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Numerical methods for hyperbolic systems with singular coefficients: well-balanced scheme, Hamiltonian preservation, and beyond

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Abstract. This paper reviews some recent numerical methods for hyperbolic equations with singular (discontinuous or measure-valued) coefficients. Such problems arise in wave propagation through interfaces or barriers, or nonlinear waves through singular geometries. The connection between the well-balanced schemes for shallow-water equations with discontinuous bottom topography and the Hamiltonian preserving schemes for Liouville equations with discontinuous Hamiltonians is illustrated. Various developments of numerical methods with applications in high frequency waves through interfaces, and in multiscale coupling between classical and quantum mechanics, are discussed.

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1. Introduction

In recent years there have been tremendous interests in developing well-balanced schemes for the Saint-Venant shallow-water equations with discontinuous topography. There have also been active research activities in numerical methods for hyperbolic equations with singular coefficients, and for high frequency waves through interfaces or barriers. The goal of this paper to review these recent developments in seemingly different areas of applications via a unified approach. Specifically, this unified point of view is based on the *well-balanced* scheme using the kinetic interpolation of shallow-water equations in the framework of Perthame and Simeoni [**37**] (also in [**4**]), and the *Hamiltonian-preserving* schemes using the interface condition that accounts for transmissions and reflections of waves and particles advocated by Jin and Wen [**18**] for Liouville equation with discontinuous Hamiltonians. This viewpoint allows us to develop new numerical methods for a large class of hyperbolic or kinetic equations with singular (discontinuous or even measure-valued)

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coefficients–either the wave speeds or source terms, and to extend their applications to problems from high frequency waves through interfaces, the computation of diffractions, to the multi-scale coupling of classical and quantum mechanics.

2. Hyperbolic equation with singular coefficients

The simplest such problem is the following hyperbolic equation

$$\begin{cases} \partial_t u + \partial_x \left(c(x)u\right) = 0, & t > 0, x \in \mathbb{R}, \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{2.1}$$

with a piecewise constant coefficient

$$c(x) = \begin{cases} c^- > 0, & x < 0, \\ c^+ > 0, & x > 0. \end{cases} \tag{2.2}$$

Such equations arise in modeling wave propagation through interfaces, where jumps in $c(x)$ correspond to interfaces between different media. This is also the simplest example of hyperbolic conservations laws with discontinuous coefficients, a subject that has generated lots of mathematical interests (see for example [**1, 5, 6, 36**]) where the mathematical framework of renormalized weak solution was used. This is not the approach we will adopt here. Rather, bearing the physical background of such problem in mind, an interface condition is needed at $x = 0$:

$$u(0^+, t) = \rho\, u(0^-, t), \tag{2.3}$$

where $\rho = 1$ corresponds to the conservation of mass u or $\rho = c^-/c^+$ for the conservation of flux cu. This is the approach that will be taken in this paper, as it was in [**40, 31**]. Such a condition will guarantee the well-posedness of the initial value problem to (2.1), see [**20**].

The characteristic of equation (2.1) is given by

$$\frac{\partial x}{\partial t} = c(x)\,, \quad x(0) = x_0 \tag{2.4}$$

Since $c(x)$ is discontinuous at $x = 0$, the classical well-posedness theory for the initial value problem of ODEs cannot be applied. For $x_0 < 0$, solution to (2.4) can be written as

$$x(t) = \begin{cases} x_0 + c_- t & \text{for} \quad t \le t_c = -x_0/c_- \\ x_1 + c_+ t & \text{for} \quad t > t_c \end{cases} \tag{2.5}$$

where x_1 can not be uniquely determined unless one specifies a condition at $x = 0$. One possible condition is that x *is continuous at 0*, then $x_1 = 0$ and one obtains a unique solution. If this is how the solution to (2.5) is defined, and one solves the PDE (2.1) by the method of characteristics, then it corresponds to the interface condition $\rho = 1$, namely, u is continuous at $x = 0$. (This is the duality solution defined in [**8**]). But for $\rho \neq 1$, it is not clear how to correspond the solution of (2.1) with the method of characteristics at $x = 0$.

When numerically solving (2.1)-(2.2), the most natural approach is the *immersed interface method* which builds the interface condition (2.3) into the numerical flux [**40, 31**] (see also [**33, 30, 38**] for immersed boundary or immersed interface methods for general problems, and the Hamiltonian-preserving methods for Liouville equations with discontinuous potentials [**18, 19, 20**]).

Let the spatial mesh be $x_{i+1/2} = (i - 1/2)\Delta x$, where $i \in \mathbb{Z}$, the set of all integers (so the interface is located at $x_{1/2} = 0$) and Δx is the mesh size. Let

$U_i(t) = U(x_i, t)$ be the numerical approximation of $u(x_i, t)$. At each cell-interface $x_{i+1/2}$ the numerical flux is allowd to be discontinuous, and we need to define $U^{\pm}_{i+1/2}$. The immersed upwind scheme proposed in [**40**] for the convection equation (2.1)-(2.2) uses the following discretization:

$$\partial_t U_j + \frac{1}{\Delta x}\left(c^-_{j+1/2}U^-_{j+1/2} - c^+_{j-1/2}U^+_{j-1/2}\right) \tag{2.6}$$

where $c^{\pm}(x_{j+1/2}) = \lim_{x\to x^{\pm}_{j+1/2}} c(x)$ and the numerical flux

$$U^-_{j+1/2} = U_j, \qquad U^+_{j+1/2} = \rho_{j+1/2}\, U^-_{j+1/2} \tag{2.7}$$

with

$$\rho_{j+1/2} = \begin{cases} 1 & \text{if } j \neq 0, \\ \rho, & \text{if } j = 0\,. \end{cases} \tag{S1}$$

Clearly if $\rho = 1$, or if there is no interface, then the above scheme is the standard upwind scheme.

Convergence and l^1 error estimates of this scheme was established in [**40, 17**].

3. Well-balanced schemes for shallow water equations with discontinuous topography

We now discuss a hyperbolic system with a singular source term. Their connection with hyperbolic equations with singular wave speed with be made clear later in this subsection.

Consider the one-dimensional shallow water equations with topography

$$\partial_t h + \partial_x(hv) = 0, \tag{3.1}$$

$$\partial_t(hv) + \partial_x\left(hv^2 + \frac{1}{2}gh^2\right) = -gh\partial_x B\,, \tag{3.2}$$

where h is the height of the water, v is the mean velocity, g is the gravitational constant, and $B(x)$ is the bottom topograph, which is allowed to be *discontinuous*. The steady state solutions satisfy

$$\partial_x(hv) = 0, \tag{3.3}$$

$$\partial_x\left(hv^2 + \frac{1}{2}gh^2\right) = -gh\partial_x B\,. \tag{3.4}$$

This is a system of ODEs that has a *measure-valued* right hand side when $B(x)$ is discontinuous. In order to define a unique solution to this ODE system we need an additional condition at the discontinuity of $B(x)$. For smooth solutions, one can deduce, from (3.3)-(3.4), the following conditions:

$$hv = C_1, \tag{3.5}$$

$$E(h, u, B) = \frac{1}{2}v^2 + gh + gB = C_2. \tag{3.6}$$

Note the first condition (3.5) is the conservation of momentum, which the second condition (3.6) is the conservation of energy E. At the discontinuity of B, these two conditions provide the jump conditions for h and v, which are needed for the ODE system (3.3)-(3.4) to have a unique solution. Such jump conditions are not provided by the equations. Rather, they are supplemented as a physical condition at the jump (interface).

A numerical method for the shallow water equations (3.1), (3.2) is called *well-balanced* [**9**] if it satisfies the steady state conditions (3.5), (3.6) exactly or with at least a second order accuracy even when the bottom function $B(x)$ contains discontinuities. Development of well-balanced schemes has been an active area of research in the last decade, see for example [**9, 8, 37, 3, 29, 10**].

A particularly interesting well-balanced scheme was introduced by Perthame and Simeoni [**37**], in which they give a *kinetic description* of the well-balance condition (3.5)-(3.6). This approach provides the bridge between the well-balanced scheme at the hydrodynamic level (the shallow-water equations) and what will be discussed at the next section. They first pointed out that the shallow water system has a kinetic formulation:

$$\partial_t M + \xi\, \partial_x M - g\, \partial_x B\, \partial_\xi M = Q(t,x,\xi) \tag{3.7}$$

where

$$M(t,x,\xi) = M(h, \xi - u) = \sqrt{h(t,x)}\, \chi\left(\frac{\xi - u(t,x)}{\sqrt{h(t,x)}} \right), \tag{3.8}$$

$$\chi(\omega) = \frac{\sqrt{2}}{\pi\sqrt{g}} \left(1 - \frac{\omega^2}{2g} \right)_+^{1/2}, \tag{3.9}$$

for some collision term $Q(t,x,\xi)$ which satisfies, for almost every (t,x),

$$\int_R Q\, d\xi = 0\,, \qquad \int_R \xi Q\, d\xi = 0\,. \tag{3.10}$$

Furthermore, the χ chosen in (3.9) is the only function such that M defined in (3.8) satisfies the steady state equation

$$\xi\, \partial_x M - g\, \partial_x B\, \partial_\xi M = 0 \tag{3.11}$$

on all steady state given by a *lake at rest*:

$$u(t,x) = 0, \quad h(t,x) + B(x) = H\,, \quad \forall t \geq 0\,. \tag{3.12}$$

Notice that (3.12) requires $u = 0$, thus satisfies the well-balanced condition (3.5)-(3.6) only for zero velocity.

The macroscopic quantities in the shallow water equations can be recovered from the kinetic variable M by taking the first three moments, defined by

$$h = \int_R M(h, \xi - u)\, d\xi\,, \tag{3.13}$$

$$hu = \int_R \xi M(h, \xi - u)\, d\xi\,, \tag{3.14}$$

$$hu^2 + \frac{1}{2} g h^2 = \int_R \xi^2 M(h, \xi - u)\, d\xi\,. \tag{3.15}$$

By multiplying the kinetic equation (3.7) with $(1, \xi)$ one obtains the shallow-water equations (2.1).

To discretize the shallow-water system, a *kinetic scheme with reflections*, a concept first appeared in [**4**], was introduced in [**37**]. Taking a finite volume discretization of the kinetic equation (3.7):

$$\partial_t f_i(\xi) + \frac{1}{\Delta x} \xi \left(M^-_{i+1/2} - M^+_{i-1/2}(\xi) \right) = 0\,, \tag{3.16}$$

The collision term Q is omitted here since we are only interested in the (macroscopic) solution to the shallow-water equations by taking $f = M$ where Q will relax to zero. The peculiar discretization for the fluxes in (3.16) is defined by upwind formulas

$$M^-_{i+1/2}(\xi) = M_i(\xi)\,\mathbf{I}_{\xi\geq 0} + M_{i+1/2}(\xi)\,\mathbf{I}_{\xi\leq 0} \tag{3.17}$$

$$M^+_{i-1/2}(\xi) = M_{i-1/2}(\xi)\,\mathbf{I}_{\xi\geq 0} + M_i(\xi)\,\mathbf{I}_{\xi\leq 0} \tag{3.18}$$

where $\mathbf{I}_A$ is the characteristic function with support at set A, and

$$M_{i+1/2}(\xi) = M_i(-\xi)\,\mathbf{I}_{|\xi|^2\leq 2g\Delta B_{i+1/2}} \tag{3.19}$$

$$+M_{i+1}\left(-\sqrt{|\xi|^2 - 2g\Delta B_{i+1/2}}\right)\,\mathbf{I}_{|\xi|^2\geq 2g\Delta B_{i+1/2}}\,, \tag{3.20}$$

$$M_{i-1/2}(\xi) = M_i(-\xi)\,\mathbf{I}_{|\xi|^2\leq 2g\Delta B_{i+1/2}} \tag{3.21}$$

$$+M_{i-1}\left(-\sqrt{|\xi|^2 - 2g\Delta B_{i-1/2}}\right)\,\mathbf{I}_{|\xi|^2\geq 2g\Delta B_{i-1/2}}\,, \tag{3.22}$$

with $\Delta B_{i+1/2} = B^+_{i+1/2} - B^- i + 1/2$. An important feature of this scheme is that *it builds the microscopic physical of particle collisions with barriers (either transmission and reflection) into the numerical flux.*

The final well-balanced scheme is obtained by taking the moments of this scheme. We omit the details here.

4. High frequency waves through barriers

4.1. The Liouville equation with discontinuous Hamiltonians. We start this section by presenting a general Liouville equation with a Hamiltonian $H(\mathbf{x}, \mathbf{p})$:

$$\partial_t w + \nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{x}} w - \nabla_{\mathbf{x}} H \cdot \nabla_{\mathbf{p}} w = 0\,. \tag{4.1}$$

The Liouville equation arises from the semiclassical limit of the Schrödinger equation, where $H = \frac{1}{2}|\mathbf{p}|^2 + V(\mathbf{x})$, or in geometric optics, with $H = c(\mathbf{x})|\mathbf{p}|$, which is the high frequency limit of the wave equation. It can also arise in the high frequency limit of any linear symmetric hyperbolic systems, including the acoustic wave, elastic wave, and electromagnetic waves, via the so-called Wigner transform, see [**42, 32, 7, 36, 39**].

When the Hamiltonian $H(\mathbf{x}, \mathbf{p})$ has a discontinuity in $\mathbf{x}$ (corresponding to the discontinuities in V or c in the aforementioned applications), the Liouville equation (4.1) contains coefficients that are discontinuous and even measure-valued. Its bicharacteristics, given by the Hamiltonian system:

$$\partial_t \mathbf{x} = \nabla_{\mathbf{p}} H\,, \tag{4.2}$$

$$\partial_t \mathbf{p} = -\nabla_{\mathbf{x}} H\,, \tag{4.3}$$

is a system of ODEs with a measure-valued right hand side that is not Lipschitz (for which the classical well-posedness theory was established), nor has a bounded variation, for which the renormalized solution was introduced by DiPerna and Lions [**6**] (see also [**1**]).

4.2. Notion of the solution. The first interesting mathematical question is about the notion of solution to such singular Liouville equation (4.1) and the underlying singular Hamiltonian system (4.2)-(4.3). It is not clear how a weak solution can be defined. A correct definition of mathematical solutions should be consistent to the physics of waves at the interfaces, namely, it should give the correct

transmission and reflection of waves through the interface, obeying Snell's Law of Refraction. Our idea in [**20**] is to provide an interface condition that connects the Liouville equations at both sides of the interface. To illustrate the basic idea, let us concentrate in one space dimension. Consider a particle or wave moving to the right with velocity $H_p > 0$ to the interface. The interface condition is then

$$w(x^+, p^+) = \alpha_T\, w(x^-, p^-) + \alpha_R\, w(x^+, -p^+)\,. \tag{4.4}$$

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

$$H(x^+, p^+) = H(x^-, p^-)\,. \tag{4.5}$$

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. The well-balanced kinetic scheme introduced by Perthame and Simeoni, as discussed in the previous section, was based on this principle. Thus *the Hamiltonian preservation here is the kinetic interpretation of the well-balancedness (which conserves the energy (3.6) at the macroscopic hydrodynamics level)!* (4.4) was also the condition used in [**2**] to connect two regions of classcial mechanics.

However, waves can be *partially* transmitted or reflected at the interface, in which case α_T and α_R are between 0 and 1. They cannot be determined at the classical (Liouville) level. Rather, they should be determined from the original wave equation before the geometric optics or high frequency limit is taken. In fact, these coefficients, normally refereed to as the scattering coefficients, can be obtained by suitable interface conditions such as the continuity of wave function and/or its flux. Thus (4.4) is a *multi-scale* coupling between the (macroscopic) Liouville equation and the (microscopic) wave (or Schrödinger) equation. Moreover, condition (4.5) is equivalent to Snell's Law of Refraction for a flat interface, as shown in [**19**].

The well-posedness of the initial value problem to the singular Liouville equation with the interface condition (4.4) was established in l^∞ and l^1 spaces in [**20**], using the method of characteristics. With the interface condition (4.4) one can solve the initial value problem using a *generalized* characteristic method, in which a characteristic, when hitting the interface, bifurcates into two branches, one corresponding to the transmission (obeying Snell's Law) and the other reflection (obeying the reflection law).

A notion of the solution to the Hamiltonian system (4.2)-(4.3), using a *probability* interpretation, was introduced in [**11**], which was the basis for a Monte-Carlo particle method in [**15**]. 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:

$$x \to x, \quad p^- \to -p^-\,. \tag{4.6}$$

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

$$x \to x, \quad p^+ \text{ is obtained from } p^- \text{ using (4.5)} \tag{4.7}$$

This probability solution allows us to go beyond the interface with the new values of (x,p) defined in (4.6)-(4.7), giving the new initial data for the waves to continue with the smooth Hamiltonian system until they hit the next interface. This is clearly the Lagrangian picture of the Eulerian solution determined by the Liouville equation (4.1) using the interface condition (4.4).

In multidimensions and with a curved interface condition, the interface condition (4.4) should be imposed along the *normal* direction of the interface, see [**12**].

4.3. Numerical flux at the interface. While the Liouville equation (4.1) can be solved by a standard finite difference or finite volume shock capturing method, 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 the correct amount of transmissions and reflections (see some numerical examples in [**19, 21**]). 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 (4.1) at the interface in [**18, 20**] is to *build the interface condition (4.4) into the numerical flux*. This is in the spirit of the immersed interface method [**33, 30**], and also the approach by Perthame and Simeoni [**37**].

Consider the one space dimension. We employ a uniform mesh with grid points at $x_{i+1/2}$, in the x-direction and $p_{j+1/2}$, in the p-direction. The cells are centered at (x_i, p_j), with $x_i = \frac{1}{2}(x_{i+1/2} + x_{i-1/2})$ and $p_j = \frac{1}{2}(p_{j+1/2} + p_{j-1/2})$. The uniform mesh size is denoted by $\Delta x = x_{i+1/2} - x_{i-1/2}, \Delta p = p_{j+1/2} - p_{j-1/2}$. The cell average of w is defined by

$$W_{ij} = \frac{1}{\Delta x \Delta p} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{p_{j-1/2}}^{p_{j+1/2}} w(x,p,t)\, dpdx.$$

Assume that the discontinuous points of the Hamiltonian H are located at the grid points. Let the left and right limits of $H(x,p)$ at point $x_{i+1/2}$ be $H^+_{i+1/2,j}$ and $H^-_{i+1/2,j}$ respectively. Note that if H is continuous at $x_{j+1/2}$, then $H^+_{i+1/2,j} = H^-_{i+1/2,j}$. We approximate H by a piecewise linear function

$$H(x) \approx H^+_{i-1/2,j} + \frac{H^-_{i+1/2,j} - H^+_{i-1/2,j}}{\Delta x}(x - x_{j-1/2}), \quad \text{for} \quad x \in [x_{j-1/2}, x_{j+1/2}].$$

We also define the averaged wave speed as $H_i = \frac{1}{2}(H^+_{i-1/2} + H^-_{i+1/2})$. The flux splitting technique is used here. The semidiscrete scheme (with time continuous) reads

$$\begin{aligned} &\partial_t W_{ij} + \frac{\partial_p H_{ij}}{\Delta x} \qquad (W^-_{i+1/2,j} - W^+_{i-1/2,j}) \\ &\qquad - \frac{H^-_{i+1/2,j} - H^+_{i-1/2,j}}{\Delta x \Delta p}(W_{i,j+1/2} - W_{i,j-1/2}) = 0, \end{aligned} \tag{4.8}$$

where the numerical flux $W_{i,j+1/2}$ are defined using the upwind discretization. We will use (4.4) to define the fluxes $W^{\pm}_{i+1/2}$.

Assume H is discontinuous at $x_{i+1/2}$. Consider the case $\partial_p H_{ij} > 0$. Using upwind scheme, $W^-_{i+1/2,j} = W_{ij}$. However, by (4.4),

$$W^+_{i+1/2,j} = \alpha^T W(x^-_{i+1/2}, p^-_j) + \alpha^R W(x^+_{i+1/2}, -p_j) \tag{4.9}$$

while p^-_j is obtained from $p^+_j = p_j$ using (4.5). The terms on the right hand side of (4.9) can be approximated by the upwind method, namely

$$W(x^-_{i+1/2}, p^-_j) = W(x_i, p^-_j)\,, \quad W(x^+_{i+1/2}, -p_j) = W(x_{i+1}, -p_j)\,.$$

Since p^-_j may not be a grid point, we have to define it approximately. One can first locate the two cell centers that bound this velocity, and then use a linear interpolation to evaluate the needed numerical flux at p^-.

The case of $p_j < 0$ is treated similarly.

Our new numerical schemes produce the solution crossing the interface defined by the mathematical solution introduced in the previous subsection, thus obtain the physically relevant solution of particle/wave transmission and reflection at the interfaces, with sharp numerical resolutions (no smearing) at the interface. In particular, in the case of geometric optics, the Snell's Law was built into the numerical flux! In addition, it allows a *hyperbolic* CFL condition $\Delta t = O(\Delta x, \Delta p)$, which is optimal for the underlying hyperbolic Liouville equation.

This idea has been applied successfully to compute the semiclassical limit of the linear Schrödinger equation with potential barriers [**18**] and the geometrical optics with complete transmission/reflection [**19**] or partial transmission/reflection [**20**]. 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 [**18**] was established in [**41**], following [**40**].

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. The framework also extends to reduced Liouville equation [**21**], where the interface condition uses directly Snell's Law to determine one side of the wave direction vector from the other side. It has also been extended to high frequency elastic waves [**12**], and high frequency waves in random media [**13**] with *diffusive interfaces*, where radiative transfer equation rather than the Liouville equation was used. It was also extended to a multi-scale coupling of the radiative transfer equation with its diffusion limit though an interface that can specularly or diffusively transmit or reflect waves [**22**].

4.4. 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. In classical mechanics one cannot observe *tunneling*, thus some quantum mechanics needs to be used to capture such a quantum phenomenon through a quantum well. 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 [**2**].

In [**14**], we introduced the following semiclassical model for thin quantum barriers:

- 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 α_T and α_R).
- solve the classical Liouville equation elsewhere, using the scattering data at the barrier in the interface condition (4.4) and the numerical method of [**18**] for a classical barrier.

To obtain the quantum scattering data, the Schrödinger equation for the complex wave function ψ:

$$i\epsilon\,\psi_t + \frac{\epsilon^2}{2}\Delta\psi - V(\mathbf{x})\psi = 0, \qquad \mathbf{x} \in \Re^n, \tag{4.10}$$

with an open boundary needs to be solved. Since we only need the scattering data, the transfer matrix method [**25**] or the quantum transmitting boundary method [**28**] can be used.

We have developed such a *decoherent* semiclassical model in one-space dimension in [**14**] and in two-space dimension space in [**15**]. Our numerical experiments confirm the validity of this approach when the well is very thin (a few ϵ's) and well-separated. In such cases, wave interference and time delay are negligible (although the time-delay can be easily incorporated into the model). The model can correctly capture tunneling, 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. For a two-dimensional numerical comparison between the solution of the Schrödinger equation (4.10) and that of the semiclassical model, see Fig.1.

Wave interference can not be captured in the de-coherent model due to the loss of phase information in the semiclassical limit where the particle density distribution satisfies the *real valued* Liouville equation (4.1) with real-valued transmission and reflection interface condition. In order to handle the wave interference through the quantum barriers, we proposed a *complex* Liouville equation with a complex interface condition using directly the quantum scattering matrix [**16**]. The complex valued scattering matrix provides necessary phase information to allow us to handle the wave interference at the quantum barrier.

4.5. Computation of diffraction. The geometric optics approximation offers good approximations when the wave length is very small, thus phenomena such as diffractions can be ignored. However, when the wave length is moderately small, the diffraction effect should not be ignored. Clearly, the interface condition (4.4) takes into account only transmission and reflection, thus one does not expect any diffractions to be captured.

Diffractions occur when waves hit an interface at a critical or tangent angle, or when waves hit a vertex. Geometrical Theory of Diffraction (GTD) was developed to include the diffraction into the theory of geometric optics [**26, 27**]. In GTD, the diffraction coefficients and decay rates of surface waves were derived. In [**23**], for smooth convex (or concave) curved interfaces, the interface condition (4.4) is modified at critical and tangent angles using these diffraction data from the GTD theory. Since these coefficients and decay rates depend on geometry and boundary conditions, the specific interface condition has to be worked out for different types

of interfaces, and at vertices. For an application of diffraction at the tip of a half-plane, see [**24**]. For multi-patched phase space method for computing creeping waves along a convex body, see [**35**].

References

[1] L. Ambrosio, Transport equation and Cauchy problem for BV vector fields, Invent. math., 158, 227-260, 2004.

[2] N. Ben Abdalla, I. Gamba and P. Degond, Coupling one-dimensional time-dependent classical and quantum transport models, J. Math. Phys. 43, 1-24, 2002.

[3] A. Bermudez and M.E. Vasquez, Upwind methods for hyperbolic conservation laws with source terms, Comput. & fluids 23, 1049-1071, (1994).

[4] R. Botchorishvili, B. Perthame and B. Vasseur, Equilibrium schemes for scalar conservation laws with stiff sources. (English summary) Math. Comp. 72, 131–157, (2003).

[5] F. Bouchut, Renormalized solutions to the Vlasov equation with coefficients of bounded variations, Arch. Rat. Mech. Anal. 157, 75-90, (2001).

[6] R.J. DiPerna and P.-L. Lions, Ordinary differential equations, transport theory and Sobolev spaces, Invent. Math. 98, No. 3, 511-547, 1989.

[7] P. Gerard, P.A. Markowich, N.J. Mauser and F. Poupaud, Homogenization limits and Wigner transforms, Comm. Pure Appl. Math. 50, 323-379, 1997.

[8] L. Gosse,A well-balanced flux-vector splitting scheme designed for hyperbolic systems of conservation laws with source terms. Comput. Math. Appl. 39 (2000), no. 9-10, 135–159.

[9] J.M. Greenberg and A.Y. Leroux, A well-balanced scheme for the numerical processing of source terms in hyperbolic equations. SIAM J. Numer. Anal. 33 (1996), no. 1, 1–16.

[10] S. Jin, A steady-state capturing method for hyperbolic systems with geometrical source terms, M2AN Math. Model. Num. Anal. 35, 631-646, (2001).

[11] S. Jin, Recent computational methods for high frequency waves in heterogeneous media, in Proceedings of 2006 Annual Meeting of the Chinese Society of Industrial and Applied Mathematics, to appear.

[12] S. Jin and X. Liao, A Hamiltonian-preserving scheme for high frequency elastic waves in heterogeneous media, J. Hyperbolic Diff. Eqn. 3, No. 4, 741-777, 2006.

[13] S. Jin, X. Liao and X. Yang, Computation of interface reflection and regular or diffuse transmission of the planar symmetric radiative transfer equation with isotropic scattering and its diffusion limit, SIAM J. Sci. Comp., 30, 1992-2017, 2008

[14] S. Jin and K. Novak, A semiclassical transport model for thin quantum barriers, Multiscale Modeling and Simulation, 5, 1063-1086, 2006.

[15] S. Jin and K. Novak, A semiclassical transport model for two-dimensional thin quantum barriers, J. Comp. Phys. 226, 1623-1644, 2007.

[16] S. Jin and K. Novak, A coherent semiclassical transport model for pure-state quantum scattering, preprint.

[17] S. Jin and P. Qi, l^1-error estimates on the immersed interface upwind scheme for linear convection equations with piecewise constant coefficients: a simple proof. Preprint.

[18] S. Jin and X. Wen, Hamiltonian-preserving schemes for the Liouville equation with discontinuous potentials, Comm. Math. Sci. 3, 285-315, 2005

[19] S. Jin and X. Wen, Hamiltonian-preserving schemes for the Liouville equation of geometrical optics with discontinuous local wave speeds, J. Comp. Phys. 214, 672-697, 2006.

[20] S. Jin and X. Wen, Hamiltonian-preserving schemes for the Liouville equation of geometrical optics with partial transmissions and reflections, SIAM J. Num. Anal. 44, 1801-1828, 2006.

[21] S. Jin and X. Wen, Computation of Transmissions and Reflections in Geometrical Optics via the Reduced Liouville Equation, Wave Motion 43(8), 667-688, 2006.

[22] S. Jin, X. Yang and G. Yuan, A domain decomposition method for a two-scale transport equation with energy flux conserved at the interface, (with X. Yang and G.W. Yuan) , Kinetic and Related Models, 1, 65-84, 2008.

[23] S. Jin and D. Yin, Computational high frequency waves through curved interfaces via the Loiuville equation and Geometric Theory of Diffraction, J. Comp. Phys. 227, 6106-6139, 2008.

[24] S. Jin and D. Yin, Computation of high frequency wave diffraction by a half plane via the Loiuville equation and Geometric Theory of Diffraction, Comm Comput Phys. 4, No. 5, 1106-1128, 2008.

[25] B. Johnson and S.T. Eng, Solving the Schrödinger equation in arbitrary quantum-well potential profiles using the transfer matrix method, IEEE J. Quantum Elect., 726, 2025-2035, 1990.
[26] J.B. Keller, Geometric theory of diffraction, J. Opt. Sco. of America 52, 116-130, 1962.
[27] J.B. Keller and R. Lewis, Asymptotic methods for partial differential equations: the reduced wave equation and Maxwell's equations, in Surveys in Applied Mathematics, edited by D. McLaughlin, J.B. Keller and G. Papanicolaou, Plenum Press, New York, 1995.
[28] C.S. Lent and D.J. Kirkner, The quantum transmitting boundary method, J. Appl. Phys. 67, 6353-6359, 1990.
[29] R.J. LeVeque, Balancing source terms and flux gradients in high-resolution Godunov methods: the quasi-steady wave-propagation algorithm, J. Comp. Phys. 146, 346-365, (1998).
[30] R.J. LeVeque and Z.L. Li, Immersed interface methods for Stokes flow with elastic boundaries, SIAM J. Sci. Comp. 18, 709-735, 1997.
[31] R.J. LeVeque and C. Zhang, The immersed interface method for acoustic wave equations with discontinuous coefficients, Wave Motion 25, 237-263 (1997).
[32] P.L. Lions and T. Paul, Sur les measures de Wigner, Revista. Mat. Iberoamericana 9, 553-618, 1993.
[33] A. Mayo. The fast solution of Poisson'sand the biharmonic equations on irregular regions, SIAM J. Sci. Comp. 21, 285-299, 1984.
[34] L. Miller, Refraction of high frequency waves density by sharp interfaces and semiclassical measures at the boundary, J. Math. Pures Appl. IX 79, 227-269, 2000.
[35] M. Motamed and O. Runborg. A multiple-patch phase space method for computing trajectories on manifolds with applications to wave propagation problems. Commun. Math. Sci. 5, 617-648, 2007
[36] G. Papanicolaou and L. Ryzhik, Waves and transport, IAS/Park City Mathematics Series, Vol. 5, L. Caffarelli and Weinan E, eds., AMS, 1998, pp. 305-382.
[37] B. Perthame and C. Simeoni, A kinetic scheme for the Saint-Venant system with a source term, Calcolo 38, 201-231 (2001).
[38] C. Peskin, The immersed boundary method, Acta Numerica, 479-517, 2002.
[39] L. Ryzhik, G. Papanicolaou and J.B. Keller, Transport equations for elastic and other waves in random media, Wave Motion 24(4), 327-370, (1996).
[40] X. Wen and S. Jin, Convergence of an immersed interface upwind scheme for linear advection equations with piecewise constant coefficients I: l^1-error estimates, J. Comp. Math., to appear.
[41] X. Wen and S. Jin, The l^1-error estimates for a Hamiltonian-preserving scheme to the Liouville equation with piecewise constant coefficients, SIAM J. Num. Anal. 46, 2688-2714, 2008.
[42] E. Wigner, On the quantum correction for thermodynamic equilibrium, Phys. Rev 40, 749-759, 1932.

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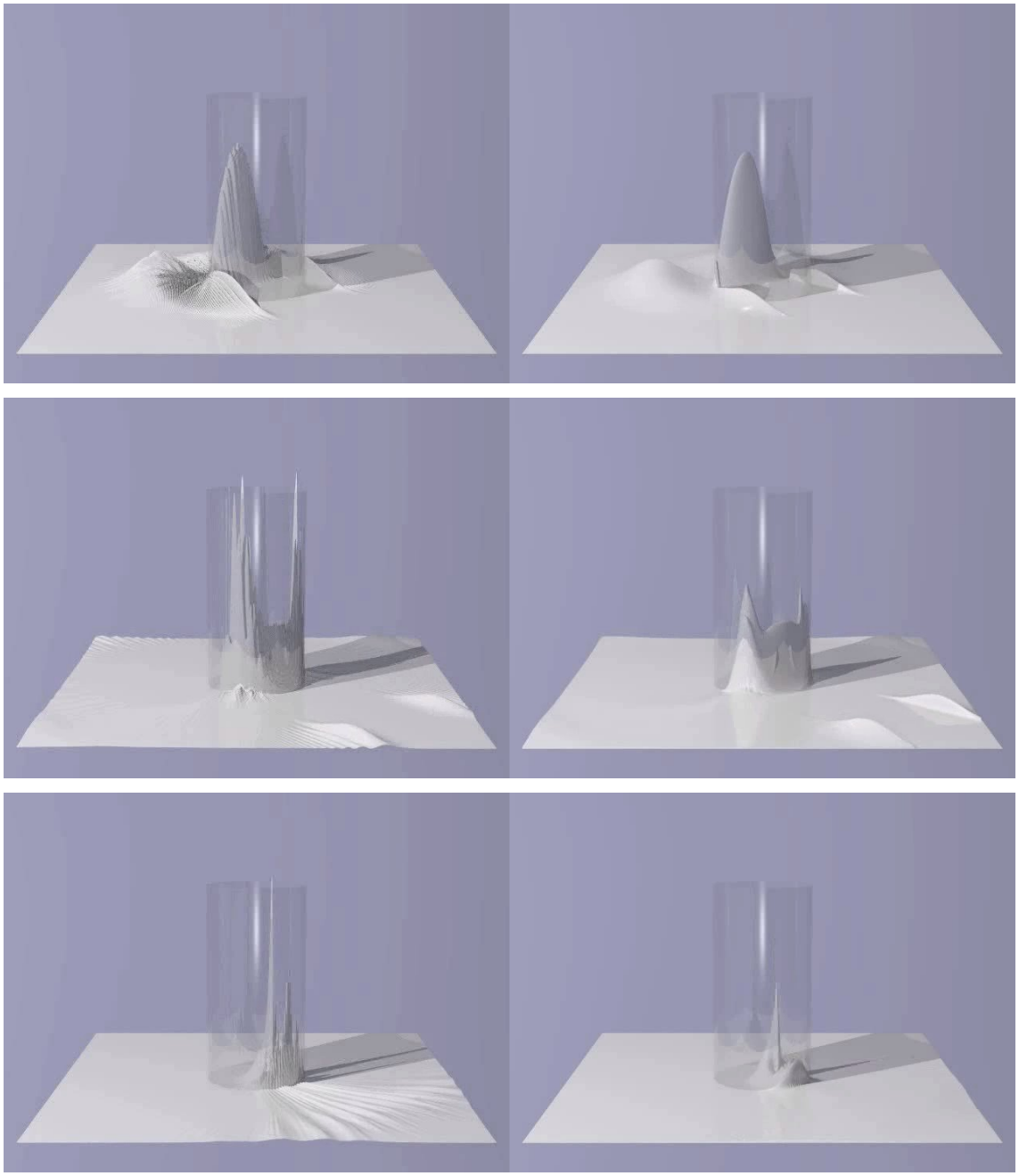

FIGURE 1. An Gaussian wave packet initially outside of the circular barrier moveing toward the barrier tunnels through the barrier, generating partially transmitted and reflected waves. The left figures are the position density of the Schrödinger equation for $\epsilon = 1/400$ at several different times, while the right figures are those computed using the decoherent semiclassical model at the same times. For details see [**15**].