Asymptotic-Preserving Schemes for Multiscale Physical Problems

Shi Jin

Shanghai Jiao Tong University, China

CIRM-Jean-Morlet Chair Program: Research School

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outlines

Lecture 1:

- mathematical connections between different physical scales,
  from quantum all the way to hydrodynamics;
- How to resolve oscillations in quantum dynamics

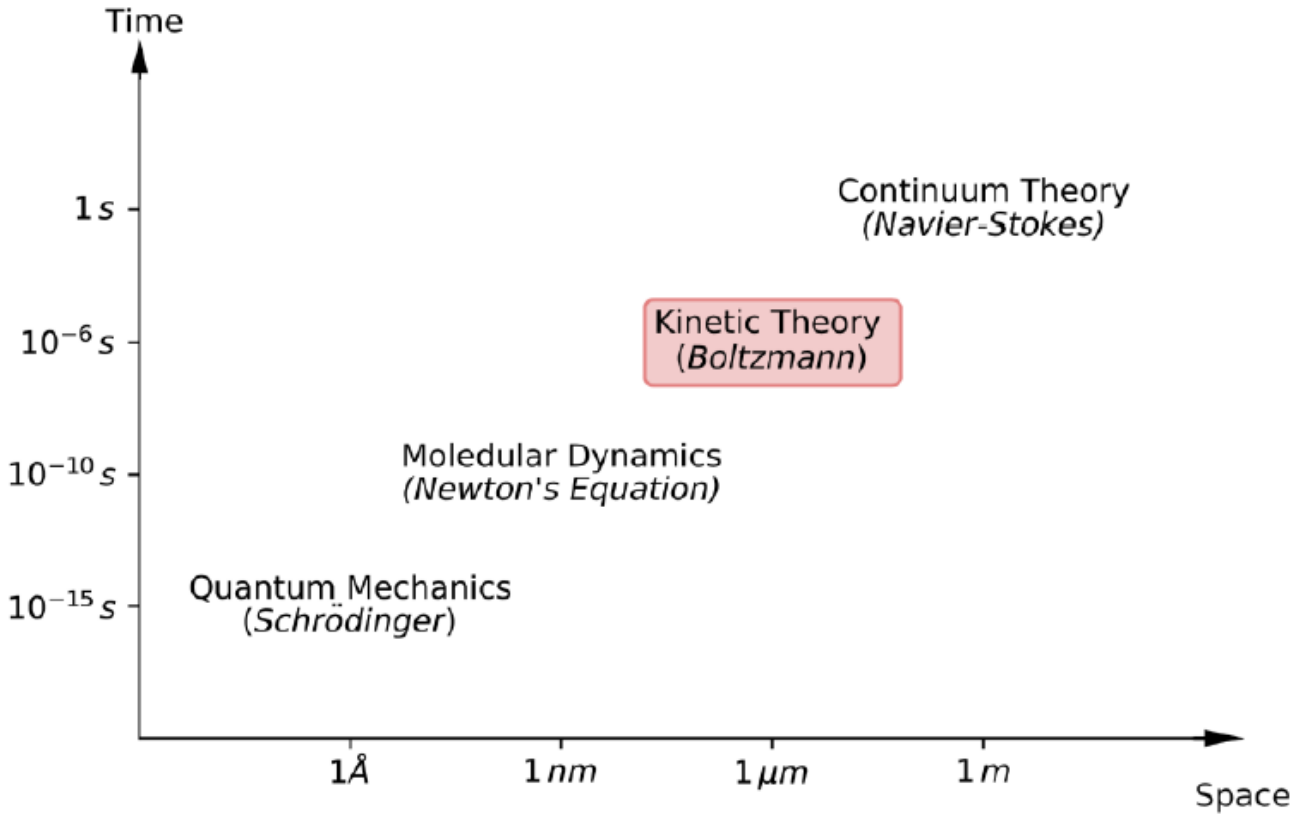
Lecture 2:

efficient numerical transitions from particles to mean-fields: random batch methods

Lecture 3:

Asymptotic-preserving schemes for multiscale kinetic equations

Four physical scales



Fundamental Physical Equations

- If relativistic effect is not considered, then these four physical laws basically cover all essential physical equations at the four different scales
- They describe the same problem at *different* scales

- If there is an external field then one needs to couple these equations with field equations

  Poisson equations (Gauss's Law) for electric field;

  Maxwell equations for electromagnetic field

  Liouville (Vlasov)-poisson systems, Vlasov-Maxwell equations, Euler-Poisson system, etc.

N-body Schrodinger equation—the first principle computation

$$i\hbar\partial_t\Phi(t,\mathbf{x},\mathbf{y}) = H\Phi(t,\mathbf{x},\mathbf{y})$$

$$H = -\sum_{j=1}^{N}\frac{\hbar^2}{2M_j}\Delta_{x_j} + H_e(\mathbf{y},\mathbf{x})$$

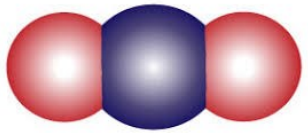
$$H_e(\mathbf{y},\mathbf{x}) = -\sum_{j=1}^{n}\frac{\hbar^2}{2m_j}\Delta_{y_j} + \sum_{j<k}\frac{1}{|y_j-y_k|} + \sum_{j<k}\frac{Z_jZ_k}{|x_j-x_k|} - \sum_{j=1}^{N}\sum_{k=1}^{n}\frac{Z_j}{|x_j-y_k|}$$

Too big to compute!

- Paul Dirac (1929): “The general theory of quantum mechanics is now complete ··· The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known , and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble”

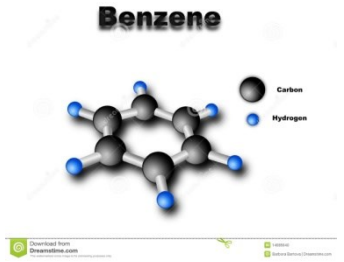
- If computer is big and fast enough to solve the N-body Schrodinger equation then we don’t need the other (more macroscopic) equations
- Quantum simulation is computational daunting!

CO2: 75 dimension



O=C=O

Benzene 162 dimensions



Dimension reduction

- Separating the computation of electrons from that of the nuclei

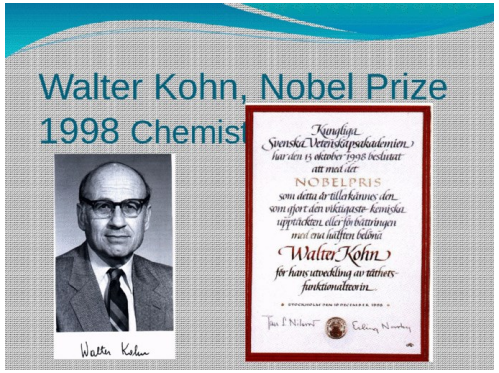
  Born-Oppenheimer approximation;

  Ehrenfest dynamics

- Mean-field approximation (approximation by 1-body system)

  Hartree theory, Hartree-Fock theory (F. Golse's course*);*

  density function theory



Newton's equation (microscopic; classical mechanics)

F=ma

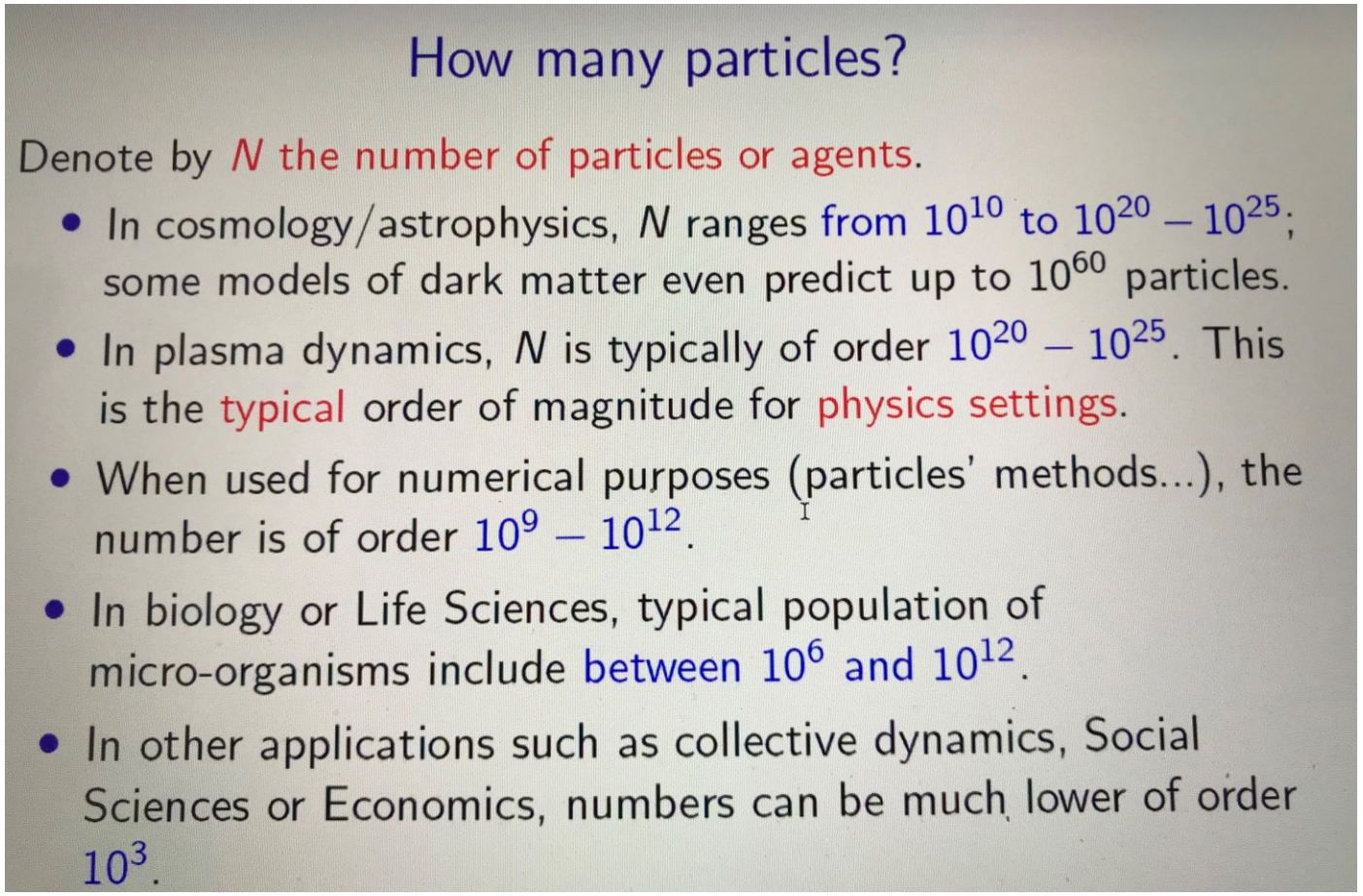
- Hamiltonian system

$$\dot{q}_i = \frac{p_i}{m_i}$$

i=1,⋯ N

$$\dot{p}_i = -\frac{\partial V}{\partial q_i} = F_i$$

How big is N?



- *P.E. Jabin*'s slide (also course by P. Degond)

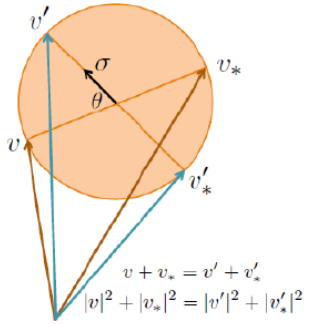
Kinetic theory (mesoscopic, statistical physics)

The Boltzmann equation (6 dimension +time!)

$f(t, \mathbf{x}, \mathbf{v})$ is the **phase space distribution function** of time t, position $\mathbf{x}$, and velocity $\mathbf{v}$

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\varepsilon} \mathcal{Q}(f, f)(\mathbf{v}), \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d, \ \mathbf{v} \in \mathbb{R}^d$$

$$\mathcal{Q}(f, f)(\mathbf{v}) = \int_{\mathbb{R}^d} \int_{S^{d-1}} B(\mathbf{v} - \mathbf{v}_*, \sigma)[f(\mathbf{v}')f(\mathbf{v}'_*) - f(\mathbf{v})f(\mathbf{v}_*)] \, \mathrm{d}\sigma \mathrm{d}\mathbf{v}_*$$



The Boltzmann's H-Theorem (entropy condition)

$$\partial_t \langle f \ln f \rangle + \nabla_x \cdot \langle v f \ln f \rangle \leq 0$$

Fluid dynamics (Euler/Navier-Stokes equations: macroscopic)

- Conservation of mass
- Conservation of momentum
- Conservation of energy

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla_x \cdot \rho u = 0, \\ \frac{\partial \rho u}{\partial t} + \nabla_x \cdot (\rho u \otimes u + p\,\mathrm{I}) = 0, \\ \frac{\partial E}{\partial t} + \nabla_x \cdot ((E + p)u) = 0, \end{cases}$$

- Equation of state

$$p = (\gamma - 1)\left(E - \frac{1}{2}\rho |u|^2\right)$$
$$\gamma = (d_v + 2)/d_v$$

- Adding viscosity and heat conductivity → Navier-Stokes equations

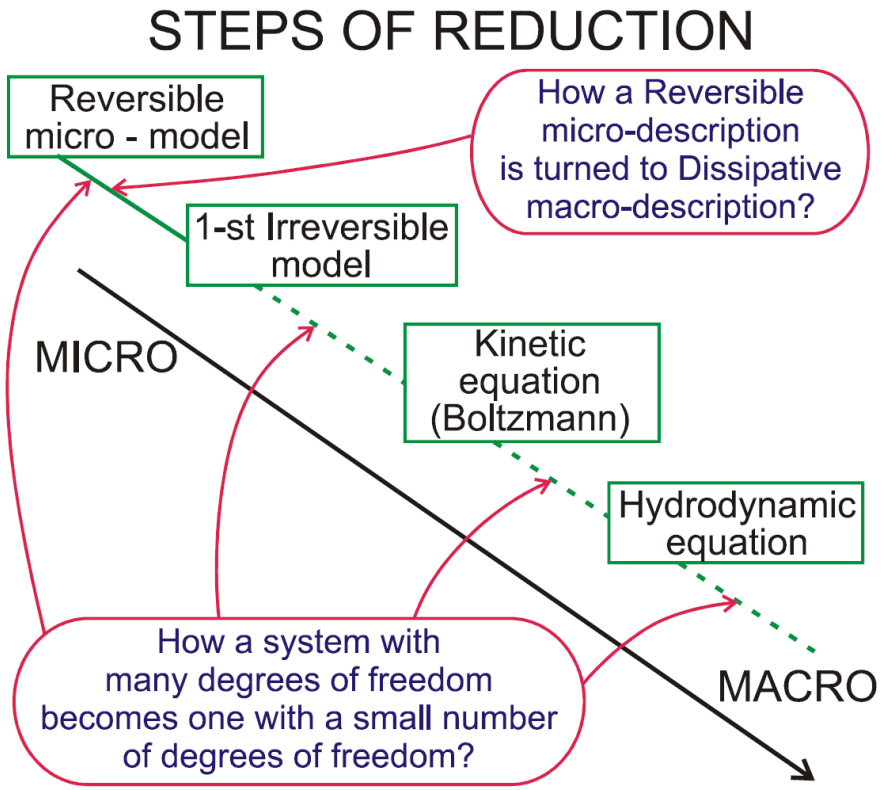
Mathematical connections between micro and macro physics

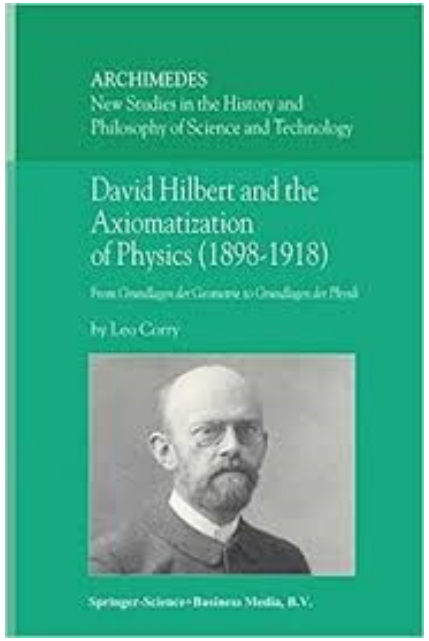
- If these equations describe the same physics, except at different scales, there must be mathematical connections between them:

  one should be able to derive mathematically from equation in one scale to the other scales!

- Exploring these mathematical connections (rigorously) between different scales has generated some of the most important results in mathematical physics and PDEs

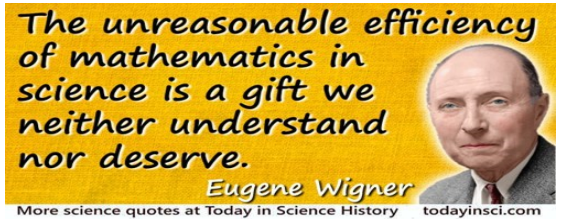
Hilbert's sixth problem (axiomatize physics)





- Hilbert's expansion of the Boltzmann equation

From quantum to classical –the Wigner transform



$$\mathrm{i}\varepsilon\partial_t u^\varepsilon = -\frac{\varepsilon^2}{2}\Delta u^\varepsilon + V(x)u^\varepsilon$$

$$w^\varepsilon[u^\varepsilon](x,\xi) := \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} u^\varepsilon\left(x+\frac{\varepsilon}{2}\eta\right)\overline{u^\varepsilon}\left(x-\frac{\varepsilon}{2}\eta\right)\mathrm{e}^{\mathrm{i}\xi\cdot\eta}\,\mathrm{d}\eta$$

Wigner transform

$$\partial_t w^\varepsilon + \xi\cdot\nabla_x w^\varepsilon - \Theta^\varepsilon[V]w^\varepsilon = 0$$

Wigner equation

$$\Theta^\varepsilon[V]f(x,\xi) := \frac{\mathrm{i}}{(2\pi)^d}\iint_{\mathbb{R}^d\times\mathbb{R}^d}\delta V^\varepsilon(x,y)f(x,\xi')\,\mathrm{e}^{\mathrm{i}\eta(\xi-\xi')}\,\mathrm{d}\eta\,\mathrm{d}\xi'$$

$$\delta V^\varepsilon := \frac{1}{\varepsilon}\left(V\left(x-\frac{\varepsilon}{2}y\right)-V\left(x+\frac{\varepsilon}{2}y\right)\right)$$

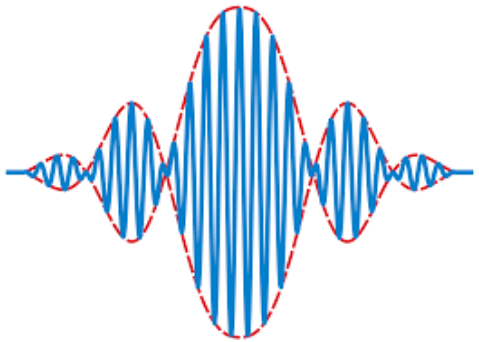
when $\varepsilon \to 0$

$$\partial_t w + \xi \cdot \nabla_\xi w - \nabla_x V(x) \cdot \nabla_\xi w = 0$$

classical Liouville equation

$$\dot{x} = \xi, \quad \dot{\xi} = -\nabla_x V(x)$$

its (bi)characteristics are
Newton's equation



when the Planck constant

$$\varepsilon \to 0$$

quantum mechanics becomes classical mechanics

P.L. Lions-Paul '93, Gerard-Markowich-Mauser-Poupaud '97

From Newton's equation to the Boltzmann equation

- N-body Newton's equation

$$\begin{cases} \dot{x}_i = v_i, \\ \dot{v}_i = -\sum\limits_{\substack{j=1\dots N \\ j\neq i}} \nabla\varphi(x_i - x_j) \end{cases}$$

$$z_1 \dots z_N = Z_N = (X_N, V_N) = (x_1 \dots x_N, v_1 \dots v_N)$$

Probability measure $W^N(Z_N)dZ_N$ on $\mathbb{R}^{3N} \times \mathbb{R}^{3N}$

- N-body Liouville equation

$$\partial_t W^N(t) = \mathcal{L}_N W^N(t) \qquad \mathcal{L}_N = -\sum_{i=1}^{N} [v_i \cdot \nabla_{x_i} + F_i \cdot \nabla_{v_i}]$$

$$F_i = -\sum_{j:j\neq i} \nabla\varphi(x_i - x_j)$$

$N \to \infty$ Limit (mean field limit)

$$f_j^N(Z_j;t) = \int dz_{j+1} \dots dz_N W^N(Z_j, z_{j+1} \dots z_N; t) \qquad j = 1 \dots N.$$

Marginal distribution

$$W^N(z_1 \dots z_i \dots z_j \dots z_N) = W^N(z_1 \dots z_j \dots z_i \dots z_N)$$

assume all particles are identical, indistinguishable

$$f_2^N(x_1, v_1, x_2, v_2) = f_1^N(x_1, v_1) f_1^N(x_2, v_2)$$

$$\varepsilon \to 0, \quad N \to \infty, \quad n\varepsilon^2 \to \text{const.}$$

molecular chaos assumption

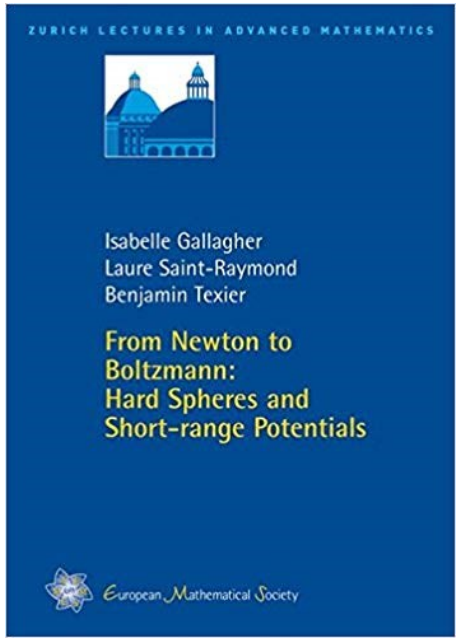
ε diameter of particles

The Boltzmann-Grad limit

$f_1^N(x_1, v_1)$ satisfies the Boltzmann equation

The proof of the Boltzmann-Grad limit is very difficult

- Lanford 1974
- Gallegher-Saint-Raymond-Texier 2013
  (valid for a fraction of mean free path)



(course by M. Pulvirenti)

From the Boltzmann equation to fluid equations

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} \mathcal{Q}(f, f)$$

ε Knudsen number (dimensionless mean free path)

- Moments

$$n = \int_{\mathbb{R}^d} f(v)\, dv, \qquad u = \frac{1}{n} \int_{\mathbb{R}^d} f(v) v\, dv, \qquad T = \frac{1}{dn} \int_{\mathbb{R}^d} f(v)|v-u|^2\, dv.$$

- Moment equations (conservations of mass, momentum and energy)—not closed!

$$\partial_t \begin{pmatrix} n \\ nu \\ E \end{pmatrix} + \nabla_x \cdot \begin{pmatrix} nu \\ nu \otimes u + \mathbb{P} \\ Eu + \mathbb{P}u + \mathbb{Q} \end{pmatrix} = 0$$

$E = \frac{1}{2} n|u|^2 + \frac{d}{2} nT$: total energy=kinetic energy + internal energy

Fluid dynamic limit $\varepsilon \to 0$

$$f \to \quad M_{(n,u,T)} = \frac{n}{(2\pi T)^{d/2}} \exp\left(-\frac{|v-u|^2}{2T}\right)$$ Local Maxwellian

Then one can close the moment equation → compressible Euler equations

By Chapman-Enskog expansion, one can expand to the next order in ε to get the Navier-Stokes equations (Euler + viscosity + heat conductivity)

Only incompressible N-S limit was rigorously proved

Bardos-Golse-Levermore (1991), Golse-Saint-Raymond (2003)

A summary

- Macroscopic equations are limits or asymptotic approximations of microscopic equations

- Microscopic (quantum or classical) equations are linear, and time reversible; meso- and macroscopic equations are nonlinear, and time irreversible

- Microscopic equations are harder for computation (too many degree of freedoms); macroscopic equations are harder for mathematical analysis (nonlinearity; Millennium problems)

Multiscale problems

- Space shuttle re-entry problem

  $\varepsilon : 10^{-8} \sim 1$ meters

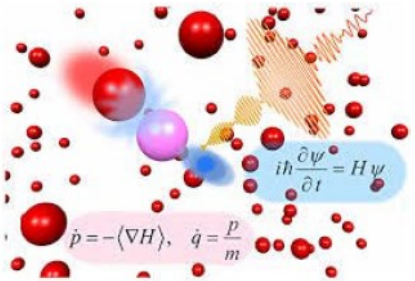
- Supersonic flights

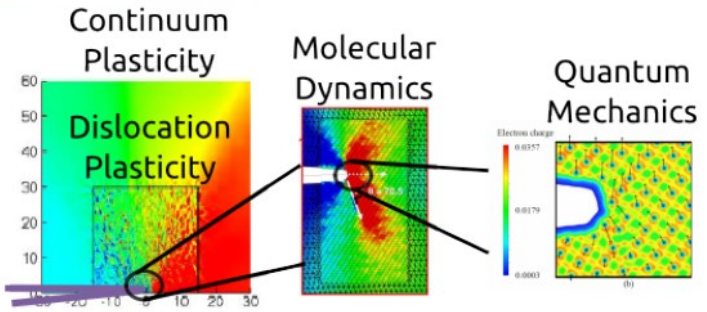
  thickness of Navier-Stokes shock profile

  not correct

- Dislocation (at which continuum assumption not valid)

- Chemical reaction—need quantum mechanics

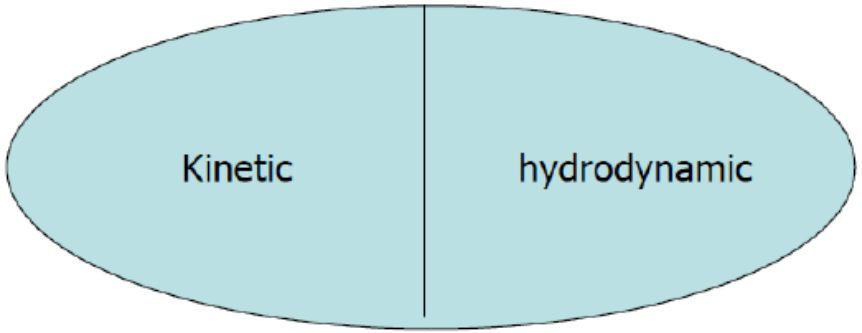




Multiscale methodology I: hybridization

- Pros: macro part computational cost small

- Cons: how to determine the location of the artificial interface and how to define the connecting (boundary or interface) conditions?



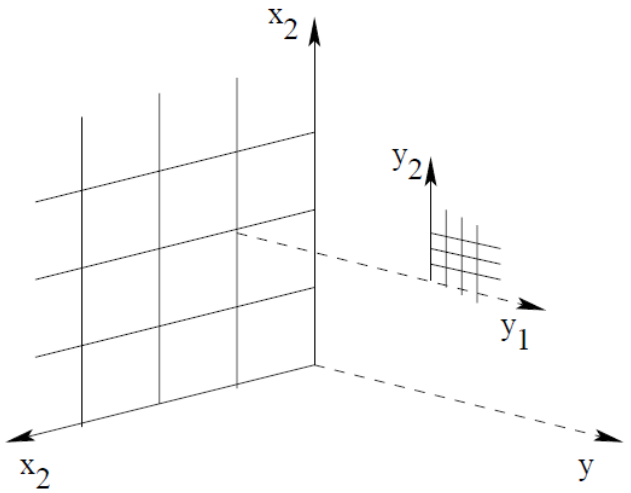
Micro→macro: taking averaging, moments, etc.

macro→ micro: no unique definition (assuming local Maxwellian?)

Neuzert, Klar, Perthame, etc.

Multiscale methodology II: heterogeneous multiscale methods

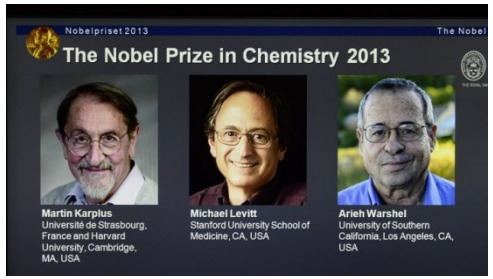
- Microscopic simulation around macroscopic meshes
  (to get equation of state, constitutive relations, forcing terms, etc.)



$$V(\mathbf{r}) = \sum_{\text{bonds}} K_b^{(1)}(b-b_0)^2 + \sum_{\text{angles}} K_\theta^{(2)}(\theta-\theta_0)^2 + \sum_{\text{dihedrals}} K_\chi^{(3)}(1+\cos(n\chi-\delta)) + \sum_{\text{nonbonded-pairs},i,j} \left[\frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}^{(4)} - \varepsilon_{ij}\left\{\left(\frac{R_{\min ij}}{r_{ij}}\right)^{12} - 2\left(\frac{R_{\min ij}}{r_{ij}}\right)^{6}\right\}^{(5)}\right]$$

Energy dependencies on:

1. Bond length
2. Bond valence angle
3. Bond dihedral angle
4. Non-bonded electrostatic interactions
5. Non-bonded van-der Waals interactions

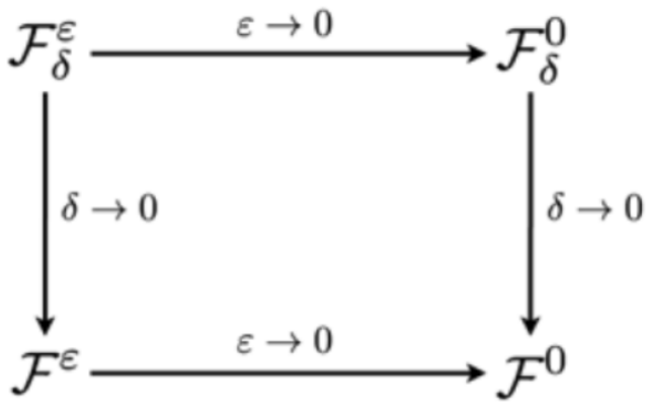


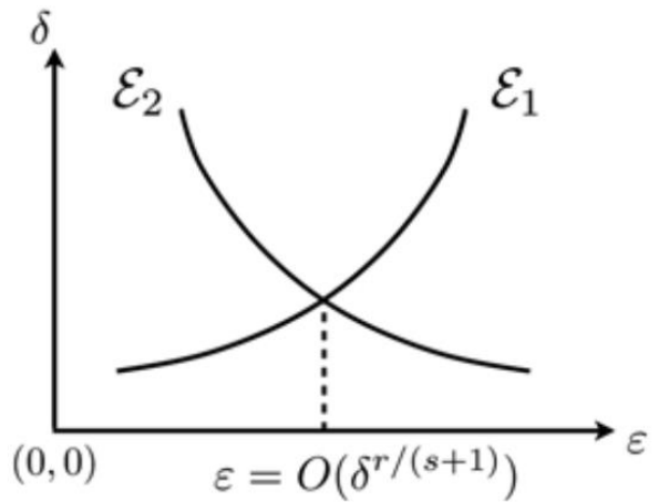
E & Engquist difficulty: marco to micro transition

Computational Methodology III: Asymptotic-preserving (AP) schemes

- Design schemes that work crossing scales—a micro-solver that automatically becomes a macro-solver in the macroscopic limit, when the numerical parameters do not resolve the microscopic scale
- Numerical schemes preserve the asymptotic transition from micro to macro scales

Uniform convergence (Golse-Jin-Levermore '99)





$$\|\mathcal{F}^{\varepsilon} - \mathcal{F}^{0}\| = O(\varepsilon)$$

a classical numerical analysis typically gives

$$\mathcal{E}_2 = \|\mathcal{F}^{\varepsilon}_{\delta} - \mathcal{F}^{\varepsilon}\| = O(\delta^{r}/\varepsilon^{s}), \quad 1 \le s \le r$$

the scheme is AP

$$\|\mathcal{F}^{\varepsilon}_{\delta} - \mathcal{F}^{0}_{\delta}\| = O(\varepsilon) \qquad \text{uniformly in} \quad \delta$$

$$\|\mathcal{F}^{0}_{\delta} - \mathcal{F}^{0}\| = O(\delta^{r}).$$

one adds up the errors

$$\mathcal{E}_1 = \|\mathcal{F}^{\varepsilon}_{\delta} - \mathcal{F}^{\varepsilon}\| = O(\varepsilon + \delta^{r})$$

By comparing the two error estimates

$$\|\mathcal{F}^{\varepsilon}_{\delta} - \mathcal{F}^{\varepsilon}\| = \min(\mathcal{E}_1, \mathcal{E}_2)$$

which has an upper bound around $\varepsilon = O(\delta^{r/(s+1)})$

$$\|\mathcal{F}^{\varepsilon}_{\delta} - \mathcal{F}^{\varepsilon}\| = O(\delta^{r/(s+1)}), \qquad \text{uniformly in} \quad \varepsilon$$

Is it always possible to allow $\Delta x, \Delta t >> \varepsilon$?

- Discrete Schrodinger → discrete Liouville

  yes for time, *no* for space

  the best one can do is $\Delta x = \mathcal{O}\left(\varepsilon^{1/2}\right)$

  (Gaussian beam/wave packet methods)

- Discrete Newton (Liouville) to discrete Boltzmann?

  some success: Molecular dynamics-random batch methods

- Discrete Boltzmann to discrete Euler/Navier-Stokes

  largely *yes*

AP I: from quantum to classical mechanics

- Difficulty of quantum simulation:
  large N: curse of dimensionality
  small $\hbar$: solution is highly oscillatory

Here we will only concentrate on the oscillation problem

The Schrodinger equation

$$\mathrm{i}\varepsilon\partial_t u^\varepsilon = -\frac{\varepsilon^2}{2}\Delta u^\varepsilon + V(x)u^\varepsilon, \quad u^\varepsilon(0,x) = u_{\mathrm{in}}^\varepsilon(x) \qquad (t,x) \in \mathbb{R}\times\mathbb{R}^d$$

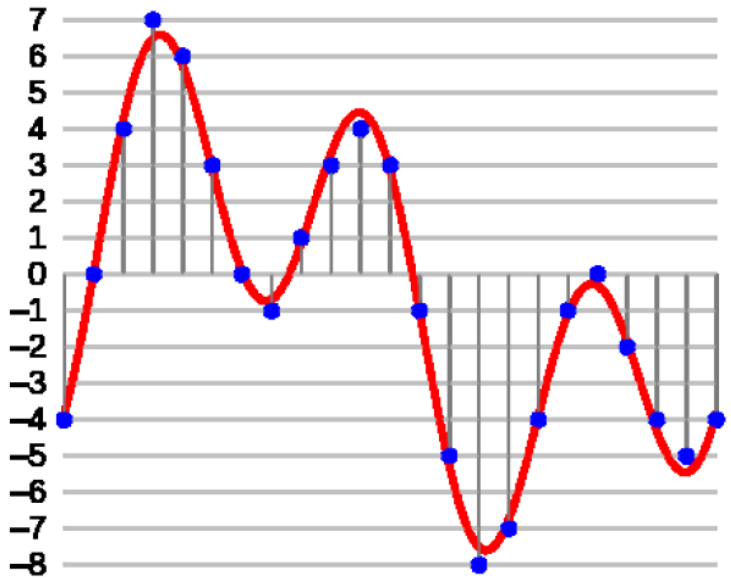
- If V(x)=0, a single plane wave solution

$$u^\varepsilon(t,x) = \exp\left(\frac{\mathrm{i}}{\varepsilon}\left(\xi\cdot x - \frac{t}{2}|\xi|^2\right)\right)$$

oscillation in both space and time!

typical mesh strategy: $k = \Delta t$ $\qquad h = o(\varepsilon), \quad k = o(\varepsilon)$

- Nyquist-Shannon sampling theorem: need a few grid points per wave length



- This is a daunting talk for most high frequency waves, including quantum dynamics, compuations in high dimensions

A time splitting spectral method

- Trotter splitting

Step 1. From time $t = t_n$ to time $t = t_{n+1}$, first solve the free Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t u^\varepsilon + \frac{\varepsilon^2}{2}\partial_{xx} u^\varepsilon = 0. \tag{5.2}$$

Step 2. On the same time interval, *i.e.*, $t \in [t_n, t_{n+1}]$, solve the ordinary differential equation (ODE)

$$\mathrm{i}\varepsilon\partial_t u^\varepsilon - V(x)u^\varepsilon = 0, \tag{5.3}$$

with the solution obtained from Step 1 as initial data for Step 2. Equation (5.3) can be solved *exactly* since $|u(t,x)|$ is left invariant under (5.3),

$$u(t,x) = |u(0,x)|\,\mathrm{e}^{\mathrm{i}V(x)t}.$$

- In step 1, one can use the spectral method and then integrate in time exactly in the Fourier space
- One can use the Strang splitting to get second order in time

$$n^{\varepsilon}(\mathbf{x}, t) = |u^{\varepsilon}(\mathbf{x}, t)|^2 \qquad J^{\varepsilon}(\mathbf{x}, t) = \varepsilon \, \mathrm{Im}(\overline{u^{\varepsilon}(\mathbf{x}, t)} \nabla u^{\varepsilon}(\mathbf{x}, t))$$

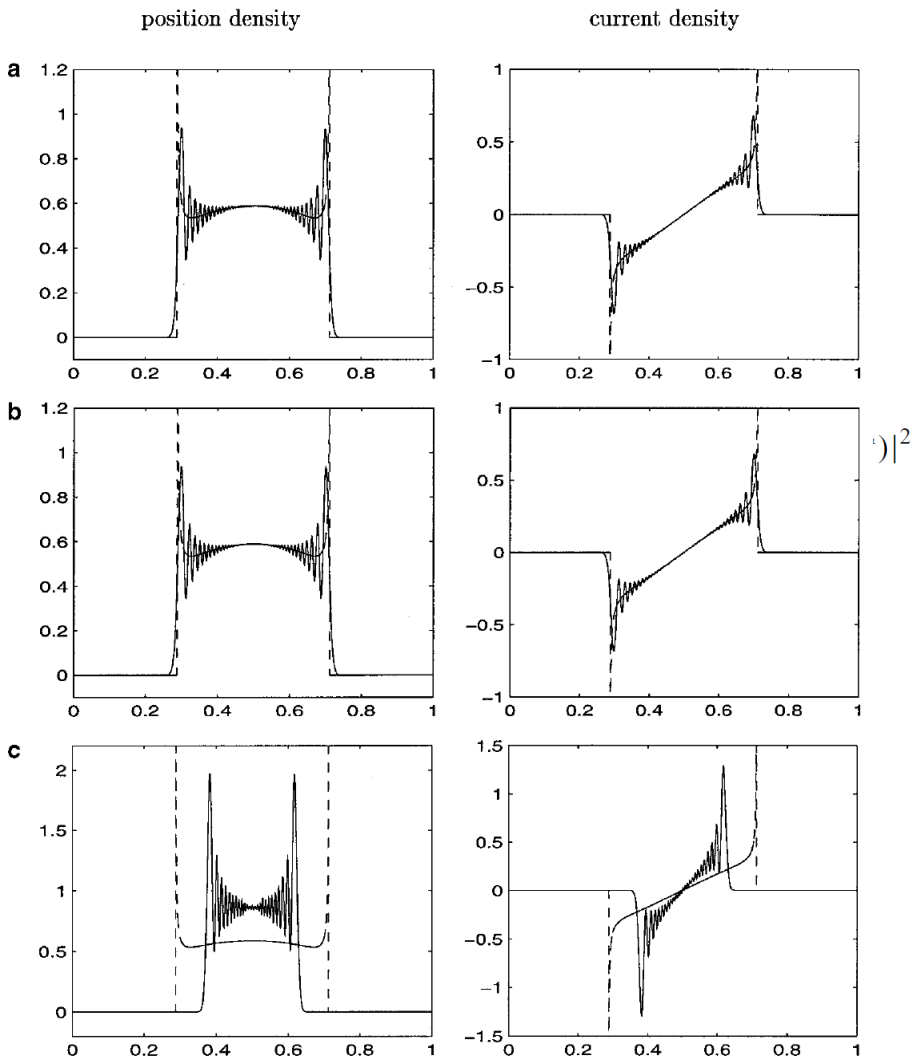


FIG. 3. Numerical solutions at $t = 0.54$ in Example 1. $\varepsilon = 10^{-3}$, $V(x) = 10$, $h = \frac{1}{512}$. (a) CNSP (2.13), $k = 0.00001$; (b) SP2 (2.9); (c) CNSP (2.13), $k = 0.0001$.

Mesh strategy

- To get accurate wave function one needs

$$k = o(\varepsilon) \qquad h = O(\varepsilon)$$

via standard numerical analysis:

$$\left\| u^{\varepsilon}(t_n) - u_I^{\varepsilon,n} \right\|_{L^2} \leq G_m \frac{T}{k} \left(\frac{h}{\varepsilon(b-a)} \right)^m + \frac{CTk}{\varepsilon}$$

- To get the correct physical observables (position density, flux, energy etc) one just needs

$$k = O(1)$$

How to prove this result? (*Bao-J-Markowich* '02)

- Recall the Wigner transform

$$w^\varepsilon(f,g)(x,\xi)=\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\bar{f}\left(x+\frac{\varepsilon}{2}\sigma\right)g\left(x-\frac{\varepsilon}{2}\sigma\right)e^{i\sigma\cdot\xi}\,d\sigma$$

the Wigner equation $$w_t^\varepsilon+\xi\cdot\nabla_x w^\varepsilon+\Theta^\varepsilon[V]w^\varepsilon=0$$

$$\Theta^\varepsilon[V]w^\varepsilon(x,\xi,t):=\frac{i}{(2\pi)^d}\int_{\mathbb{R}^d_\alpha}\frac{V\left(x+\frac{\varepsilon}{2}\alpha\right)-V\left(x-\frac{\varepsilon}{2}\alpha\right)}{\varepsilon}\hat{w}^\varepsilon(x,\alpha,t)e^{i\alpha\cdot\xi}\,d\alpha$$

As $\varepsilon\to 0$ one gets the semiclassical limit (the Liouville equation)

$$w_t^0+\xi\cdot\nabla_x w^0-\nabla_x V(x)\cdot\nabla_\xi w^0=0$$

Assume spatially continuous, since at each step the time integration is conducted exactly, the splitting scheme, upon Wigner transform, can be viewed as the splitting of the Wigner equation as:

Step 1:

$$w_t^\varepsilon + \xi \cdot \nabla_x w^\varepsilon = 0, \quad t \in [t_n, t_{n+1}]$$

Step 2:

$$w_t^\varepsilon + \Theta^\varepsilon[V] w^\varepsilon = 0, \quad t \in [t_n, t_{n+1}].$$

As $\varepsilon \to 0$ these two steps reach the following limit

Step 1:

$$w_t^0 + \xi \cdot \nabla_x w^0 = 0, \quad t \in [t_n, t_{n+1}]$$

Step 2:

$$w_t^0 - \nabla_x V \cdot \nabla_\xi w^0 = 0, \quad t \in [t_n, t_{n+1}].$$

Which is the splitting scheme for the Liouville equation.

The above limit is taken with k fixed, thus k can be independent of ε (AP in time!)

Only for Physical observables, not wave function

the moments of Wigner transform only give (all) the physical observables

- Position density
- Current density
- Energy density

$$\rho^\varepsilon(t,x) = \int_{\mathbb{R}^d} w^\varepsilon(t,x,\xi)\,\mathrm{d}\xi$$

$$j^\varepsilon(t,x) = \int_{\mathbb{R}^d} \xi w^\varepsilon(t,x,\xi)\,\mathrm{d}\xi$$

$$e^\varepsilon(t,x) = \int_{\mathbb{R}^d} H(x,\xi) w^\varepsilon(t,x,\xi)\,\mathrm{d}\xi \qquad H(x,\xi) = \frac{1}{2}|\xi|^2 + V(x)$$

Wave function cannot be completely recovered (loss of constant phase, for example)

A more rigorous analysis (*Golse-J-Paul*, JFoCM)

Definition 2.4. *For all ρ and ρ', Borel probability measures on $\mathbf{R}^{2d}$, we set*

$$\mathrm{dist}_{\mathrm{MK},2}(\rho,\rho') := \inf_{\pi\in\Pi(\rho,\rho')}\left(\int_{\mathbf{R}^{2d}}(|q-q'|^2+|p-p'|^2)\pi(dqdpdq'dp')\right)^{1/2},$$

where $\Pi(\rho,\rho')$ designates the set of couplings of ρ and ρ'. More precisely, $\Pi(\rho,\rho')$ is the set of Borel probability measures on $\mathbf{R}^{2d}\times\mathbf{R}^{2d}$ with first and second marginals ρ and ρ' resp., i.e. such that

$$\int_{\mathbf{R}^{2d}\times\mathbf{R}^{2d}}(\phi(q,p)+\phi'(q',p'))\pi(dqdpdq'dp')$$
$$=\int_{\mathbf{R}^{2d}}\phi(q,p)\rho(dqdp)+\int_{\mathbf{R}^{2d}}\phi'(q',p')\rho'(dq'dp')$$

for all $\phi,\phi'\in C_b(\mathbf{R}^{2d})$.

Monge-Kantorovich or Wasserstein distance with exponent 2

Definition 2.4. *For all ρ and ρ', Borel probability measures on $\mathbf{R}^{2d}$, we set*

$$\mathrm{dist}_{\mathrm{MK},2}(\rho,\rho') := \inf_{\pi\in\Pi(\rho,\rho')}\left(\int_{\mathbf{R}^{2d}}(|q-q'|^2+|p-p'|^2)\pi(dqdpdq'dp')\right)^{1/2},$$

where $\Pi(\rho,\rho')$ designates the set of couplings of ρ and ρ'. More precisely, $\Pi(\rho,\rho')$ is the set of Borel probability measures on $\mathbf{R}^{2d}\times\mathbf{R}^{2d}$ with first and second marginals ρ and ρ' resp.,

Let $R\in\mathcal{D}(\mathfrak{H})$. The Wigner transform of R is

$$W_\hbar(R)(x,\xi) := \frac{1}{(2\pi)^d}\int_{\mathbf{R}^d} r(x+\tfrac{1}{2}\hbar y, x-\tfrac{1}{2}\hbar y)e^{-i\xi\cdot y}dy$$

where $r\equiv r(x,y)$ is the integral kernel of R

Husimi operator $\tilde{W}_\hbar(R) := e^{\hbar\Delta_{x,\xi}/4}W_\hbar(R)$

- Theorem

$$\begin{aligned}&\mathrm{dist}_{\mathrm{MK},2}(\tilde{W}_\hbar(R^n), \tilde{W}_\hbar(R(n\Delta t)))\\ &\leq C_T\Delta t + 2\sqrt{d\hbar}\left(1+\exp\left(\tfrac{1}{2}T(1+\max(1,\mathrm{Lip}(\nabla V)^2))\right)\right)\end{aligned}$$

from here one can also deduce a error uniform in $\hbar$

How about spatial discretization?

- The best one can do is $\Delta x = \mathcal{O}\left(\varepsilon^{1/2}\right)$

  via Gaussian beam/Gaussian wave-packet methods (*Heller '81, Popov '82, Ralston '82*)

$$\varphi^{\varepsilon}(t,x,y) = A(t,y)\,\mathrm{e}^{\mathrm{i}T(t,x,y)/\varepsilon}$$

$$T(t,x,y) = S(t,y) + p(t,y)\cdot(x-y) + \frac{1}{2}(x-y)^{\top}M(t,y)(x-y) + \mathcal{O}(x-y|^3)$$

Plug this ansatz to the Schrodinger equation and ignore higher order terms in x-y and ε

$$\frac{\mathrm{d}y}{\mathrm{d}t} = p, \qquad \frac{\mathrm{d}p}{\mathrm{d}t} = -\nabla_y V,$$

$$\frac{\mathrm{d}M}{\mathrm{d}t} = -M^2 - \nabla_y^2 V,$$

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{1}{2}|p|^2 - V, \qquad \frac{\mathrm{d}A}{\mathrm{d}t} = -\frac{1}{2}\big(\mathrm{Tr}(M)\big)A$$

Key: complex Riccati equation prevents blow-up→ no caustics!

- M is complex, and chosen to have positive definite imaginary part→ Gaussian
- Gaussian beam decomposition of initial data

Tanushev ‘08

Theorem 8.2. Let the initial data be given by

$$u_{\text{in}}^{\varepsilon}(x) = a_{\text{in}}(x)\,\mathrm{e}^{\mathrm{i}S_{\text{in}}(x)/\varepsilon},$$

with $a_{\text{in}} \in C^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ and $S_{\text{in}} \in C^3(\mathbb{R}^d)$, and define

$$\varphi^{\varepsilon}(x, y_0) = a_{\text{in}}(y_0)\,\mathrm{e}^{\mathrm{i}T(x,y_0)/\varepsilon},$$

where

$$T(x, y_0) = T_\alpha(y_0) + T_\beta \cdot (x - y_0) + \frac{1}{2}(x - y_0)^\top T_\gamma\,(x - y_0),$$
$$T_\alpha(y_0) = S_{\text{in}}(y_0), \quad T_\beta(y_0) = \nabla_x S_{\text{in}}(y_0), \quad T_\gamma(y_0) = \nabla_x^2 S_{\text{in}}(y_0) + \mathrm{i}\,\mathrm{Id}.$$

Then

$$\left\| u_{\text{in}}^{\varepsilon} - (2\pi\varepsilon)^{-d/2} \int_{\mathbb{R}^d} r_\theta(\cdot - y_0)\varphi^{\varepsilon}(\cdot, y_0)\,\mathrm{d}y_0 \right\|_{L^2} \leq C\varepsilon^{\frac{1}{2}},$$

where $r_\theta \in C_0^\infty(\mathbb{R}^d)$, $r_\theta \geq 0$ is a truncation function with $r_\theta \equiv 1$ in a ball of radius $\theta > 0$ around the origin, and C is a constant related to θ.

- One first partition the domain into subdomain with width of $\mathcal{O}(\varepsilon^{1/2})$, putting one Gaussian beam in each of these subdomains, with initial condition

$$\begin{aligned} y(0,y_0) &= y_0, \quad p(0,y_0) = \nabla_x S_{\text{in}}(y_0), \\ M(0,y_0) &= \nabla_x^2 S_{\text{in}}(y_0) + \mathrm{i}\,\mathrm{Id}, \\ S(0,y_0) &= S_{\text{in}}(y_0), \quad A(0,y_0) = a_{\text{in}}(y_0) \end{aligned}$$

  which evolves according to the Guassian beam dynamics, and in the end superimpose all the beams to form an approximate solution to the Schrodinger equation

$$u_{\text{G}}^{\varepsilon}(t,x) = (2\pi\varepsilon)^{-d/2} \int_{\mathbb{R}^d} r_\theta(x - y(t,y_0)) \varphi^{\varepsilon}(t,x,y(t,y_0))\,\mathrm{d}y_0.$$

- Need to re-initialize once the width of Gaussian beam is over $\mathcal{O}(\varepsilon^{1/2})$
- Can expand T to higher order to get higher order approximation

convergence

- Liu-Runborg-Tanushev '11

Theorem 8.4. If $u^\varepsilon(t,x)$ denotes the exact solution to the Schrödinger equation (2.1) and $u^\varepsilon_{\mathrm{G,k}}$ is the kth-order Gaussian beam superposition, then

$$\sup_{|t|<T} \|u^\varepsilon(t,\cdot) - u^\varepsilon_{\mathrm{G,k}}(t,\cdot)\| \le C(T)\varepsilon^{k/2}, \tag{8.14}$$

for any $T > 0$.

- Eulerian version: *Leung-Qian* '09, *J-Wu-Yang* '11
- Non-truncative Gaussian wave packet transform: *Russo-Smereka* '13
- (phase-space) Frozen Gaussian beams—using Gaussian with fixed width

(*Heller '81, Herman-Kluk '84, Lu-Yang '11*)

$$\psi^\varepsilon(y_0,p_0) = \int_{\mathbb{R}^d} u^\varepsilon_{\mathrm{in}}(y)\, \mathrm{e}^{-(\mathrm{i}p_0\cdot(y-y_0)-\frac{1}{2}|y-y_0|^2)/\varepsilon}\, \mathrm{d}y.$$

$$u^\varepsilon_{\mathrm{FG}}(t,x) = (2\pi\varepsilon)^{-3d/2} \iint_{\mathbb{R}^d\times\mathbb{R}^d} a(t,y_0,p_0)\psi(y_0,p_0)\, \mathrm{e}^{(\mathrm{i}p(t)\cdot(x-y(t))-\frac{1}{2}|x-y(t)|^2)/\varepsilon}\, \mathrm{d}p_0\, \mathrm{d}y_0$$

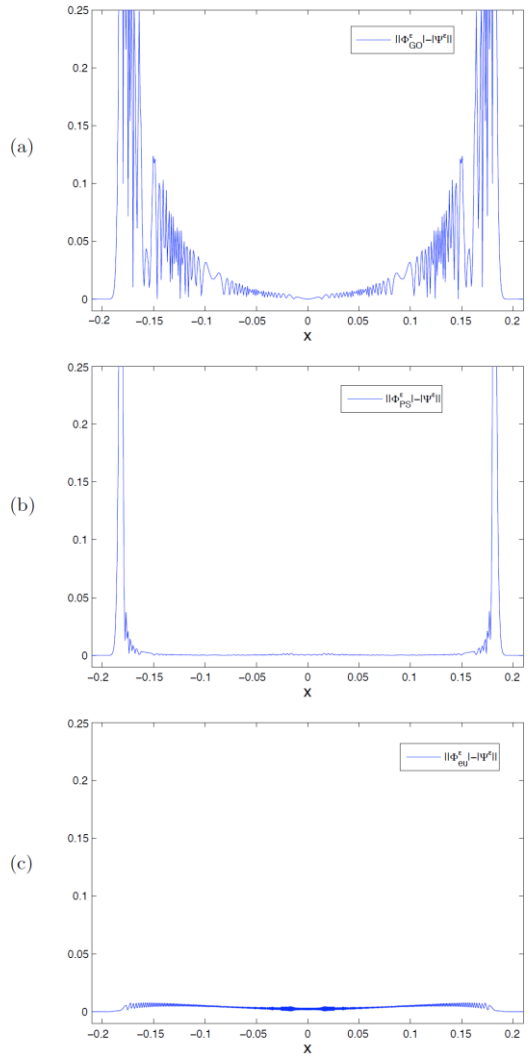


Figure 9.1. Example 9.4: numerical errors between the solution of the Schrödinger equation and (a) the geometrical optics solution, (b) the geometrical optics with phase shift built in, and (c) the Gaussian beam method. Caustics are around $x = \pm 0.18$.

From *J-Wu-Yang (CMS '08)*

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