitudes a_j are calculated using the identity

$$A_0^{-1}(x) = \sum_{j\in J}\mathbf{b}_j(x,k)\otimes\mathbf{b}_j(x,k).$$

Then (5.28) implies that $a_0^{12}(0,x,k)=a_0^{21}(0,x,k)=0$ and

$$a_0^{jj}(0,x,k) = a_\pm(0,x,k) = |\chi(x)|^2 f(k), \quad j=1,2. \qquad (5.35)$$

5.3.5 Mode Decomposition and Refocusing

We can use the above result to recast (5.29) as

$$\mathbf{u}^B(\xi;x_0) = (F(T,\cdot;x_0)*\mathbf{S})(\xi), \qquad (5.36)$$

where

$$F(T,\xi;x_0) = \sum_{m,n=1}^{2}\int_{\mathbb{R}^3} e^{ik\cdot\xi} a_0^{mn}(T,x_0;k)\Gamma\mathbf{b}_m(x_0,k)\otimes\mathbf{b}_n(x_0,k)A_0(x_0)\Gamma\frac{dk}{(2\pi)^3}$$
$$+\int_{\mathbb{R}^3} e^{ik\cdot\xi} a_+(T,x_0;k)\Gamma\mathbf{b}_+(x_0,k)\otimes\mathbf{b}_+(x_0,k)A_0(x_0)\Gamma\frac{dk}{(2\pi)^3} \qquad (5.37)$$
$$+\int_{\mathbb{R}^3} e^{ik\cdot\xi} a_-(T,x_0;k)\Gamma\mathbf{b}_-(x_0,k)\otimes\mathbf{b}_-(x_0,k)A_0(x_0)\Gamma\frac{dk}{(2\pi)^3}.$$

This expression can be used to assess the quality of the refocusing. When $F(T,\xi;x_0)$ has a narrow support in ξ, refocusing is good. When its support in ξ grows larger, its quality degrades. The spatial decay of the kernel $F(t,\xi;x_0)$ in ξ is directly related to the smoothness in k of its Fourier transform in ξ:

$$\hat F(T,k;x_0) = \sum_{m,n=1}^{2} a_0^{mn}(T,x_0;k)\Gamma\mathbf{b}_m(x_0,k)\otimes\mathbf{b}_n(x_0,k)A_0(x_0)\Gamma\frac{dk}{(2\pi)^3}$$
$$+\Gamma\left[a_+(T,x_0;k)\mathbf{b}_+(x_0,k)\otimes\mathbf{b}_+(x_0,k)+a_-(T,x_0;k)\mathbf{b}_-(x_0,k)\otimes\mathbf{b}_-(x_0,k)\right]A_0(x_0)\Gamma.$$

Namely, for F to decay in ξ, one needs $\hat F(k)$ to be smooth in k. However, the eigenvectors b_j are singular at $k=0$ as can be seen from the explicit expressions (5.32). Therefore, a priori $\hat F$ is not smooth at $k=0$. This means that in order to obtain good refocusing one needs the original signal to have no low frequencies: $\hat S(k)=0$ near $k=0$. Low frequencies in the initial data will not refocus well.

We can further simplify (5.36)-(5.37) is we assume that the initial condition is irrotational. Taking Fourier transform of both sides in (5.36), we obtain that

$$\hat{\mathbf{u}}^B(k;x_0) = \sum_{j,n\in J} a_j(T,x_0,k)\hat S_n(k)(A_0(x_0)\Gamma b_n(x_0,k)\cdot b_j(x_0,k))\Gamma b_j(x_0,k) \qquad (5.38)$$

where we have defined

$$\hat{\mathbf{S}}(k) = \sum_{n \in J} \hat{S}_n(k) \mathbf{b}_n(x_0, k). \tag{5.39}$$

Irrotationality of the initial condition means that $\hat{S}_1$ and $\hat{S}_2$ identically vanish, or equivalently that

$$\mathbf{S}(x) = \begin{pmatrix} \nabla \phi(x) \\ p(x) \end{pmatrix} \tag{5.40}$$

for some pressure $p(x)$ and potential $\phi(x)$. Remarking that $\Gamma \mathbf{b}_\pm = -\mathbf{b}_\mp$ and by irrotationality that $(A_0(x_0)\hat{\mathbf{S}}(k) \cdot \mathbf{b}_{1,2}(k)) = 0$, we use (5.33) to recast (5.38) as

$$\hat{\mathbf{u}}^B(k; x_0) = a_-(T, x_0, k)\hat{S}_+(k)\mathbf{b}_+(x_0, k) + a_+(T, x_0, k)\hat{S}_-(k)\mathbf{b}_-(x_0, k). \tag{5.41}$$

Decomposing the initial condition $\mathbf{S}(x)$ as

$$\mathbf{S}(x) = \mathbf{S}_+(x) + \mathbf{S}_-(x), \qquad \text{such that} \quad \hat{\mathbf{S}}_\pm(k) = \hat{S}_\pm(k)\mathbf{b}_\pm(x_0, k),$$

the back-propagated signal takes the form

$$\mathbf{u}^B(\xi; x_0) = (\hat{a}_-(T, x_0, \cdot) * \mathbf{S}_+(\cdot))(\xi) + (\hat{a}_+(T, x_0, \cdot) * \mathbf{S}_-(\cdot))(\xi) \tag{5.42}$$

where $\hat{a}_\pm$ is the Fourier of $a_\pm$ in k. This form is much more tractable than (5.36)-(5.37). It is also almost as general. Indeed, rotational modes do not propagate in the high frequency regime. Therefore, they are exactly back-propagated when $\chi(x_0) = 1$ and $f(x) = \delta(x)$, and not back-propagated at all when $\chi(x_0) = 0$. All the refocusing properties are thus captured by the amplitudes $a_\pm(T, x_0, k)$. Their evolution equation characterizes how waves propagate in the medium and their initial conditions characterize the recording array.

5.3.6 Homogeneous Media

In homogeneous media with $c(x) = c_0$ the amplitudes $a_\pm(T, x, k)$ satisfy the free transport equation [96, 101]

$$\frac{\partial a_\pm}{\partial t} \pm c_0 \hat{k} \cdot \nabla_x a_\pm = 0 \tag{5.43}$$

with initial data $a_\pm(0, x, k) = |\chi(x)|^2 f(k)$ as in (5.35). They are therefore given by

$$a_\pm(t, x_0, k) = |\chi(x_0 \mp c_0 \hat{k} t)|^2 \hat{f}(k). \tag{5.44}$$

These amplitudes become more and more singular in k as time grows since their gradient in k grows linearly with time. The corresponding kernel $F = F_H$ decays therefore more slowly in ξ as time grows. This implies that the quality of the refocusing degrades with time. For sufficiently large times, all the energy has left the domain Ω (assumed to be bounded), and the coefficients $a_\pm(t, x_0, k)$ vanish. Therefore the back-propagated signal $\mathbf{u}^B(\xi; x_0)$ also vanishes, which means that there is no refocusing at all. The same conclusions could also be drawn by analyzing (5.14) directly in a homogeneous medium. This is the situation in the numerical experiment presented in Fig. 5.3: in a homogeneous medium, the back-propagated signal would vanish.

5.3.7 Heterogeneous Media and Radiative Transport Regime

The results of the preceding sections show how the back-propagated signal $\mathbf{u}^B(\xi; x_0)$ is related to the propagating modes $a_\pm(T, x_0, k)$ of the Wigner matrix $W(T, x_0, k)$. The form assumed by the modes $a_\pm(T, x_0, k)$, and in particular their smoothness in k, will depend on the hypotheses we make on the underlying medium; i.e., on the density $\rho(x)$ and compressibility $\kappa(x)$ that appear in the matrix $A(x)$. We have seen that partial measurements in homogeneous media yield poor refocusing properties. We now show that refocusing is much better in random media.

We consider here the radiative transport regime, also known as weak coupling limit. There, the fluctuations in the physical parameters are weak and vary on a scale comparable to the scale of the initial condition. Density and compressibility assume the form

$$\rho(x) = \rho_0 + \sqrt{\varepsilon}\rho_1(\frac{x}{\varepsilon}) \qquad \text{and} \qquad \kappa(x) = \kappa_0 + \sqrt{\varepsilon}\kappa_1(\frac{x}{\varepsilon}). \tag{5.45}$$

The functions ρ_1 and κ_1 are assumed to be mean-zero spatially homogeneous processes. The average (with respect to realizations of the medium) of the propagating amplitudes $a_\pm$, denoted by $\bar{a}_\pm$, satisfy in the high frequency limit $\varepsilon \to 0$ a radiative transfer equation (RTE), which is a linear Boltzmann equation of the form

$$\begin{aligned} &\frac{\partial \bar{a}_\pm}{\partial t} \pm c_0 \hat{k} \cdot \nabla_x \bar{a}_\pm = \int_{\mathbb{R}^3} \sigma(k,p)(\bar{a}_\pm(t,x,p) - \bar{a}_\pm(t,x,k))\delta(c_0(|k|-|p|))dp \\ &\bar{a}_\pm(0,x,k) = |\chi(x)|^2 \hat{f}(k). \end{aligned} \tag{5.46}$$

The scattering coefficient $\sigma(k,p)$ depends on the power spectra of ρ_1 and κ_1. We refer to [101] for the details of the derivation and explicit form of $\sigma(k,p)$. The above result remains formal for the wave equation and requires averaging over the realizations of the random medium although this is not necessary in the physical and numerical time reversal experiments. A rigorous derivation of the linear Boltzmann equation (which also requires averaging over realizations) has only been obtained for the Schrödinger equation; see [23, 102]. Nevertheless, the above result formally characterizes the filter $F(T, \xi; x_0)$ introduced in (5.37) and (5.42).

The transport equation (5.46) has a smoothing effect best seen in its integral formulation. Let us define the total scattering coefficient $\Sigma(k) = \int_{\mathbb{R}^3} \sigma(k,p)\delta(c_0(|k|-|p|))dp$. Then the transport equation (5.46) may be rewritten as

$$\begin{aligned} &\bar{a}_\pm(t,x,k) = \bar{a}_\pm(0, x \mp c_0\hat{k}t, k)e^{-\Sigma(k)t} \\ &+ \frac{|k|^2}{c_0} \int_0^t ds \int_{S^2} \sigma(k, |k|\hat{\mathbf{p}})\bar{a}_\pm(s, x \mp c_0(t-s)\hat{k}, |k|\hat{\mathbf{p}})e^{-\Sigma(k)(t-s)} d\Omega(\hat{\mathbf{p}}). \end{aligned} \tag{5.47}$$

Here $\hat{\mathbf{p}} = p/|p|$ is the unit vector in direction of p and $d\Omega(\hat{\mathbf{p}})$ is the surface element on the sphere S^2. The first term in (5.47) is the ballistic part that undergoes no scattering. It has no smoothing effect, and, moreover, if $a(0,x,k)$ is not smooth in x, as may be the case for (5.35), the discontinuities in x translate into discontinuities in k at later times as in (5.44) in a homogeneous medium. However, in contrast to the homogeneous medium case, the ballistic term decays exponentially in time, and does not affect the refocused signal for sufficiently long times $t \gg 1/\Sigma$. The second term in (5.47) exhibits a smoothing effect. Namely the operator $\mathcal{L}g$ defined by

$$\mathcal{L}g(t,x,k) = \frac{|k|^2}{c_0} \int_0^t ds \int_{S^2} \sigma(k,|k|\hat{\mathbf{p}})g(s, x \mp c_0(t-s)\hat{k}, |k|\hat{\mathbf{p}})e^{-\Sigma(k)(t-s)} d\Omega(\hat{\mathbf{p}})$$

is regularizing, in the sense that the function $\tilde{g} = \mathcal{L}g$ has at least 1/2-more derivatives than g (in some Sobolev scale). The precise formulation of this smoothing property is given by the averaging lemmas [34, 51] and will not be dwelt upon here. Iterating (5.47) n times we obtain

$$\bar{a}_{\pm}(t,x,k) = a^0_{\pm}(t,x,k) + a^1_{\pm}(t,x,k) + \cdots + a^n_{\pm}(t,x,k) + \mathcal{L}^{n+1}\bar{a}_{\pm}(t,x,k). \tag{5.48}$$

The terms $a^0_{\pm}, \ldots, a^n_{\pm}$ are given by

$$a^0_{\pm}(t,x,k) = \bar{a}_{\pm}(0, x \mp c_0\hat{k}t, k)e^{-\Sigma(k)t}, \quad a^j_{\pm}(t,x,k) = \mathcal{L}a^{j-1}_{\pm}(t,x,k).$$

They describe, respectively, the contributions from waves that do not scatter, scatter once, twice, ... It is straightforward to verify that all these terms decay exponentially in time and are negligible for times $t \gg 1/\Sigma$. The last term in (5.48) has at least $n/2$ more derivatives than the initial data a_0, or the solution (5.44) of the homogeneous transport equation. This leads to a faster decay in ξ of the Fourier transforms $\hat{a}_{\pm}(T,x_0,\xi)$ of $a_{\pm}(T,x_0,k)$ in k. This gives a qualitative explanation as to why refocusing is better in heterogeneous media than in homogeneous media. A more quantitative answer requires to solve the transport equation (5.46).

5.3.8 Diffusion Regime

It is known for times t much longer than the scattering mean free time $\tau_{sc} = 1/\Sigma$ and distances of propagation L very large compared to $l_{sc} = c_0\tau_{sc}$ that solutions to the radiative transport equation (5.46) can be approximated by solutions to a diffusion equation, provided that $c(x) = c_0$ is independent of x [19, 48]. More precisely, we let $\delta = l_{sc}/L \ll 1$ be a small parameter and rescale time and space variables as $t \to t/\delta^2$ and $x \to x/\delta$. In this limit, the wave direction is completely randomized so that

$$\bar{a}_+(t,x,k) \approx \bar{a}_-(t,x,k) \approx a(t,x,|k|),$$

where a solves

$$\begin{aligned} &\frac{\partial a(t,x,|k|)}{\partial t} - D(|k|)\Delta_x a(t,x,|k|) = 0, \\ &a(0,x,|k|) = |\chi(x)|^2 \frac{1}{4\pi|k|^2}\int_{\mathbb{R}^3} \hat{f}(q)\delta(|q|-|k|)dq. \end{aligned} \tag{5.49}$$

The diffusion coefficient $D(|k|)$ may be expressed explicitly in terms of the scattering coefficient $\sigma(k,p)$ and hence related to the power spectra of ρ_1 and κ_1. We refer to [101] for the details. For instance, let us assume for simplicity that the density is not fluctuating, $\rho_1 \equiv 0$, and that the compressibility fluctuations are delta-correlated, so that $\mathbb{E}\{\hat{\kappa}_1(p)\hat{\kappa}_1(q)\} = \kappa_0^2\hat{R}_0\delta(p+q)$. Then we have

$$\sigma(k,p) = \frac{\pi c_0^2|k|^2\hat{R}_0}{2}, \qquad \Sigma(|k|) = 2\pi^2 c_0|k|^4\hat{R}_0 \tag{5.50}$$

and

$$D(|k|) = \frac{c_0^2}{3\Sigma(|k|)} = \frac{c_0}{6\pi^2|k|^4\hat{R}_0} \tag{5.51}$$

Let us assume that there are no initial rotational modes, so that the source $\mathbf{S}(x)$ is decomposed as in (5.40). Using (5.41), we obtain that

$$\hat{\mathbf{u}}^B(k;x_0) = a(T,x_0,|k|)\hat{\mathbf{S}}(k). \tag{5.52}$$

When $f(x)$ is isotropic so that $\hat{f}(k) = \hat{f}(|k|)$, and the diffusion coefficient is given by (5.51), the solution of (5.49) takes the form

$$a(T, x_0, |k|) = \hat{f}(|k|)\Big(\frac{3\pi|k|^4\hat{R}_0}{2c_0T}\Big)^{3/2}\int_{\mathbb{R}^3} \exp\Big(-\frac{3\pi^2|k|^4\hat{R}_0|x_0 - y|^2}{2c_0T}\Big)|\chi(y)|^2 dy. \qquad (5.53)$$

When $f(x) = \delta(x)$, and $\Omega = \mathbb{R}^3$, so that $\chi(x) \equiv 1$, we retrieve $a(T, x_0, k) \equiv 1$, hence the refocusing is perfect. When only partial measurement is available, the above formula indicates how the frequencies of the initial pulse are filtered by the one-step time reversal process. Notice that both the low and high frequencies are damped. The reason is that low frequencies scatter little from the underlying medium so that it takes a long time for them to be randomized. High frequencies strongly scatter with the underlying medium and consequently propagate little so that the signal that reaches the recording array Ω is small unless recorders are also located at the source point: $x_0 \in \Omega$. In the latter case they are very well measured and back-propagated although this situation is not the most interesting physically. Expression (5.53) may be generalized to other power spectra of medium fluctuations in a straightforward manner using the formula for the diffusion coefficient in [101].

5.3.9 Numerical Results

The numerical results in Fig. 5.3 show that some signal refocuses at the location of the initial source after the time reversal procedure. Based on the above theory however, we do not expect the refocused signal to have exactly the same shape as the original one. Since the location of the initial source belongs to the recording array ($\chi(x_0) = 1$) in our simulations, we expect from our theory that high frequencies will refocus well but that low frequencies will not. This

Figure 5.4: Zoom of the initial source and the refocused signal for the numerical experiment of Fig. 5.3.

is confirmed by the numerical results in Fig. 5.4, where a zoom in the vicinity of $x_0 = \mathbf{0}$ of the initial source and refocused signal are represented. Notice that the numerical simulations are presented here only to help in the understanding of the refocusing theory and do not aim at reproducing the theory in a quantitative manner. The random fluctuations are quite strong in our numerical simulations and it is unlikely that the diffusive regime will be valid. The refocused signal on the right figure looks however like a high-pass filter of the signal in the left figure, as expected from theory.

5.4 Refocusing of Classical Waves

The theory presented in section 5.3 provides a quantitative explanation for the results observed in time reversal physical and numerical experiments. However, the time reversal procedure is by no means necessary to obtain refocusing. Time reversal is associated with the specific choice (5.12) for the matrix Γ in the preceding section, which reverses the direction of the acoustic velocity and keeps pressure unchanged. Other choices for Γ are however possible. When nothing is done at time T, i.e., when we choose $\Gamma = I$, no refocusing occurs as one might expect. It turns out that $\Gamma = I$ is more or less the only choice of a matrix that prevents some sort of refocusing. Section 5.4.1 presents the theory of refocusing for acoustic waves, which is corroborated by numerical results presented in Section 5.4.2. Sections 5.4.3 and 5.4.4 generalize the theory to other linear hyperbolic systems.

5.4.1 General Refocusing of Acoustic Waves

In one-step time reversal, the action of the "intelligent" array is captured by the choice of the signal processing matrix Γ in (5.13). Time reversal is characterized by Γ given in (5.12). A passive array is characterized by $\Gamma = I$. This section analyzes the role of other choices for Γ, which we let depend on the receiver location so that each receiver may perform its own kind of signal processing.

The signal after time reversal is still given by (5.13), where $\Gamma(y')$ is now arbitrary. At time $2T$, after back-propagation, we are free to multiply the signal by an arbitrary invertible matrix to analyze the signal. It is convenient to multiply the back-propagated signal by the matrix $\Gamma_0 = \mathrm{Diag}(-1,-1,-1,1)$ as in classical time reversal. The reconstruction formula (5.15) in the localized source limit is then replaced by

$$\mathbf{u}^B(\xi; x_0) = \int_{\mathbb{R}^9} \Gamma_0 G(T, x_0 + \varepsilon\xi; y)\Gamma(y')G(T, y'; x_0 + \varepsilon z)\chi(y, y')\mathbf{S}(z)dydy'dz \tag{5.54}$$

with $\chi(y, y')$ defined by (5.16). To generalize the results of section 5.3, we need to define an appropriate adjoint Green's matrix G_*. As before, this will allow us to remove the matrix Γ between the two Green's matrices in (5.54) and to interchange the order of points in the second Green's matrix. We define the new adjoint Green's function $G_*(t, x; y)$ as the solution to

$$\begin{gathered}\frac{\partial G_*(t, x; y)}{\partial t} A(x) + \frac{\partial G_*(t, x; y)}{\partial x^j} D^j = 0 \\ G_*(0, x; y) = \Gamma(x)\Gamma_0 A^{-1}(x)\delta(x - y).\end{gathered} \tag{5.55}$$

Following the steps of section 5.3.3, we show that

$$G_*(t, x, y) = \Gamma(y)G(t, y; x)A^{-1}(x)\Gamma_0. \tag{5.56}$$

The only modification compared to the corresponding derivation of (5.18) is to multiply (5.19) on the left by $\Gamma(x)$ and on the right by Γ_0 so that $\Gamma(y)$ appears on the left in (5.20). The re-transmitted signal may now be recast as

$$\mathbf{u}^B(\xi; x_0) = \int_{\mathbb{R}^9} \Gamma_0 G(T, x_0 + \varepsilon\xi; y)G_*(T, x_0 + \varepsilon z; y')\Gamma_0^{-1} A(x_0 + \varepsilon z)\chi(y, y')\mathbf{S}(z)dydy'dz. \tag{5.57}$$

Therefore the only modification in the expression for the re-transmitted signal compared to the time reversed signal (5.22) is in the initial data for (5.55), which is the only place where the matrix $\Gamma(x)$ appears.

The analysis in Sections 5.3.3-5.3.7 requires only minor changes, which we now outline. The back-propagated signal may still be expressed in term of the Wigner distribution (compare to (5.27))

$$\mathbf{u}^B(\xi; x_0) = \int_{\mathbb{R}^6} e^{ik\cdot(\xi - z)}\Gamma_0 W_\varepsilon(T, x_0 + \varepsilon\frac{z + \xi}{2}, k)\Gamma_0 A(x_0 + \varepsilon z)\mathbf{S}(z)\frac{dzdk}{(2\pi)^3}. \tag{5.58}$$

The Wigner distribution is defined as before by (5.25) and (5.26). The function Q is defined as before as the solution of (5.4) with initial data $Q(0, x; q) = \chi(x)e^{iq\cdot x/\varepsilon}I$, while Q_* solves (5.17) with the initial data $Q_*(0, x; q) = \Gamma(x)\Gamma_0 A^{-1}(x)\chi(x)e^{-iq\cdot x/\varepsilon}$. The initial Wigner distribution is now given by

$$W(0, x, k) = |\chi(x)|^2\Gamma(x)\Gamma_0 A^{-1}(x)\hat{f}(k). \tag{5.59}$$

Lemma 5.3.1 and Proposition 5.3.2 also hold, and we obtain the analog of (5.29)

$$\mathbf{u}(\xi; x_0) = \int_{\mathbb{R}^6} e^{ik\cdot(\xi - z)} \Gamma_0 W(T, x_0, k) \Gamma_0 A_0(x_0) \mathbf{S}(z) dz dk. \tag{5.60}$$

The limit Wigner distribution $W(T, x_0, k)$ admits the mode decomposition (5.34) as before. If we assume that the source $\mathbf{S}(x)$ has the form (5.40) so that no rotational modes are present initially, we recover the refocusing formula (5.41):

$$\hat{\mathbf{u}}^B(k; x_0) = a_-(T, x_0, k)\hat{S}_+(k)b_+(x_0, k) + a_+(T, x_0, k)\hat{S}_-(k)b_-(x_0, k). \tag{5.61}$$

The initial conditions for the amplitudes $a_\pm$ are replaced by

$$\begin{aligned} a_\pm(0, x, k) &= \mathrm{Tr}\left[A_0(x)W(0, x, k)A_0(x)b_\pm(x_0, k)b_\pm^*(x_0, k)\right] \\ &= |\chi(x)|^2 \hat{f}(k)(A_0(x)\Gamma(x)b_\mp(x, k) \cdot b_\pm(x, k)). \end{aligned} \tag{5.62}$$

Observe that when $\Gamma(x) = \Gamma_0$, we get back the results of Section 5.3.7. When the signal is not changed at the array, so that $\Gamma = I$, the coefficients $a_\pm(0, x, k) \equiv 0$ by orthogonality (5.33) of the eigenvectors $\mathbf{b}_j$. We thus obtain that no refocusing occurs when the "intelligent" array is replaced by a passive array, as expected physically.

Another interesting example is when only pressure p is measured, so that the matrix $\Gamma = \mathrm{Diag}(0, 0, 0, 1)$. Then the initial data is

$$a_\pm(0, x, k) = \frac{1}{2}|\chi(x)|^2 \hat{f}(k),$$

which differs by a factor 1/2 from the full time reversal case (5.35). Therefore the re-transmitted signal $\mathbf{u}^B$ also differs only by a factor 1/2 from the latter case, and the quality of refocusing as well as the shape of the re-propagated signal are exactly the same. The same observation applies to the measurement and reversal of the acoustic velocity only, which corresponds to the matrix $\Gamma = \mathrm{Diag}(-1, -1, -1, 0)$. The factor 1/2 comes from the fact that only the potential energy or the kinetic energy is measured in the first and second cases, respectively. For high frequency acoustic waves, the potential and kinetic energies are equal, hence the factor 1/2. We can also verify that when only the first component of the velocity field is measured so that $\Gamma = \mathrm{Diag}(-1, 0, 0, 0)$, the initial data is

$$a_\pm(0, x, k) = |\chi(x)|^2 \hat{f}(k) \frac{k_1^2}{2|k|^2}. \tag{5.63}$$

As in the time reversal setting of Section 5.3, the quality of the refocusing is related to the smoothness of the amplitudes $a_\pm$ in k. In a homogeneous medium they satisfy the free transport equation (5.43), and are given by

$$a_\pm(t, x, k) = |\chi(x - c_0\hat{k}t)|^2 \hat{f}(k)(A_0(x - c_0\hat{k}t)\Gamma(x - c_0\hat{k}t)b_\mp(x - c_0\hat{k}t, k) \cdot b_\pm(x - c_0\hat{k}t, k)).$$

Once again, we observe that in a uniform medium $a_\pm$ become less regular in k as time grows, thus refocusing is poor.

The considerations of Section 5.3.7 show that in the radiative transport regime the amplitudes $a_\pm$ become smoother in k also with initial data given by (5.62). This leads to a better refocusing as explained in Section 5.3.5. Let us assume that the diffusion regime of Section 5.3.8 is valid and that the kernel f is isotropic $\hat{f}(k) = \hat{f}(|k|)$. This requires in particular that $A_0(x)$ be independent of x. We obtain that $a_\pm(T, x_0, k) = \tilde{a}(T, x_0, |k|)$, thus the refocusing formula (5.61) reduces to

$$\hat{\mathbf{u}}^B(k; x_0) = \tilde{a}(T, x_0, |k|)\hat{\mathbf{S}}(k). \tag{5.64}$$

The difference with the case treated in Section 5.3.8 is that $\tilde{a}(T, x, |k|)$ solves the diffusion equation (5.49) with new initial conditions given by

$$\begin{aligned}\tilde{a}(0, x, |k|) &= \frac{|\chi(x)|^2}{4\pi|k|^2}\int_{\mathbb{R}^3}\hat{f}(|q|)(A_0\Gamma(x)\mathbf{b}_-(q)\cdot\mathbf{b}_+(q))\delta(|q|-|k|)dq \qquad (5.65)\\ &= \frac{|\chi(x)|^2}{4\pi|k|^2}\int_{\mathbb{R}^3}\hat{f}(|q|)(A_0\Gamma(x)\mathbf{b}_+(q)\cdot\mathbf{b}_-(q))\delta(|q|-|k|)dq.\end{aligned}$$

When only the first component of the velocity field is measured, as in (5.63), the initial data for $\tilde{a}$ is

$$\tilde{a}(0, x, |k|) = \frac{1}{6}|\chi(x)|^2\hat{f}(|k|).$$

Therefore even time reversing only one component of the acoustic velocity field produces a re-propagated signal that is equal to the full re-propagated field up to a constant factor.

More generally, we deduce from (5.65) that a detector at x will contribute some refocusing for waves with wavenumber $|k|$ provided that

$$\int_{S^2}\hat{f}(|k|\hat{q})(A_0\Gamma(x)\mathbf{b}_\mp(\hat{q})\cdot\mathbf{b}_\pm(\hat{q}))d\Omega(\hat{q}) \neq 0.$$

When $f(x) = f(|x|)$ is radial, this property becomes independent of the wavenumber $|k|$ and reduces to $\int_{S^2}(A_0\Gamma(x)\mathbf{b}_\mp(\hat{q})\cdot\mathbf{b}_\pm(\hat{q}))d\Omega(\hat{q}) \neq 0$.

5.4.2 Numerical Results

Let us come back to the numerical results presented in Fig. 5.3 and 5.4. We now consider two different processings at the recording array. The first array is passive, corresponding to $\Gamma = I$, and the second array only measures pressure so that $\Gamma = \mathrm{Diag}(0, 0, 0, 1)$. The zoom in the vicinity of $x_0 = \mathbf{0}$ of the "refocused" signals is given in Fig. 5.5. The left figure shows

Figure 5.5: Zoom of the refocused signals for the numerical experiment of Fig. 5.3 with processing $\Gamma = I$ (left), with a maximal amplitude of roughly $4\,10^{-3}$ and $\Gamma = \mathrm{Diag}(0, 0, 0, 1)$ (right), with a maximal amplitude of roughly 0.035.

no refocusing, in accordance with physical intuition and theory. The right figure shows that refocusing indeed occurs when only pressure in recorded (and its time derivative is set to 0 in the solution of the wave equation presented in the appendix). Notice also that the refocused signal is roughly one half the one obtained in Fig. 5.4 as predicted by theory.

5.4.3 Refocusing of Other Classical Waves

The preceding sections deal with the refocusing of acoustic waves. The theory can however be extended to more complicated linear hyperbolic systems of the form (5.4) with $A(x)$ a positive definite matrix, D^j symmetric matrices, and $\mathbf{u} \in \mathbb{C}^m$. These include electromagnetic and elastic waves. Their explicit representation in the form (5.4) and expressions for the matrices $A(x)$ and D^j in these cases may be found in [101]. For instance, the Maxwell equations

$$\begin{aligned}\frac{\partial E}{\partial t} &= \frac{1}{\epsilon(x)}\,\mathrm{curl}\;H\\ \frac{\partial H}{\partial t} &= -\frac{1}{\mu(x)}\mathrm{curl}\;E\end{aligned}$$

may be written in the form (5.4) with $\mathbf{u} = (E, H) \in \mathbb{C}^6$ and the matrix

$$A(x) = \mathrm{Diag}(\epsilon(x), \epsilon(x), \epsilon(x), \mu(x), \mu(x), \mu(x)).$$

Here $\epsilon(x)$ is the dielectric constant (not to be confused with the small parameter ε), and $\mu(x)$ is the magnetic permeability. The 6×6 dispersion matrix $L(x, k)$ for the Maxwell equations is given by

$$L(x,k) = -\begin{pmatrix} 0 & 0 & 0 & 0 & -k_3/\epsilon(x) & k_2/\epsilon(x) \\ 0 & 0 & 0 & k_3/\epsilon(x) & 0 & -k_1/\epsilon(x) \\ 0 & 0 & 0 & -k_2/\epsilon(x) & k_1/\epsilon(x) & 0 \\ 0 & k_3/\mu(x) & -k_2/\mu(x) & 0 & 0 & 0 \\ -k_3/\mu(x) & 0 & k_1/\mu(x) & 0 & 0 & 0 \\ k_2/\mu(x) & -k_1/\mu(x) & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Generalization of our results for acoustic waves to such general systems is quite straightforward so we concentrate only on the modifications that need be made. The time reversal procedure is exactly the same as before: a signal propagates from a localized source, is recorded, processed as in (5.13) with a general matrix $\Gamma(y')$, and re-emitted into the medium. The re-transmitted signal is given by (5.54). Furthermore, the equation for the adjoint Green's matrix (5.55), the definition of the Wigner transform in Section 5.3.4, and the expression (5.60) for the re-propagated signal still hold.

The analysis of the re-propagated signal is reduced to the study of the Wigner distribution, which is now modified. The mode decomposition must be generalized. We recall that

$$L(x,k) = A_0^{-1}(x) k_j D^j$$

is the $m \times m$ dispersion matrix associated with the hyperbolic system (5.4). Since $L(x, k)$ is symmetric with respect to the inner product $\langle \mathbf{u}, \mathbf{v} \rangle_{A_0} = (A_0 \mathbf{u} \cdot \mathbf{v})$, its eigenvalues are real and its eigenvectors form a basis. We assume the existence of a time reversal matrix Γ_0 such that (5.21) holds with $\Gamma = \Gamma_0$ and such that $\Gamma_0^2 = I$. For example, for electromagnetic waves $\Gamma_0 = \mathrm{Diag}(1, 1, 1, -1, -1, -1)$. Then the spectrum of L is symmetric about zero and the eigenvalues $\pm\omega^\alpha$ have the same multiplicity. We assume in addition that L is isotropic so that its eigenvalues have the form $\omega_\pm^\alpha(x, k) = \pm c^\alpha(x)|k|$, where $c_\alpha(x)$ is the speed of mode α. We denote by r_α their respective multiplicities, assumed to be independent of x and k for $k \neq 0$. The matrix L has a basis of eigenvectors $\mathbf{b}_\pm^{\alpha,j}(x, k)$ such that

$$L(x,k)\mathbf{b}_\pm^{\alpha,j}(x,k) = \pm\omega^\alpha(x,k)\mathbf{b}_\pm^{\alpha,j}(x,k), \quad j = 1, \ldots, r_\alpha,$$

and $b_\pm^{\alpha,j}$ form an orthonormal set with respect to the inner product $\langle , \rangle_{A_0}$. The different ω_α correspond to different types of waves (modes). Various indices $1 \le j \le r_\alpha$ refer to different polarizations of a given mode. The eigenvectors $b_+^{\alpha,j}$ and $b_-^{\alpha,j}$ are related by

$$\Gamma_0 \mathbf{b}_+^{\alpha,j}(x,k) = \mathbf{b}_-^{\alpha,j}(x,k), \quad \Gamma_0 \mathbf{b}_-^{\alpha,j}(x,k) = \mathbf{b}_+^{\alpha,j}(x,k). \tag{5.66}$$

Proposition 5.3.3 is then generalized as follows [96, 101]:

Proposition 5.4.1 *There exist scalar functions $a_\pm^{\alpha,jm}(t, x, k)$ such that*

$$W(t,x,k) = \sum_{\pm,\alpha,j,m} a_\pm^{\alpha,jm}(t,x,k)\mathbf{b}_\pm^{\alpha,j}(x,k) \otimes \mathbf{b}_\pm^{\alpha,m}(x,k). \tag{5.67}$$

Here the sum runs over all possible values of $\pm$, α, and $1 \le j, m \le r_\alpha$.

The main content of this proposition is again that the cross terms $\mathbf{b}_{\pm}^{\alpha,j}(x,k)\otimes\mathbf{b}_{\mp}^{\beta,m}(x,k)$ do not contribute, as well as the terms $\mathbf{b}_{\pm}^{\alpha,j}(x,k)\otimes\mathbf{b}_{\pm}^{\alpha',m}(x,k)$ when $\alpha\neq\alpha'$. This is because modes propagating with different speeds do not interfere constructively in the high frequency limit.

We may now insert expression (5.67) into (5.60) and obtain the following generalization of (5.61)

$$\begin{aligned}\hat{\mathbf{u}}^B(k;x_0) = \sum_{\alpha,j,m}\Big[&a_{-}^{\alpha,mj}(T,x_0,k)\hat{S}_{+}^{\alpha,j}(x_0,k)\mathbf{b}_{+}^{\alpha,m}(x_0,k)\\ &+a_{+}^{\alpha,mj}(T,x_0,k)\hat{S}_{-}^{\alpha,j}(x_0,k)\mathbf{b}_{-}^{\alpha,m}(x_0,k)\Big],\end{aligned}\tag{5.68}$$

where $\hat{S}_{\pm}^{\alpha,j}(k)=(A(x_0)\hat{\mathbf{S}}(k)\cdot\mathbf{b}_{\pm}^{\alpha,j}(x_0,k))$. This formula tells us that only the modes that are present in the initial source ($\hat{S}_{\pm}^{\alpha,j}(k)\neq 0$) will be present in the back-propagated signal but possibly with a different polarization, that is, $j\neq m$.

The initial conditions for the modes $a_{\pm}^{\alpha,jm}$ are given by

$$a_{\pm}^{\alpha,jm}(0,x,k)=|\chi(x)|^2\hat{f}(k)(A(x)\Gamma(x)\mathbf{b}_{\mp}^{\alpha,m}(x,k)\cdot\mathbf{b}_{\pm}^{\alpha,j}(x,k)),\tag{5.69}$$

which generalizes (5.62). When $\Gamma(x)\equiv I$, we again obtain that $a_{\pm}^{\alpha,jm}(0,x,k)\equiv 0$, i.e., there is no refocusing as physically expected. When $\Gamma(x)\equiv\Gamma_0$, we have for all α that

$$a_{\pm}^{\alpha,jm}(0,x,k)=|\chi(x)|^2\hat{f}(k)\delta_{jm}.$$

In a uniform medium the amplitudes $a_{\pm}^{\alpha,jm}$ satisfy an uncoupled system of free transport equations (5.43):

$$\frac{\partial a_{\pm}^{\alpha,jm}}{\partial t}\pm c_\alpha\hat{k}\cdot\nabla_x a_{\pm}^{\alpha,jm}=0,\tag{5.70}$$

which have no smoothing effect, and hence refocusing in a homogeneous medium is still poor. When $f(x)=\delta(x)$ and $\Omega=\mathbb{R}^3$, so that $\chi(x)\equiv 1$, we still have that $a_{\pm}^{\alpha,jm}(T,x_0,k)=\delta_{jm}$ and refocusing is again perfect, that is, $\mathbf{u}^B(\xi;x_0)=\mathbf{S}(\xi)$, as may be seen from (5.68).

5.4.4 The diffusive regime

The radiative transport regime holds when the matrices $A(x)$ have the form

$$A(x)=A_0(x)+\sqrt{\varepsilon}A_1\Big(\frac{x}{\varepsilon}\Big),$$

as in (5.45). Then the $r_\alpha\times r_\alpha$ coherence matrices $w_{\pm}^{\alpha}$ with entries $w_{\pm,jm}^{\alpha}=a_{\pm}^{\alpha,jm}$ satisfy a system of matrix-valued radiative transport equations (see [101] for the details) similar to (5.46). The matrix transport equations simplify considerably in the diffusive regime, such as the one considered in Section 5.3.8 when waves propagate over large distances and long times. We assume for simplicity that $A_0=A_0(x)$ and $\Gamma=\Gamma(x)$ are independent of x. Polarization is lost in this regime, that is, $a^{\alpha,jm}(t,x,k)=0$ for $j\neq m$ and wave energy is equidistributed over all directions. This implies that

$$a_{+}^{\alpha,jj}(t,x,k)=a_{-}^{\alpha,jj}(t,x,k)=a_\alpha(t,x,|k|)$$

so that $a^{\alpha,jj}$ is independent of $j=1,\dots,r_\alpha$ and of the direction $\hat{k}=k/|k|$. Furthermore, because of multiple scattering, a universal equipartition regime takes place so that

$$a_\alpha(t,x_0,|k|)=\phi(t,x_0,c_\alpha|k|),\tag{5.71}$$

where $\phi(t,x,\omega)$ solves a diffusion equation in x like (5.49) (see [101]). The diffusion coefficient $D(\omega)$ may be expressed explicitly in terms of the power spectra of the medium fluctuations [101]. Using (5.69) and (5.71), we obtain when f is isotropic the following initial data for the function ϕ

$$\phi(0,x,\omega) = \frac{1}{4\pi}|\chi(x)|^2 \int_{S^2} \frac{2}{|\alpha|} \sum_{j,\omega_\alpha>0} \hat{f}\Big(\frac{\omega}{c_\alpha}\Big)(A_0\Gamma \mathbf{b}_-^{\alpha,j}(\hat{k}), \mathbf{b}_+^{\alpha,j}(\hat{k}))d\Omega(\hat{k}), \tag{5.72}$$

where $|\alpha|$ is the number of non-vanishing eigenvalues of $L(x,k)$, and $d\Omega(\hat{k})$ is the Lebesgue measure on the unit sphere S^2.

Let us assume that non-propagating modes are absent in the initial source $\mathbf{S}(x)$, that is, $\hat{S}_0^j(k) = 0$ with the subscript zero referring to modes corresponding to $\omega_0 = 0$. Then (5.68) becomes

$$\hat{\mathbf{u}}(k;x_0) = \sum_{\alpha,j} \phi(T,x_0,c_\alpha|k|)\left[\hat{S}_+^{\alpha,j}(k)\mathbf{b}_+^{\alpha,j}(x_0,k) + \hat{S}_-^{\alpha,j}(k)\mathbf{b}_-^{\alpha,j}(x_0,k)\right]. \tag{5.73}$$

This is an explicit expression for the re-propagated signal in the diffusive regime, where ϕ solves the diffusion equation (5.49) with initial conditions (5.72).

5.5 Conclusions

This chapter presents a theory that quantitatively describes the refocusing phenomena in time reversal acoustics as well as for more general processings of acoustic and other classical waves. We show that the back-propagated signal may be expressed as the convolution (5.1) of the original source $\mathbf{S}$ with a filter F. The quality of the refocusing is therefore determined by the spatial decay of the kernel F. For acoustic waves, the explicit expression (5.37) relates F to the Wigner distribution of certain solutions of the wave equation. The decay of F is related to the smoothness in the phase space of the amplitudes $a_j(t,x,k)$ defined in Proposition 5.3.3. The latter satisfy free transport equations in homogeneous media, which sharpens the gradients of a_j and leads to poor refocusing. In contrast, the amplitudes a_j satisfy the radiative transport equation (5.46) in heterogeneous media, which has a smoothing effect. This leads to a rapid spatial decay of the filter F and a better refocusing. For longer times, a_j satisfies a diffusion equation. This allows for an explicit expression (5.52)-(5.53) of the time reversed signal. The same theory holds for more general waves and more general processing procedures at the recording array, which allows us to describe the refocusing of electromagnetic waves when only one component of the electric field is measured, for instance.

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