Recent computational methods for high frequency waves in heterogeneous media

Shi Jin*

ABSTRACT

In this note, we review our recent results on the Eulerian computation of high frequency waves in heterogeneous media. We cover three recent methods: the moment method, the level set method, and the computational methods for interface problems in high frequency waves. These approaches are all based on high frequency asymptotic limits.

§1. Introduction

High frequency wave computation is a classical field of applied mathematics, with many important applications in acoustic waves, elastic waves, optics, and electromagnatism, etc.. The main computational challenge in these problems is that one cannot afford to numerically resolve the small wave length. Approximate models based on asymptotic methods are often used.

One of the most important computational methods for high frequency waves uses geometric optics. A classical way of solving geometric optics

*Department of Mathematics, University of Wisconsin-Madison, Madison, WI 53706, USA. Email address: jinmath.wisc.edu. This work was supported by NSF grant DMS-0608720, and a Van Vleck Distinguished Research Prize from the University of Wisconsin-Madison.

is the Lagrangian framework, which uses *ray tracing* that traces the trajectory of particles. This method is easy to implement, since one just needs to solve a system of ODEs–which is a Hamiltonian system. The disadvantage of it is that the method loses accuracy when the rays diverge, in which case a complicated regridding is needed.

The Eulerian methods, based on solving partial differential equations (PDEs) on *fixed grids*, provide uniformly accurate numerical solutions regardless of the ray behavior, thus have many attractive advantages when compared with the traditional Lagrangian method by ray tracing.

In this note, we will review several of our recently introduced Eulerian computational methods for high frequency waves. Specifically, we will review the moment methods, the level set methods and the computational methods for interface problems in high frequency waves.

For recent comprehensive reviews on high frequency wave computations, see [18, 52].

§2. The high frequency limit

As an example, consider the linear Schrödinger equation with the high frequency initial data,

$$i\epsilon\,\psi_t + \frac{\epsilon^2}{2}\Delta\psi - V(\mathbf{x})\psi = 0, \qquad \mathbf{x} \in \Re^n, \tag{2.1}$$

$$\psi(\mathbf{x}, 0) = A_0(\mathbf{x}) e^{i\frac{S_0(\mathbf{x})}{\epsilon}}. \tag{2.2}$$

In (2.1)(2.2) $\psi(\mathbf{x}, t)$ is the complex-valued wave function, ϵ is the rescaled Planck constant, and $V(\mathbf{x})$ denotes the potential. In the semiclassical regime, where the Planck constant ϵ is small, the wave function ψ and the related physical observables become oscillatory of wave length $O(\epsilon)$. Mathematically, the rapid oscillations will forbid any strong convergence, and the limits have to be defined in the weak sense.

A related problem is the wave equation:

$$u_{tt} - c(\mathbf{x})^2 \Delta u = 0 \tag{2.3}$$

where $c(\mathbf{x})$ is the local wave speed of the medium ($c_0/c(\mathbf{x})$, with c_0 a reference sound speed, is the index of refraction). When the essential frequencies of the wave field are relatively high, the wavelengths are small compared to the overall size of the physical domain.

In a direct numerical simulation of these problems, one needs a few grid points per wavelength in order to guarantee the numerical convergence [4, 45]. For sufficiently high frequencies, such a direct simulation in not feasible, especially in high space dimension, thus methods based on approximations of these equations are needed. Geometrical optics studies the high frequency limit, $\epsilon \to 0$, of solution to (2.3) in the form $u(\mathbf{x}, t) \sim A(\mathbf{x}, t) e^{i\phi(\mathbf{x},t)/\epsilon}$, where A is the amplidude of the wave while S is the phase. The similar limit for (2.1) is referred to as the semiclassical limit of the Schrödinger equation.

A classical approach for an Eulerian computation is the WKB (Wentzel-Kramers-Brillouin) method, which, by assuming the form of solution of (2.1)(2.2) to be $\psi^\epsilon(\mathbf{x}, t) = A(\mathbf{x}, t) e^{iS(\mathbf{x},t)/\epsilon}$, yields, to the leading order, an eikonal equation for the phase S and a linear transport equation for the position density $|A|^2$:

$$\partial_t S + \frac{1}{2}|\nabla S|^2 + V(\mathbf{x}) = 0, \tag{2.4}$$

$$\partial_t(|A|^2) + \nabla \cdot (|A|^2 \nabla S) = 0. \tag{2.5}$$

The eikonal equation is a nonlinear Hamilton-Jacobi equation. Even for smooth initial data, its solution may become singular in finite time, which corresponds to the formation of caustics (in the context of hyperbolic conservation law, which is the gradient of the Hamilton-Jacobi equation (2.4), it corresponds to the formation of shocks). Beyond this singularity, modern 'shock-capturing' numerical methods for the eikonal

equation (2.4) will select the very stable *viscosity solution* [13, 16], which is *not* the *dispersive* semiclassical limit of the Schrödinger equation, since it violates the superposition principle, an essential property of the linear Schrödinger equation. In fact, beyond the caustics, the solution becomes multivalued or multiphased, as can be studied by the classical stationary phase method [15].

A mathematically convenient tool to study the semiclassical limit, beyond the caustics, is the Wigner transform [59]:

$$W[\phi,\psi](\mathbf{x},\mathbf{p},t) = \frac{1}{(2\pi)^n}\int_{\Re^n} e^{i\mathbf{p}\cdot\mathbf{y}}\phi\Big(\mathbf{x}-\frac{\epsilon\mathbf{y}}{2}\Big)\overline{\psi}\Big(\mathbf{x}+\frac{\epsilon\mathbf{y}}{2}\Big)d\mathbf{y}. \qquad (2.6)$$

The moments of the Wigner function W give the physical observables, such as

$$\text{position density} \quad |\psi|^2 = \int W[\psi,\psi]\,d\mathbf{p} \qquad (2.7)$$

$$\text{current} \quad \epsilon\,\mathrm{Im}(\overline{\psi}\nabla\psi) = \int \mathbf{p}W[\psi,\psi]\,d\mathbf{p} \qquad (2.8)$$

$$\text{energy} \quad -\frac{\epsilon^2}{2}\mathrm{Re}(\overline{\psi}\Delta\psi) + \frac{\epsilon^2}{2}|\nabla\psi|^2 = \int |\mathbf{p}|^2 W[\psi,\psi]\,d\mathbf{p}\,, \qquad (2.9)$$

where $\overline{\psi}$ is the complex conjugate of ψ. For ψ^ϵ satisfying (2.1)(2.2), and a *smooth potential* $V(\mathbf{x})$, $W^\epsilon = W[\psi^\epsilon,\psi^\epsilon]$ can be shown to converge weakly towards a measure-valued solution of the Liouville or Vlasov equation in classical mechanics [21, 42]:

$$\partial_t w + \mathbf{p}\cdot\nabla_{\mathbf{x}} w - \nabla V\cdot\nabla_{\mathbf{p}} w = 0\,, \qquad (2.10)$$

$$w(\mathbf{x},\mathbf{p},0) = |A_0(x)|\delta(\mathbf{p}-\nabla S_0(\mathbf{x}))\,. \qquad (2.11)$$

The Liouville equation (2.10) naturally unfolds the caustics, and is the correct semiclassical limit *globally in time*. If one uses the ansatz

$$w(\mathbf{x},\mathbf{p},t) = \rho(\mathbf{x},t)\delta(\mathbf{p}-\mathbf{u}(\mathbf{x},t)) \qquad (2.12)$$

in (2.10) and takes the first two moments, one obtains the *pressureless gas* equations

$$\rho_t + \nabla \cdot \rho \mathbf{u} = 0\,, \tag{2.13}$$

$$\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla V = 0\,, \tag{2.14}$$

which are equivalent to (2.4)(2.5) with $\mathbf{u} = \nabla S$ for smooth solutions. The ansatz (2.12) is no longer good after the formation of caustics. In fact, the correct solution is multivalued, which is a superposition of the (smooth) solution to (2.13)-(2.14), in the physical space (see [26, 53]).

The initial value problem (2.10)-(2.11) is the starting point of the numerical methods to be described below. Most of recent computational methods are derived from, or related to, this equation. The main advantage here is that (2.10)-(2.11) filters out the $O(\epsilon)$ oscillations, thus allows a numerical mesh size *independent of* ϵ. However, there are several major difficulties in its numerical approximation:

- High dimensionality. The Liouville equation is defined in the phase space, thus the memory requirement exceeds the current computational capability.
- Singularity. The initial data (2.11) is a delta function. The solution at later time remains a delta function (for single valued solution) or a sum of delta functions (for multi-valued solutions beyond caustics [26, 53], which is poorly resolved numerically.
- Potential barrier. If $V(\mathbf{x})$ is discontinuous, corresponding to a potential barrier, there are subtle analytical and numerical issues with respect to (2.10) since it is a linear hyperbolic equation with a *measure-valued* coefficient ∇V.

In the past few years, several new numerical methods have been introduced to overcome these difficulties. Below we will review the moment

methods, the level set methods and methods for discontinuous potentials.

§3. *The moment method*

A classical approach in kinetic theory to reduce the dimension of the Boltzmann equation is to use moment closure. This can be done using a local Maxwellian, which yields the compressible Euler equations defined in the physical space, or some other *ad-hoc* density distributions [25, 40, 48] which yield higher order moment equations. For multivalued solution of (2.4)-(2.5) or (2.13)-(2.14), with $N < \infty$ phases, as shown in [26, 53], the semiclassical limit of (2.1)-(2.2), away from the caustics, takes the form

$$w(\mathbf{x}, \mathbf{p}, t) = \sum_{k=1}^{N} \rho_k(\mathbf{x}, t)\delta(\mathbf{p} - \mathbf{u}_k(\mathbf{x}, t)) \,, \tag{3.1}$$

where each $(\rho_k, \mathbf{u}_k)$ satisfies the pressureless gas equations (2.13)-(2.14). Using distribution (3.1) one can close the Liouville equation (2.10) in the *physical* space, resulting a system of $(d+1)N$ weakly hyperbolic equations for a $d-$dimensional problem [26].

For example, in one space dimension, define the moment variables

$$m_l(x, t) = \int p^l w(x, p, t)\, dp \,, \quad l = 0, 1, \cdots, 2N \tag{3.2}$$

Multiplying the Liouville equation (2.10) by p^l (for $l = 0, 1, \cdots, 2N-1$), and integrating over p, one gets the following moment system

$$\partial_t m_0 + \partial_x m_1 = 0 \tag{3.3}$$

$$\partial_t m_1 + \partial_x m_2 = -m_0 \partial_x V \tag{3.4}$$

$$\cdots\cdots\cdots \tag{3.5}$$

$$\partial_t m_{2N-1} + \partial_x m_{2N} = -(2N-1) m_{2N-2} \partial_x V \tag{3.6}$$

With the special distribution function (3.1), one can express the last moment m_{2N} as a function of the first $2N$ moments:

$$m_{2N} = g(m_0, m_1, \cdots, m_{2N-1}) \tag{3.7}$$

Thus the above moment system is closed. Moreover, it was shown in [26] that this $2N \times 2N$-system is *weakly* hyperbolic, in the sense that the Jacobian matrix of the flux is a Jordan Block, with only N-distinct eigenvalues $u_1, u_2, \cdots, u_N$.

By solving the moment system numerically, one produces the multivalued solution to (2.13)-(2.14). In [26] explicit flux function g in (3.7) was given for $N \leq 5$. For larger N a numerical procedure was proposed in [26] for evaluating g.

The moment method for multivalued solution of Burger's equation was first introduced by Brenier and Corrias [6, 7], and used computationally by Engquist and Ronborg [17] and Gosse [22] for multivalued solutions in geometrical optics, which is the high frequency limit of the wave equation (2.3).

Since the moment system is weakly hyperbolic, with phase jumps which are *undercompressive shocks* [23], standard shock capturing schemes such as the Lax-Friedrichs scheme and the Godunov scheme face severe numerical difficulties as in pressureless gas equations [8, 17]. Following our work for pressureless gas system [8], a kinetic scheme derived from the Liouville equation (2.10), with the closure (3.1), was used in [26] for this moment system, which outperforms both the Lax-Friedrichs and Godunov schemes.

The multivalued solution also arises in the high frequency approximation of nonlinear waves, for example, in the modeling of electron transport in vacuum electronic devices [24]. There the underlying equations are the Euler-Poisson equations, which is a coupled nonlinear hyperbolic-eliptic system. A similar moment method was introduced in [41] which

uses the moment closure ansatz (3.7) for the Vlasov-Poisson system. See also [57]. The validity of the semiclassical limit from the Schrödinger-Poisson system to the Vlasov-Poisson system remains a theoretical challenge, although it was studied numerically [29].

The moment systems lead to an Eulerian method defined in the physical space, thus offers greater efficiency compared with the computation in the phase space. However, when the number of phases becomes very large, or in high space dimensions, the moment systems become very complex. It is also hard to estimate, *a priori*, the total number of phases in high space dimension, which is needed to construct the moment equations. Moreover, the caustics for the moment system are *undercompressive shocks* [23], which are difficult to analyze and hard to compute accurately. These provide very interesting yet challenging numerical problems for the future.

§4. *The level set methods*

One of the recently introduced numerical methods for multivalued solution in the high frequency limit is the level set method. This method is rather general, applicable to the computation of multivalued solutions of any (scalar) multi-dimensional quasilinear hyperbolic equations and Hamilton-Jacobi equations.

We now review the level set method, following the derivation of [34]. See also [10]. The original mathematical formulation is classical, see for example [12].

Let $u(\mathbf{x}, t) \in \Re$ be a scalar satisfying an initial value problem of an n-dimensional first order hyperbolic PDE with source term:

$$\partial_t u + \mathbf{F}(u) \cdot \nabla_{\mathbf{X}} u + q(\mathbf{x}, u) = 0\,, \tag{4.1}$$

$$u(\mathbf{x}, 0) = u_0(\mathbf{x})\,. \tag{4.2}$$

Here $\mathbf{F}(u) : \Re \to \Re^n$ is a vector, and $q : \Re^{n+1} \to \Re$, B is the source term. Introduce a level set function $\phi(\mathbf{x}, p, t)$ in $n+1$ dimension, whose zero level set is the solution u:

$$\phi(\mathbf{x}, p, t) = 0 \qquad \text{at} \quad p = u(\mathbf{x}, t)\,. \tag{4.3}$$

Therefore one evolves the entire solution u as the zero level set of ϕ. Simple calculation gives

$$\partial_t \phi + \mathbf{F}(p) \cdot \nabla_{\mathbf{X}} \phi - q(\mathbf{x}, p)\, \partial_p \phi = 0\,. \tag{4.4}$$

This is the level set equation. It resembles a Liouville equation, which is linear hyperbolic with variable coefficients, with the solution governed by the characteristics, even beyond the singularity of u. By solving this linear transport equation, and then finding the zero level set of ϕ, we generate the multivalued solution to u.

For smooth initial data $u_0(x)$, the initial condition for ϕ can be chosen simply as

$$\phi(\mathbf{x}, p, 0) = p - u_0(\mathbf{x})\,. \tag{4.5}$$

However, if the initial data are discontinuous, such as in the Riemann problem, such a choice of the initial level set will miss the line that connects the two constant states, thus forming a vacuum. In this case, a good choice for the initial level set function is the *signed distance function* [54].

Similar idea can also be applied to Hamilton-Jacobi equations. Consider the time dependent, n-dimensional Hamilton-Jacobi equation

$$\partial_t S + H(\mathbf{x}, \nabla_{\mathbf{X}} S) = 0\,, \tag{4.6}$$

$$S(0, \mathbf{x}) = S_0(\mathbf{x})\,. \tag{4.7}$$

Introduce $\mathbf{u} = (u_1, \cdots, u_n) = \nabla_{\mathbf{x}} S$. Taking the gradient on (4.6), one gets an equivalent (at least for smooth solutions) form of the Hamilton-Jacobi equation

$$\partial_t \mathbf{u} + \nabla_{\mathbf{x}} H(\mathbf{x}, \mathbf{u}) = 0\,, \tag{4.8}$$

$$\mathbf{u}(\mathbf{x}, 0) \equiv \mathbf{u}_0(\mathbf{x}) = \nabla_{\mathbf{x}} S_0(\mathbf{x})\,. \tag{4.9}$$

We use n level set functions $\phi_i = \phi_i(\mathbf{x}, \mathbf{p}, t)$, $i = 1, \cdots, d$, where $\mathbf{p} = (p_1, \cdots, p_d) \in \Re^d$, such that the intersection of their zero level sets yields $\mathbf{u}$, namely,

$$\phi_i(\mathbf{x}, \mathbf{p}, t) = 0 \qquad \text{at} \quad \mathbf{p} = \mathbf{u}(\mathbf{x}, t)\,, \qquad i = 1, \cdots, n\,. \tag{4.10}$$

Then ϕ_i solves the following initial value problem of the Liouville equation for Hamiltonian $H(\mathbf{x}, \mathbf{p})$:

$$\partial_t \phi_i + \nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{x}} \phi_i - \nabla_{\mathbf{x}} H \cdot \nabla_{\mathbf{p}} \phi_i = 0\,, \quad i = 1, \cdots, n\,. \tag{4.11}$$

$$\phi_i(\mathbf{x}, \mathbf{p}, 0) = p_i - u_i(\mathbf{x}, 0) \tag{4.12}$$

It is the Liouville equation. When $H = \frac{1}{2}|\mathbf{p}|^2 + V(\mathbf{x})$, it corresponds to the semiclassical limit (2.10) of the linear Schrödinger equation (2.1), while for geometrical optics limit of the wave equation (2.3) $H = c(\mathbf{x})|\mathbf{p}|$. The intersection of the zero level sets of all ϕ_i give the multivalued solution of $\mathbf{u}$.

While the eiconal (Hamilton-Jacobi) equation gives the multivalued velocity $\mathbf{u}$, it is desirable to also compute multivalued density, energy, etc. A simple idea was introduced in [30, 31]. This method is equivalent to a decomposition of the measure-valued initial data (2.11), namely, we solve $\phi(\mathbf{x}, \mathbf{p}, t)$ satisfying the Liouville equation (2.10) with initial data

$$\phi(\mathbf{x}, \mathbf{p}, 0) = \rho_0(\mathbf{x}) \tag{4.13}$$

and $\psi_i(\mathbf{x}, \mathbf{p}, t) \in \Re^n \quad (i = 1, \cdots, n)$ satisfying the same Liouville equation, with initial data (4.12). A simple mathematical argument shows

that the solution to (2.10)-(2.11) is simply

$$w(\mathbf{x},\mathbf{p},t) = \phi(\mathbf{x},\mathbf{p},t)\Pi_{i=1}^{n}\delta(\psi_i(\mathbf{x},\mathbf{p},t))\,, \tag{4.14}$$

while the moments can be recovered through

$$\rho(\mathbf{x},t) = \int \phi(\mathbf{x},\mathbf{p},t)\Pi_{i=1}^{n}\delta(\psi_i(\mathbf{x},\mathbf{p},t))d\mathbf{p}, \tag{4.15}$$

$$\mathbf{u}(\mathbf{x},t) = \frac{1}{\rho(\mathbf{x},t)}\int \mathbf{p}\phi(\mathbf{x},\mathbf{p},t)\Pi_{i=1}^{d}\delta(\psi_i(\mathbf{x},\mathbf{p},t))d\mathbf{p}. \tag{4.16}$$

Thus the only time we have to deal with the delta-function is at the output, while during the evolution we solve ϕ and ψ_i which are l^∞ functions! This avoids the singularity problem mentioned earlier, and gives numerical methods with much better resolution than the one based directly on (2.10)-(2.11) by approximating the initial delta-function numerically and then marching on time. This idea has been successfully applied to the semiclassical limit of Schrödinger equation [30], and to general linear symmetric hyperbolic systems (including the geometrical optics) in [31].

Another advantage of this level set approach is that we only need to care about the zero level sets, thus the technique of local level set methods [1, 11, 50], which restricts the computation to a narrow band around the zero level set, can be used to reduce the computational cost to $O(N \ln N)$ for N computational points in the physical space. This is an nice alternative for dimension reduction of the Liouville equation.

The Liouville-based methods were also proposed earlier but for the computation of only the *wave fronts*, see [19, 20, 49]. Here it was shown that it can actually be used to construct the *entire solution*. When solution with many initial data need to be computed, fast algorithms can be used, see [20, 60].

So far the level set methods have not formulated for nonlinear hyperbolic systems (not the type of (4.8) which is the gradient of the Hamilton-Jacobi equations), except for 1-d Euler-Poisson equations [44] where a

three dimensional Liouville equation has to be used for a 1-d calculation of multivalued solutions.

For a recent review on these level set methods see also [43].

§5. *Computation of high frequency waves through potential barriers or interfaces*

When the medium is heterogeneous, the potential V or the local wave speed c could be *discontinuous*, creating a sharp potential barrier or interface where waves can be partially reflected and partially transmitted as in Snell-Descartes' Law of Refraction. This gives rise to new numerical challenges not faced in the smooth potential case. Clearly, the semiclassical limit (2.10)-(2.11) does not hold at the barrier. Analytical study of the semiclassical limit with interface was carried out in [3, 47]. When V or c is discontinuous, the Liouville equation (4.11) contains characteristics that are discontinuous and even measure-valued. Its bicharacteristics, given by the Hamiltonian system:

$$\partial_t \mathbf{x} = \nabla_{\mathbf{p}} H\,, \tag{5.1}$$

$$\partial_t \mathbf{p} = -\nabla_{\mathbf{x}} H \tag{5.2}$$

is a system of ODEs with the right hand side that are not Lipschitz (for which the classical well-posedness theory was established). It does not even have a bounded variation, for which the renormalized solution was introduced by DiPerna and Lions [14] (see also [2]).

5.1. Notion of the solution

One first needs to introduce a notion of solution to such singular Liouville equation (2.10) and the underlying singular Hamiltonian system (5.1)-(5.2). One can then design robust numerical methods for such

problems that capture such solutions. The solution so constructed will be physically relevant, namely, it should give the correct transmission and reflection of waves through the barrier, obeying Snell's Law of Refraction.

In [37], we provide an interface condition to connect the Liouville equations at both sides of the interface. Let us concentrate in one space dimension. Consider a particle moving with velocity $p > 0$ to the barrier. The interface condition is

$$w(x^+, p^+) = \alpha_T w(x^-, p^-) + \alpha_R w(x^+, -p^+) \tag{5.3}$$

Here the superscripts "$\pm$" represent the right and left limits of the quantities, $\alpha_T \in [0,1]$ and $\alpha_R \in [0,1]$ are the transmission and reflection coefficients respectively, satisfying $\alpha_R + \alpha_T = 1$. $x^+ = x^-$ (for a sharp interface), while p^+ and p^- are connected by the *Hamiltonian preserving* condition:

$$H(x^+, p^+) = H(x^-, p^-) \tag{5.4}$$

We remark that in classical mechanics, the Hamiltonian $H = \frac{1}{2}p^2 + V(x)$ is conserved along the particle trajectory, even across the barrier. In this case, $\alpha_T, \alpha_R = 0$ or 1, namely, a particle can be either transmitted or reflected.

In geometric optics, condition (5.4) is equivalent to Snell's Law of Refraction for a flat interface [36]. The coefficients α_T and α_R are between 0 and 1, namely, waves can be partially transmitted or reflected. They can be determined from the original wave equation (2.3) before the geometric optics limit is taken. Thus (5.3) is a *multiscale* coupling between the (more macroscopic) Liouville equation and the (microscopic) wave equation.

The well-posedness of the initial value problem to the singular Liouville equation with the interface condition (5.3) was established in [37], using the method of characteristics. To determine a solution at (x, p, t)

one traces back along the characteristics determined by the Hamiltonian system (5.1)-(5.2) until hitting the interface. At the interface, the solution bifurcates with the interface condition (5.3), one corresponds to the transmission and the other reflection, and this process continues until one arrives the line of $t = 0$. The interface condition (5.3) thus provides a generalized characteristic method.

We will also introduce a notion of the solution to the Hamiltonian system (5.1)-(5.2), using a *probability* interpretation. Basically, one solves the system using a standard ODE or Hamiltonian solver, but at the interface, we introduce the following *Monte-Carlo* solution (we give the solution in the case of $p^- > 0$; the other case is similar):

- with probability α_R, the particle (wave) is reflected with

$$x \to x, \quad p^- \to -p^- . \tag{5.5}$$

- with probability α_T, the particle (wave) is transmitted, with

$$x \to x, \quad p^+ \text{ is obtained from } p^- \text{ using (5.4)} \tag{5.6}$$

Although the original problem is deterministic, this probability solution allows us to go beyond the interface with the new value of (x, p) defined in (5.5)-(5.6). This is clearly the Lagrangian picture of the Eulerian solution determined by using the interface condition (5.3). This solution also motivates a (Monte-Carlo) particle method for thin quantum barriers, see [33].

5.2. Numerical flux at the interface

While the Liouville equation (4.11) can be solved by a standard finite difference or finite volume shock capturing methods, such schemes face difficulties when the Hamiltonian is discontinuous, since ignoring the discontinuity of the Hamiltonian during the computation will result in

solutions inconsistent with the notion of the (physically relevant) solution defined in the preceding subsection. Even with a smoothed Hamiltonian, it is usually impossible–at least in the case of *partial* transmission and reflection–to obtain transmission and reflection with the correct transmission and reflection coefficients. A smoothed Hamiltonian will also give a severe time step constraint like $\Delta t \sim O(\Delta x \Delta p)$, where $\Delta t, \Delta x$ and δp are time step, mesh sizes in the x- and p-directions respectively. This is a parabolic type CFL condition, despite that we are solving a hyperbolic problem!

Our idea of approximating the Liouville equation (4.11) at the interface in [35, 37] is to *build the interface condition (5.3) into the numerical flux*. This is in the spirit of the Immersed interface method [46, 39]. It was also motived by an idea of Perthame and Simeoni for a well-balanced kinetic scheme for shallow water equations with bottom topography [51]. Our new numerical schemes overcome the aforementioned analytic and numerical difficulties. In particular, they have the following important properties:

- they produce the solution crossing the interface defined by the mathematical solution introduced in the previous subsection, thus obtain physically relevant solution of particle/wave transmission and reflection at the interfaces. In particular, in the case of geometric optics, this solution is consistent to Snell-Descartes' Law of Refraction at the interface. The Snell's Law was built into the numerical flux!
- It allows a *hyperbolic* CFL condition $\Delta t = O(\Delta x, \Delta p)$.

This idea has been applied successfully to compute the semiclassical limit of the linear Schrödinger equation with potential barriers [35] and the geometrical optics with complete transmission/reflection [36] or partial transmission/reflection [37]. Positivity, and both l^1 and l^∞ stabilities

were also established, under the "good" (hyperbolic) CFL condition. For piecewise constant Hamiltonians, an l^1-error estimate of the first order finite difference of the type introduced in [35] was established in [56], following [55].

This is the *first* Eulerian numerical methods for high frequency waves that are able to capture correctly the transmission and reflection of waves through the barriers or interfaces. It has also been extended to high frequency elastic waves [27], and high frequency waves in random media [28] with diffusive interfaces.

5.3 Thin quantum barriers

A correct modeling of electron transport in nanostructures, such as resonant tunneling diodes, superlattices or quantum dots, require the treatment of quantum phenomena in localized regions of the devices, while the rest of the device is governed by classical mechanics. The quantum barrier that separates the quantum and classical regions differ from a classical barrier, in that a quantum wave can transmit through any barrier, a phenomenon known as tunneling. While solving the Schrödinger equation in the entire physical domain is too expensive, it is rather attractive to use a *multiscale* approach, namely, solve the quantum mechanics in the quantum well, and classical mechanics outside the well [5]. It is highly desirable to have a semiclassical computational model for quantum barriers, with a cost slightly higher than a classical approach, but much less than a quantum approach. In [32], we introduced the following semiclassical model:

- solve the time-independent Schrödinger equation–either analytically if possible, or numerically– for the local barrier/well to determine the scattering data (transmission and reflection coefficients)
- solve the classical Liouville equation elsewhere, using the scatter-

ing data at the barrier for the interface condition (5.3) and the numerical method of [35] for a classical barrier.

Our 1d [32] and 2d [33] results indicate the success of this approach when the well is very thin (a few ϵ's) and well-separated. It can correctly capture both transmitted and reflected waves that a classical Liouville equation cannot, and the results agree (in the sense of weak convergence) with the solution obtained by solving directly the Schrödinger equation with small ϵ with a much less cost.

Currently, more study is underway, in particular, for highly resonant wells, time delay, phase information, and higher dimensional problems.

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