Semiclassical computational methods for non-adiabatic quantum dynamics with uncertainty

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The prototype PDEs to be solved

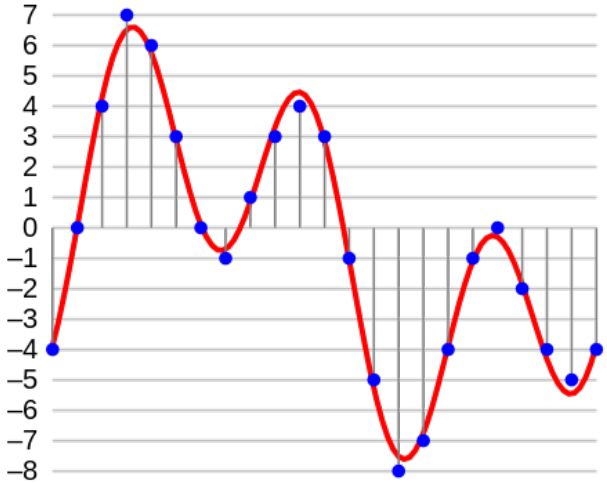
$$\partial_t u + A(x)\partial_x u + R(u) = \frac{iE(t,x)}{\varepsilon} Du + Cu, \quad u(t=0,x) = u_0(x)$$

$$A(x) = \begin{pmatrix} a_1(x) & 0 \\ 0 & a_2(x) \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}, \quad C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$$

- Systems of linear transport equations with oscillatory forces or initial data
- The system is coupled through the force
- Part of the force simulates the (non-adiabatic) phase information;
- The interaction term resembles the Berry connection in quantum dynamics
- Random uncertainty in band-gap, or initial data
- Solutions highly oscillatory in space, time and uncertainty variables

Computational difficulty

- 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

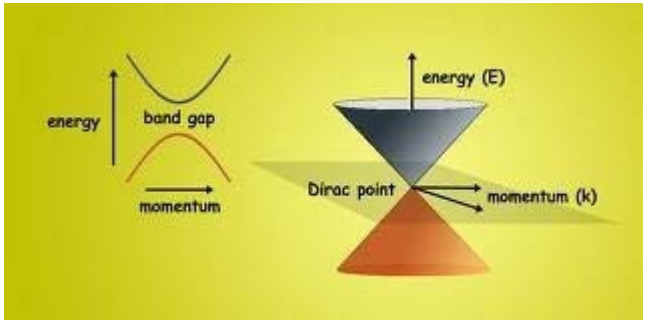
Goal

develop schemes that can get the correct (pointwise) solutions without resolving the oscillations and the numerical schemes converge uniformly in \epsilon

-- defies the Nyquist-Shannon sampling restriction in certain degree

Motivation:
Band crossings: non-adiabatic qunatum phenomena

Inter-band transition is a general quantum mechanical Phenomenon; it causes difficulties in semi-classical approximations



- Born-Oppenheimer approximation: non-adiabatic surface hopping
- Bloch decomposition in quantum dynamic with periodic potentials: crossing of Bloch bands or influence of external potentials
- elastic and electromagnetic waves with polarization effect
- Graphene: coupling of different bands near the Dirac point; effect of electric potential
- In this talk we concentrate on surface hopping

The N-body Schrodinger equation

$$i\hbar\partial_t \Phi(t, \mathbf{x}, \mathbf{y}) = H\Phi(t, \mathbf{x}, \mathbf{y}),$$
$$\Phi(0, \mathbf{x}, \mathbf{y}) = \Phi_0(\mathbf{x}, \mathbf{y}).$$

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

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

Dimension curse: 75 dimension for CO2; 162 dimension for benzene

The Born-Oppenheimer approximation


- After non-dimensionlization:

$$i\varepsilon\partial_t\Phi(t,\mathbf{x},\mathbf{y}) = -\sum_{j=1}^{N}\frac{\varepsilon^2}{2}\Delta_{x_j}\Phi(t,\mathbf{x},\mathbf{y}) + H_e(\mathbf{y},\mathbf{x})\Phi(t,\mathbf{x},\mathbf{y}).$$

Where $\varepsilon = \sqrt{\frac{m}{M}}$ is typically between 0.01 and 0.1

- First solve an electronic eigenvalue problem (DFT, etc.)

$$H_e(\mathbf{y},\mathbf{x})\varphi_k(\mathbf{y};\mathbf{x}) = E_k(\mathbf{x})\varphi_k(\mathbf{y};\mathbf{x}) \quad \forall \mathbf{x}\in\mathbb{R}^N,\ k=1,2,\ldots.$$

$$\int_{-\infty}^{\infty}\varphi_i^*(\mathbf{y};\mathbf{x})\varphi_j(\mathbf{y};\mathbf{x})d\mathbf{y} \equiv \langle\varphi_i(\mathbf{y};\mathbf{x})|\varphi_j(\mathbf{y};\mathbf{x})\rangle_{\mathbf{y}} = \delta_{ij},$$

The nucleonic Schrodinger equation

- Project to the electronic eigenspace:

$$\Phi(t,\mathbf{x},\mathbf{y}) = \sum_k \chi_k(t,\mathbf{x})\varphi_k(\mathbf{y};\mathbf{x}).$$

$$i\varepsilon\frac{\partial}{\partial t}\chi_k(t,\mathbf{x}) = \left[-\sum_{j=1}^{N}\frac{\varepsilon^2}{2}\Delta_{x_j} + E_k(\mathbf{x})\right]\chi_k(t,\mathbf{x}) + \sum_l C_{kl}\chi_l(t,\mathbf{x}),$$

- where $$C_{kl} \equiv \left\langle \varphi_k \middle| -\sum_{j=1}^{N}\frac{\varepsilon^2}{2}\Delta_{x_j}\varphi_l \right\rangle_{\mathbf{y}} - \sum_{j=1}^{N}\varepsilon^2\langle\varphi_k|\nabla_{x_j}\varphi_l\rangle_{\mathbf{y}}\cdot\nabla_{x_j}$$

describe inter-band transitions which are associated with chemical reaction such as charge transfer, photoisomerization, or photodissociation, etc.

The B-O (or adiabatic) approximation

- Assume $\{E_k(\mathbf{x})\}$ are well separated (adiabatic):

  then one can ignore C_{kl} to obtain:

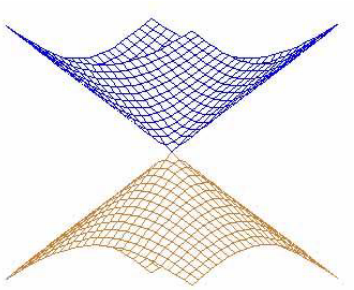
$$i\varepsilon\frac{\partial}{\partial t}\chi_k(t,\mathbf{x}) = \left[-\sum_{j=1}^{N}\frac{\varepsilon^2}{2}\Delta_{x_j} + E_k(\mathbf{x})\right]\chi_k(t,\mathbf{x})$$

Then the classical limit $\varepsilon \to 0$ can be taken easily.

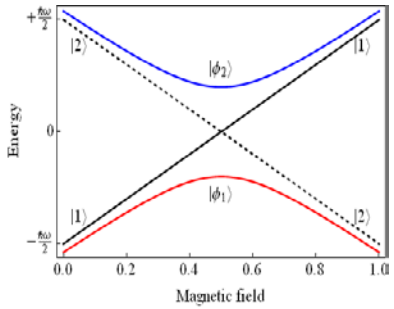
- Mathematical study of the adiabatic B-O approximation and band crossing: Gerard, Hagedorn, Lasser, Spohn, Teufel, Fermanian…
- However, when $\{E_k(\mathbf{x})\}$ are not well-separated, one cannot ignore C_{kl} since the non-adiabatic quantum transition is significant. Then the B-O approximation breaks down and one needs improved models

Transition between electronic states

conical crossing



avoided crossing



The Landau-Zener formula

The **Landau–Zener formula** is an analytic solution to the equations of motion governing the transition dynamics of a 2-level quantum mechanical system, with a time-dependent Hamiltonian varying such that the energy separation of the two states is a linear function of time. The formula, giving the probability of a diabatic (not adiabatic) transition between the two energy states, was published separately by Lev Landau, Clarence Zener, Ernst Stueckelberg, and Ettore Majorana, in 1932 (from Wikipedia)

The surface hopping method (Tully ‘71)

- Particles follow the classical trajectory determined by the classical Hamiltonian; at crossing region they “hop” with transition probability to different energy level (Hamiltonian system for different potential surfaces)
- A Monte-Carlo procedure; or particle splitting

- It does not give correct discription of interference (for example when two particles arrive in the hopping points at the same time)

A two-level nucleonic Schrodinger system

$$i\varepsilon\partial_t\psi^\varepsilon(t,\mathbf{x}) = \left(-\frac{\varepsilon^2}{2}\Delta_{\mathbf{x}} + V(\mathbf{x})\right)\psi^\varepsilon(t,\mathbf{x}), \quad (t,\mathbf{x}) \in \mathbb{R}^+ \times \mathbb{R}^2,$$

$$V(\mathbf{x}) = \frac{1}{2}\mathrm{tr}V(\mathbf{x}) + \begin{pmatrix} v_1(\mathbf{x}) & v_2(\mathbf{x}) \\ v_2(\mathbf{x}) & -v_1(\mathbf{x}) \end{pmatrix}$$

The Hamiltonian is given by $H = -\frac{\varepsilon^2}{2}\Delta_{\mathbf{x}} + V(\mathbf{x})$. The dimensionless semiclassical parameter $\varepsilon > 0$ is given by $\varepsilon = \sqrt{\frac{m}{M}}$, where m and M are the masses of an electron and a nucleus, respectively. Then, all oscillations are roughly characterized by the frequency $1/\varepsilon$, which typically ranges between 100 and 1,000. Hereafter, we will treat ε as a small parameter and discuss the semiclassical limit of the Schrödinger equations (12) and (13).

The potential $V(\mathbf{x})$ has eigenvalues $\lambda^{(\pm)} = \mathrm{tr}V(\mathbf{x}) \pm \sqrt{v_1(\mathbf{x})^2 + v_2(\mathbf{x})^2}$. Two energy levels are called *crossing at a point* $\mathbf{x}_* \in \mathbb{R}^2$ if $\lambda^+(\mathbf{x}_*) = \lambda^-(\mathbf{x}_*)$. Such a crossing is called *conical* if the vectors $\nabla_{\mathbf{x}} v_1(\mathbf{x}_*)$ and $\nabla_{\mathbf{x}} v_2(\mathbf{x}_*)$ are linearly independent. If all the crossings are conical, the crossing set $S = \{\mathbf{x} \in \mathbb{R}^2 | \lambda^+(\mathbf{x}) = \lambda^-(\mathbf{x})\}$ is a submanifold of *codimension two* in $\mathbb{R}^2$ [11].

The Wigner transform

$$W^{\varepsilon}(\psi^{\varepsilon})(\mathbf{x},\mathbf{k}) = (2\pi)^{-2}\int_{\mathbb{R}^2} e^{i\mathbf{y}\cdot\mathbf{k}}\psi^{\varepsilon}\left(\mathbf{x}-\frac{\varepsilon}{2}\mathbf{y}\right)\otimes\bar{\psi}^{\epsilon}(\mathbf{x}+\frac{\varepsilon}{2}\mathbf{y})d\mathbf{y}$$

$$\lim_{\varepsilon\to 0} W^{\varepsilon}(t,\mathbf{x},\mathbf{k}) \rightharpoonup u(t,\mathbf{x},\mathbf{k}),$$

which is called the *Wigner measure* or *semiclassical measure*. We now precisely describe this limit.

First, for the Schrödinger equation (12), the complex 2×2 matrix-valued symbol is given by

$$P(\mathbf{x},\mathbf{k}) = \frac{i}{2}|\mathbf{k}|^2 + iV(\mathbf{x}),$$

where $\mathbf{k}$ is the conjugate variable to the position variable $\mathbf{x}$. The two eigenvalues of $-iP(\mathbf{x},\mathbf{k})$ are

$$\lambda_1(\mathbf{x},\mathbf{k}) = \frac{|\mathbf{k}|^2}{2} + \mathrm{tr}V(\mathbf{x}) + \sqrt{v_1(\mathbf{x})^2+v_2(\mathbf{x})^2},$$

and

$$\lambda_2(\mathbf{x},\mathbf{k}) = \frac{|\mathbf{k}|^2}{2} + \mathrm{tr}V(\mathbf{x}) - \sqrt{v_1(\mathbf{x})^2+v_2(\mathbf{x})^2}.$$

Semiclassical limit (adiabatic case)

For $(\mathbf{x},\mathbf{k}) \in \Omega$, we denote by $\chi_\tau(\mathbf{x},\mathbf{k})$ the column eigenvector corresponding to the eigenvalue $\lambda_\tau(\mathbf{x},\mathbf{k})$ and the matrix $\Pi_\tau(\mathbf{x},\mathbf{k}) = \chi_\tau(\mathbf{x},\mathbf{k})(\chi_\tau(\mathbf{x},\mathbf{k}))^T$ is the orthogonal projection onto the eigenspace associated to $\lambda_\tau(\mathbf{x},\mathbf{k})$.

By Theorem 6.1 of [8], outside the crossing set S, the Wigner measure $u(t,\cdot)$ commutes with the projectors Π_τ and thus can be decomposed as

$$u(t,\cdot) = \Pi_1 u(t,\cdot)\Pi_1 + \Pi_2 u(t,\cdot)\Pi_2.$$

Since the eigenspaces are one-dimensional, the decomposition is simplified to be

$$u(t,\cdot) = u_1(t,\cdot)\Pi_1 + u_2(t,\cdot)\Pi_2,$$

where the scalar function $u_\tau(t,\mathbf{x},\mathbf{k})$, determined by projection

$$u_\tau(t,\mathbf{x},\mathbf{k}) = \mathrm{tr}(\Pi_\tau u(t,\mathbf{x},\mathbf{k}))$$

$$\partial_t u_\tau + \nabla_{\mathbf{k}}\lambda_\tau \cdot \nabla_{\mathbf{x}} u_\tau - \nabla_{\mathbf{x}}\lambda_\tau \cdot \nabla_{\mathbf{k}} u_\tau = 0,$$

- Lions-Paul, Gerard-Markowich-Mauser-Poupaud, Keller-Papanicolaou-Ryzhik, …

The Landau Zener transition probability

- This analysis is not valid at hopping point thus cannot handle interband transtion.
- The Landau-Zener probability of transition between the two bands:

$$T(\mathbf{x}_0, \mathbf{k}_0) = \exp\left(-\frac{\pi}{\varepsilon}\frac{(\mathbf{v}(\mathbf{x}_0) \wedge \nabla_{\mathbf{x}}\mathbf{v}(\mathbf{x}_0)\mathbf{k}_0)^2}{|\nabla_{\mathbf{x}}\mathbf{v}(\mathbf{x}_0)\mathbf{k}_0|^3}\right)$$

- Even by incorporating the Landau-Zener probability (surface hopping method) it still does not decribe correctly the interference (Berry connection, Berry phase, etc.

A semiclassical model for avoided crossing (Chai-Li-Jin-Morandi, MMS 2014)

- The surface hopping algorithm does not account for phase information, thus cannot handle resonance, and dynamic phase factor such as Berry phase, Berry connection etc. when two wave packets arrive at the crossing points at the same time from different bands (related to quantum hall effect)

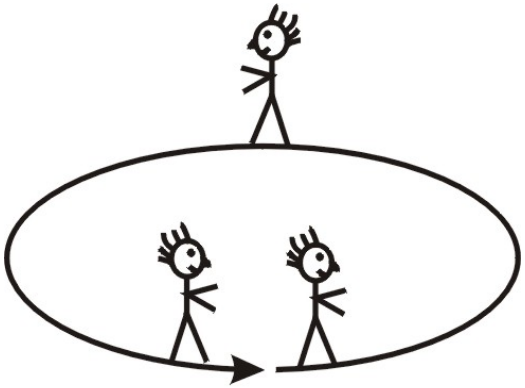


Abb. 1: Der "klassische" Mensch.

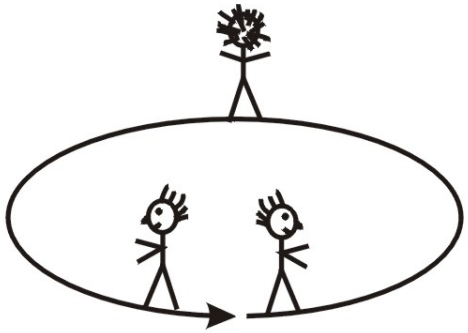
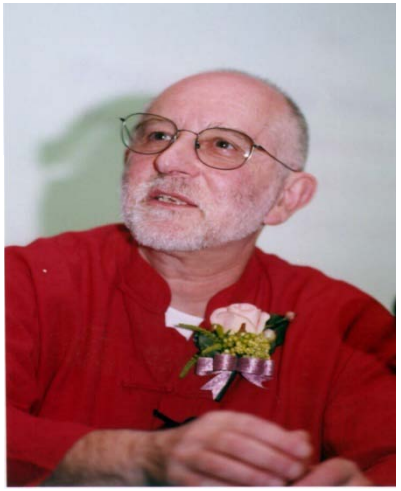


Abb. 2: Der "quantenmechanische" Mensch.

http://www.teilchen.at/kdm/45



Sir Michael Berry

The main idea: evolve the entire Wigner matrix semiclassically

- The previous model only keeps track of the "diagonal terms" of the Wigner matrix corresponding to the projection onto the two eigenspaces of the Hamiltonian
- But the off-diagonal term contains important inter-band transition information that should not be ignored

The semiclassical model

- Via the Wigner transform and the Weyl quantization, we expand the Wigner equation in ε to obtain the following asymptotic model after ignoring $O(\varepsilon^2)$ terms

$$\frac{\partial f^+}{\partial t} = -\boldsymbol{p}\cdot\nabla_{\boldsymbol{x}} f^+ + \nabla_{\boldsymbol{x}}(U+E)\cdot\nabla_{\boldsymbol{p}} f^+ + \bar{b}^i f^i + b^i \overline{f^i},$$

$$\frac{\partial f^-}{\partial t} = -\boldsymbol{p}\cdot\nabla_{\boldsymbol{x}} f^- + \nabla_{\boldsymbol{x}}(U-E)\cdot\nabla_{\boldsymbol{p}} f^- - \bar{b}^i f^i - b^i \overline{f^i},$$

$$\frac{\partial f^i}{\partial t} = -\boldsymbol{p}\cdot\nabla_{\boldsymbol{x}} f^i + \nabla_{\boldsymbol{x}} U\cdot\nabla_{\boldsymbol{p}} f^i + b^i(f^- - f^+) + (b^+ - b^-) f^i + \frac{2E}{\mathrm{i}\varepsilon} f^i$$

- It is a system of Liouville equations (thus hyperbolic) with oscillatory forcing terms that describe inter-band transitions
- The coefficients of f^i : $(b^+(\boldsymbol{x}(t)) - b^-(\boldsymbol{x}(t))) - \frac{2\mathrm{i}}{\varepsilon} E(\boldsymbol{x}(t))$

  are exactly the time derivative of the Berry phase

Classical approaches for oscillations

- No known numerical methods that can defy Shanon's Sampling System for both time and space oscillations
- Classical appraoches:

  geometric optics/WKB: not good after caustics

  multivalued solution (Sparber-Markowich-Mauser) : cannot handle quantum interference

  Gaussian beam/wavepackets $\Delta x, \Delta t = O(\sqrt{\varepsilon})$.

  these methods also don not work for large ε

Review: Jin-Markowich-Sparber, Mathematical and Computational Methods for Semiclassical Schrodinger equations, ***Acta Numerica***, 2011

Our idea

- Consider a toy problem

$$\partial_t u + A(x)\partial_x u + R(u) = \frac{iE(t,x)}{\varepsilon} Du + Cu, \quad u(t=0,x) = u_0(x)$$

$$A(x) = \begin{pmatrix} a_1(x) & 0 \\ 0 & a_2(x) \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}, \quad C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$$

- Use a nonlinear geometric optics (NGO) ansatz

$$U(t,x,S(t,x)/\varepsilon) = u(t,x).$$

Keller, Diperna, Majda, Rauch, Joyt, etc. 80-90): Mathematical theory, no one uses it for computation

$$\partial_t S + a_2 \partial_x S = E, \quad S(0,x) = 0,$$

$$\partial_t U_1 + a_1 \partial_x U_1 + \frac{1}{\varepsilon}[(a_1 - a_2)\partial_x S + E]\partial_\tau U_1 + R_1(U_1, U_2) = C_{11}U_1 + C_{12}U_2,$$

$$\partial_t U_2 + a_2 \partial_x U_2 + R_2(U_1, U_2) = -\frac{E}{\varepsilon}[\partial_\tau U_2 + iU_2] + C_{21}U_1 + C_{22}U_2.$$

Setting $V_2 = e^{i\tau}U_2$, we finally obtain

$$\begin{cases} \partial_t U_1 + a_1 \partial_x U_1 + R_1(U_1, e^{-i\tau}V_2) - C_{11}U_1 - C_{12}e^{-i\tau}V_2 = -\dfrac{1}{\varepsilon}[E + (a_1 - a_2)\partial_x S]\partial_\tau U_1, \\ \\ \partial_t V_2 + a_2 \partial_x V_2 + e^{i\tau}R_2(U_1, e^{-i\tau}V_2) - C_{21}e^{i\tau}U_1 - C_{22}V_2 = -\dfrac{E}{\varepsilon}\partial_\tau V_2. \end{cases}$$

- Unlike in geometric optics, no caustics, phase equation is linear, do not throw away terms: uniformly accurate in epsilon
- Choose initial data such that (Kreiss ‘80, Croseilles-Lemou-Mehat ‘13) (for time oscillations)
- 1) match the initial data of f
- 2) solution is smooth (up to second order in epsilon)

- Using Chapman-Enskog expansion for the equation:

$$U_1(t,x,\tau) = U_1^0(t,x) + \frac{i\varepsilon C_{12} e^{-i\tau}}{E(t,x) + (a_1(x) - a_2(x))\partial_x S(t,x)} V_2^0(t,x) + O(\varepsilon^2)$$

$$U_2(t,x,\tau) = V_2^0(t,x) e^{-i\tau} - \frac{i\varepsilon C_{21}}{E(t,x)} U_1^0(t,x) + O(\varepsilon^2).$$

- Ignore the $O(\varepsilon^2)$ term and then match the initial condition

$$\begin{cases} U_1(0,x,\tau) = f_1^{in} + \dfrac{i\varepsilon E C_{12}}{E^2 - \varepsilon^2 C_{12} C_{21}} \left(e^{-i\tau} - 1\right) f_2^{in}, \\ \\ U_2(0,x,\tau) = \dfrac{i\varepsilon E C_{21}}{E^2 - \varepsilon^2 C_{12} C_{21}} \left(e^{-i\tau} - 1\right) f_1^{in} + e^{-i\tau} f_2^{in} \end{cases}$$

- Spectral approximation in τ (due to periodicity of solution in τ) and upwind type finite difference approximations
- Interpolation to get u from U
- We can prove that U and u has the same limit and the method converges strongly in maximum norm (first order in space and time) uniformly in ε
- Same strategy applied to the two band semiclassical model for surface hopping

$$\partial_t f^+ + p\cdot\nabla_x f^+ - \nabla_x(U+E)\cdot\nabla_p f^+ = \overline{b}^i f^i + b^i\overline{f}^i,$$
$$\partial_t f^- + p\cdot\nabla_x f^- - \nabla_x(U-E)\cdot\nabla_p f^- = -\overline{b}^i f^i - b^i\overline{f}^i,$$
$$\partial_t f^i + p\cdot\nabla_x f^i + \nabla_x U\cdot\nabla_p f^i = -i\frac{2E}{\varepsilon} f^i + b^i(f^- - f^+) + (b^+ - b^-)f^i$$

Numerical examples

- Underresolved time oscillations

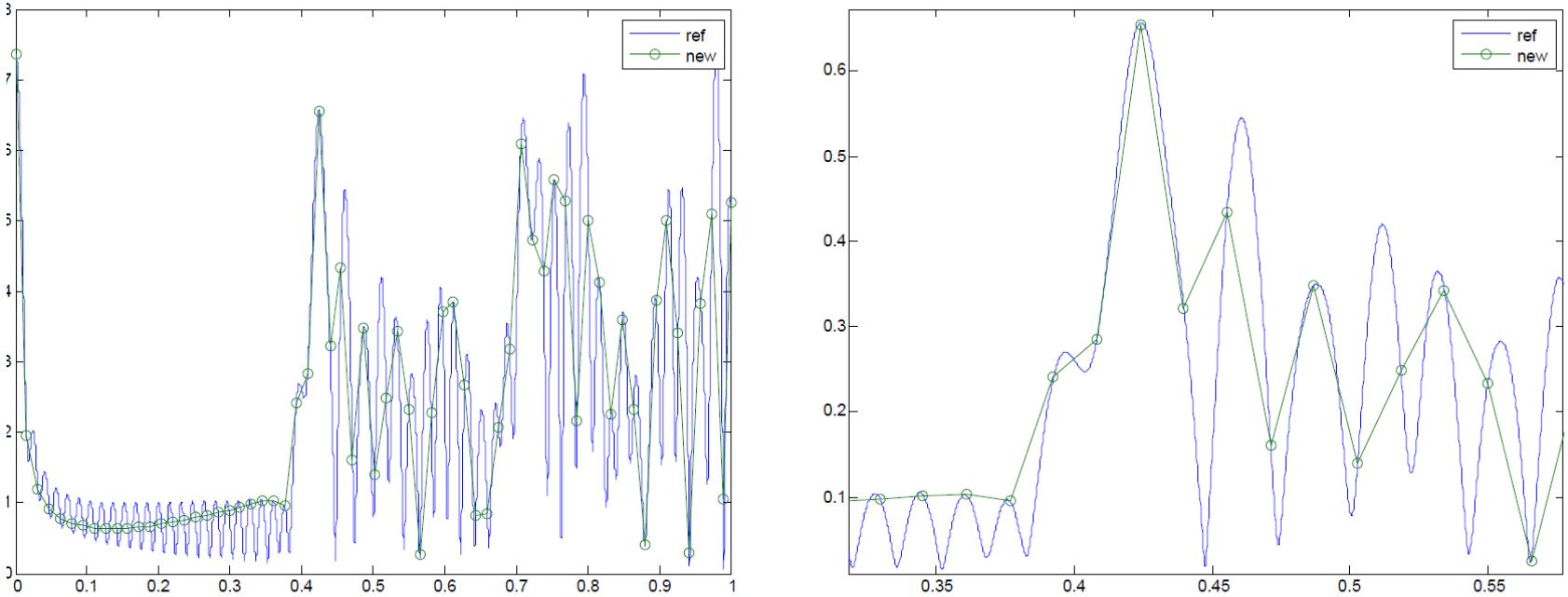
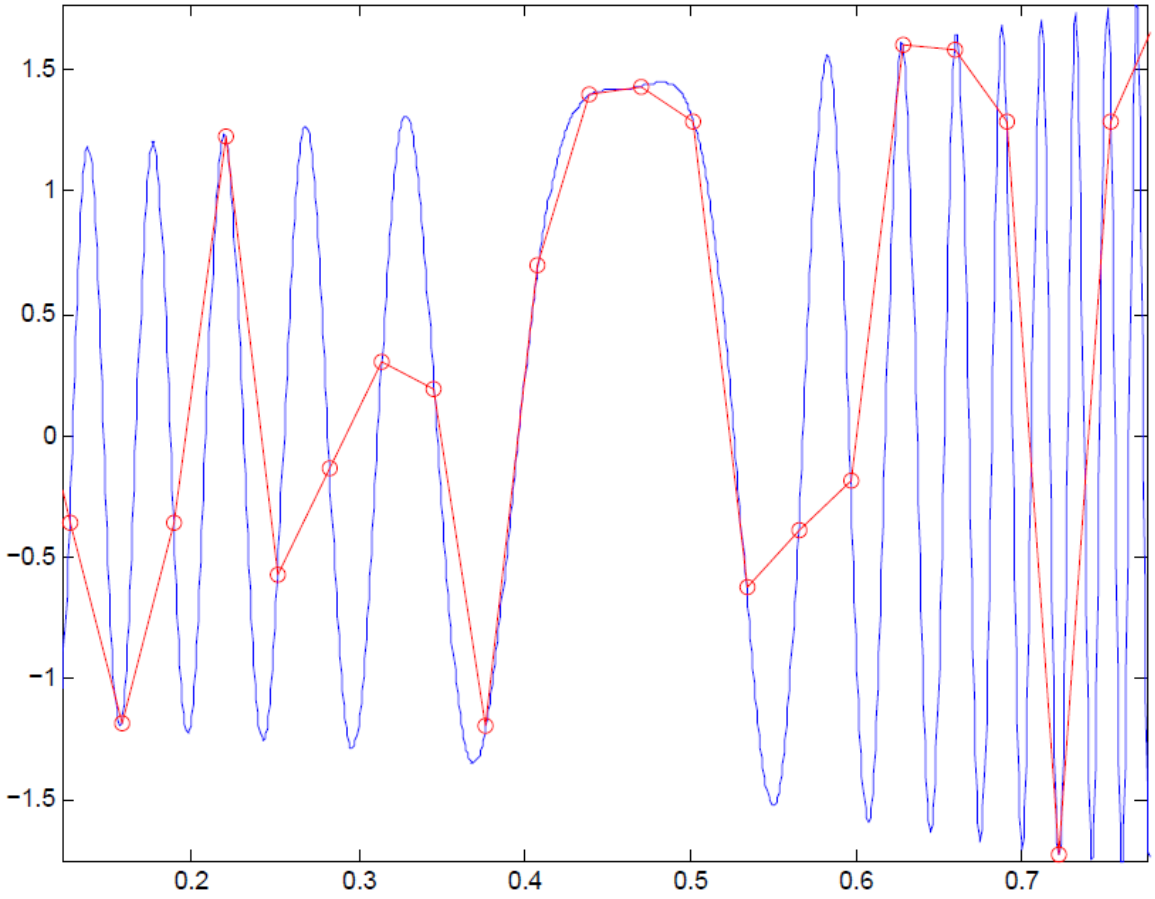


Figure 8: Time history of $\mathcal{R}$. Comparison between a reference solution and the solution of the new method (*with* initial correction and exact computation for S), for $\varepsilon = 5 \cdot 10^{-3}$, $t_f = 1$. The right part is a zoom of the left part.

Underresolved spatial oscillations



- We are defying Shanon's Sampling Theorem in both time and space!

Uncertainty in oscillatory coefficients

$$\partial_t u + c(x)\partial_x u + r(u) = \frac{ia(x,\mathbf{z})}{\varepsilon}u, \qquad u(0,x,\mathbf{z}) = u_{in}(x,\mathbf{z})$$

- a(x,z) arises in potential energy surface which are obtained by empirical laws or numerical approximations thus usually are uncertain
- z random variable with a given PDF
- Solving directly: for constant c, analytic solution is

$$u(t,x,\mathbf{z}) = e^{\frac{ia(\mathbf{z})}{\varepsilon}t}u_{in}(x-ct,\mathbf{z})$$

$$\partial_{\mathbf{z}}^q u = O(1/\varepsilon^q)$$

Generalized polynomial chaos (gPC) approach

- The PC or generalized PC (gPC) approach first introduced by Wiener, followed by Cameron-Martin, and generalized by Ghanem and Spanos, Xiu and Karniadakis etc. has been shown to be very efficient in many UQ applications when the solution has enough regularity in the random variable
- Let z be a random variable with pdf $\rho(z) > 0$
- Let $\Phi_m(z)$ be the orthonormal polynomials of degree m corresponding to the weight $\rho(z) > 0$

$$\int \Phi_i(z)\Phi_j(z)\rho(z)\,dz = \delta_{ij}$$

The Wiener-Askey polynomial chaos for random variables (table from Xiu-Karniadakis SISC 2002)

	Random variables ζ	Wiener-Askey chaos $\{\Phi(\zeta)\}$	Support
Continuous	Gaussian	Hermite-Chaos	$(-\infty, \infty)$
	Gamma	Laguerre-Chaos	$[0, \infty)$
	Beta	Jacobi-Chaos	$[a, b]$
	Uniform	Legendre-Chaos	$[a, b]$
Discrete	Poisson	Charlier-Chaos	$\{0, 1, 2, \dots\}$
	Binomial	Krawtchouk-Chaos	$\{0, 1, \dots, N\}$
	Negative Binomial	Meixner-Chaos	$\{0, 1, 2, \dots\}$
	Hypergeometric	Hahn-Chaos	$\{0, 1, \dots, N\}$

TABLE 4.1

The correspondence of the type of Wiener-Askey polynomial chaos and their underlying random variables ($N \geq 0$ is a finite integer).

Generalized polynomial chaos stochastic Galerkin (gPC-sG) methods

- Take an orthonormal polynomial basis $\{\Phi_j(z)\}$ in the random space
- Expand functions into Fourier series and truncate:

$$f(z) = \sum_{j=0}^{\infty} f_j \phi_j(z) \approx \sum_{j=0}^{K} f_j \phi_j(z) := f^K(z).$$

- Substitute into system, Galerkin projection. Then one gets a deterministic system of the gPC coefficients $(f_0, \ldots, f_K)$

Accuracy and efficiency

- We will consider the gPC-stochastic Galerkin (gPC-SG) method
- Under suitable regularity assumptions this method has a spectral accuracy
- Much more efficient than Monte-Carlo samplings (halfth-order)

How about NGO-gPC?

$$\partial_t V + c(x)\partial_x V + e^{-i\tau} r(e^{i\tau} V) = -\frac{a(x, \mathbf{z})}{\varepsilon}\partial_\tau V$$

- The l-th derivative in z satisfies almost the sameequation as the l-th derivative in x, so the z-regularity is the same as the x-regularity (smooth only to second order)

  ➔ no spectral accuracy!

Our new idea

$$V(t,x,\mathbf{z},\tau) = W(S(t,x,\mathbf{z}),x,\mathbf{z},\tau), \tag{2.33}$$

where S solves (2.20). Then, W is the solution to the following problem:

$$\begin{aligned}
&\partial_s W + \frac{c}{a(x,\mathbf{z})}\partial_x W + \frac{1}{a(x,\mathbf{z})}e^{-i\tau}r(e^{i\tau}W) = -\frac{1}{\varepsilon}\partial_\tau W,\\
&W(0,x,\mathbf{z},\tau) = V(0,x,\mathbf{z},\tau) = u_{in}(x,\mathbf{z}) + \frac{\varepsilon}{a(x,\mathbf{z})}\Big[\mathcal{G}(0,u_{in},\mathbf{z}) - \mathcal{G}(\tau,u_{in},\mathbf{z})\Big],\\
&\text{with } \mathcal{G}(\tau,u_{in},\mathbf{z}) = \mathcal{L}^{-1}(\mathcal{I}-\Pi)[e^{-i\tau}r(e^{i\tau}u_{in}(x,\mathbf{z}))]\,.
\end{aligned} \tag{2.34}$$

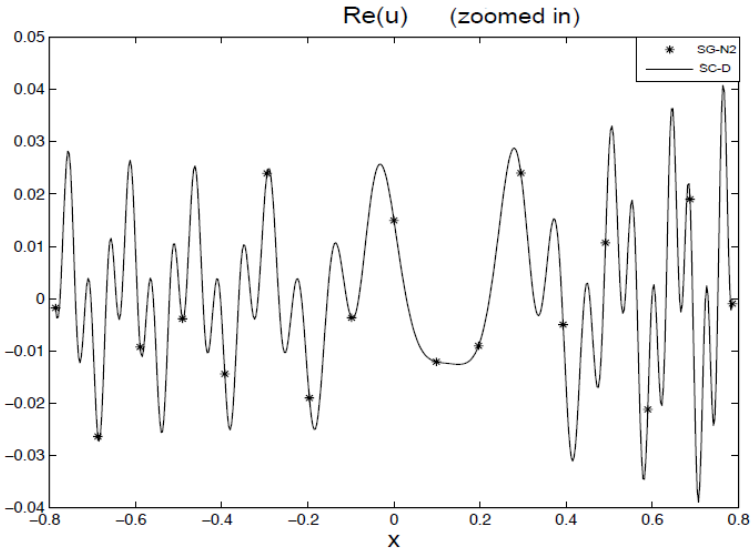
Uniform regularity in x and z!

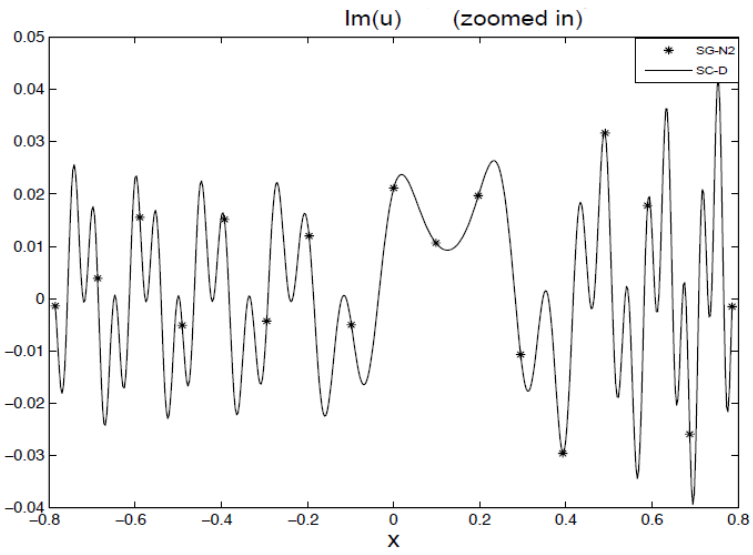
Proposition 2.1 *Let W be the solution of (2.34) on $[0,\bar{T}]$, $\bar{T}>0$, with periodic boundary condition in x and τ. Then, up to the second order derivative in s, and arbitrary order in x and $\mathbf{z}$ derivatives of W are bounded uniformly in $\varepsilon \in [0,1]$, that is, $\exists C>0$ independent of ε such that, $\forall s \in [0,\bar{T}]$*

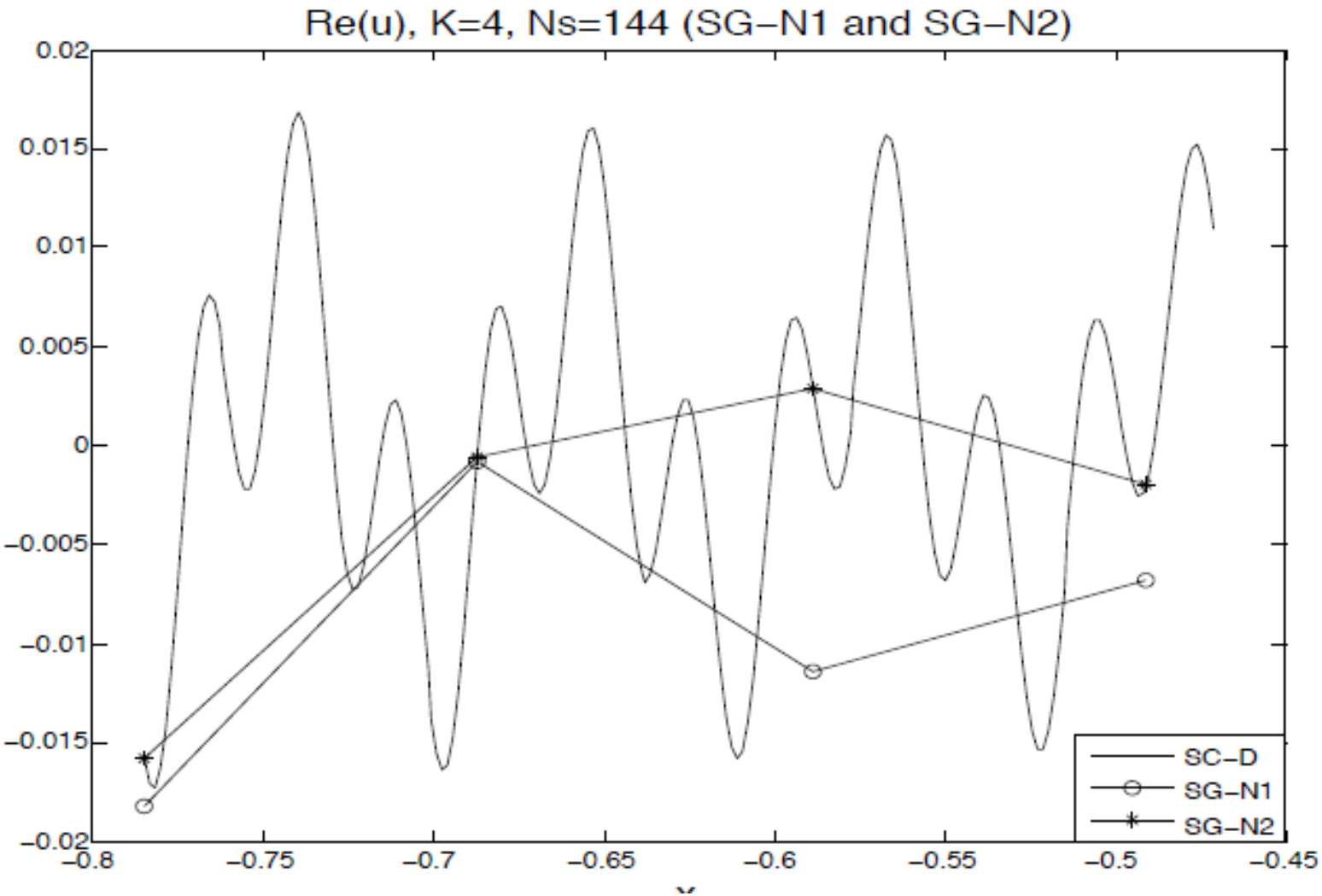
$$\|\partial_s^p \partial_x^q \partial_{\mathbf{z}}^r W(s)\|_{L^\infty_{\tau,x}(L^2(\pi(\mathbf{z})d\mathbf{z}))} \leq C, \quad for \quad p=0,1,2, \quad and \quad q,r \in \mathbb{N}.$$

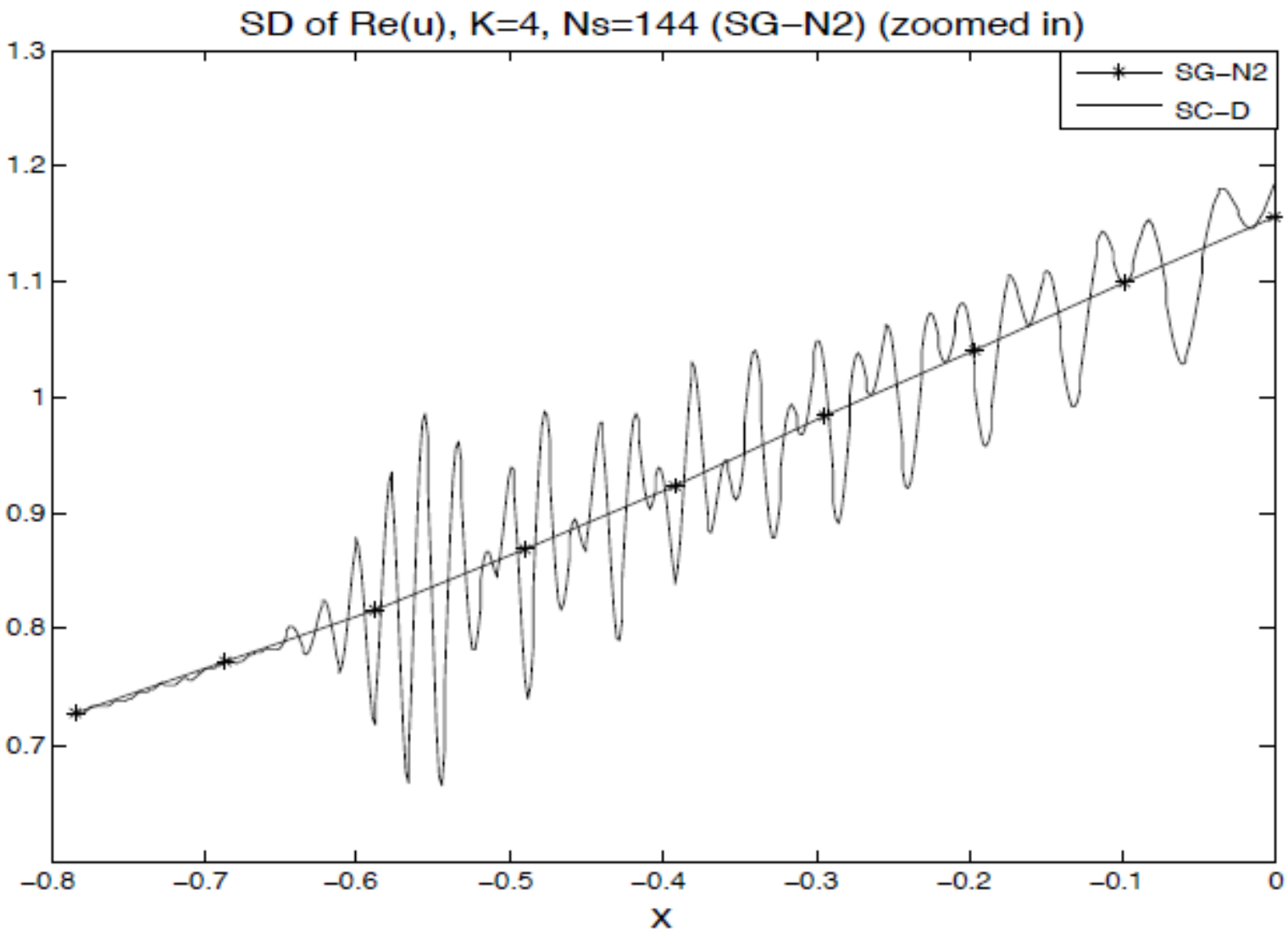
- This implies we can get a scheme of arbitrary high order accuracy in x and z, uniformly in ε

$$||W - \sum_{j=1}^{K} \tilde{W}_j \tilde{\psi}_j||_{L^2(\pi(\mathbf{z})d\mathbf{z})} \leq \frac{C}{K^q}, \quad \forall q \text{ positive integer},$$


Re(u) (zoomed in)
SG-N2
SC-D
0.05
0.04
0.03
0.02
0.01
0
−0.01
−0.02
−0.03
−0.04
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
x


Im(u) (zoomed in)
SG-N2
SC-D
0.05
0.04
0.03
0.02
0.01
0
−0.01
−0.02
−0.03
−0.04
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
x


Re(u), K=4, Ns=144 (SG−N1 and SG−N2)
0.02
0.015
0.01
0.005
0
−0.005
−0.01
−0.015
−0.02
−0.8
−0.75
−0.7
−0.65
−0.6
−0.55
−0.5
−0.45
SC−D
SG−N1
SG−N2


SD of Re(u), K=4, Ns=144 (SG−N2) (zoomed in)
SG−N2
SC−D
1.3
1.2
1.1
1
0.9
0.8
0.7
−0.8
−0.7
−0.6
−0.5
−0.4
−0.3
−0.2
−0.1
0
x

Some comments

- All numerical parameters (mesh size, time step, polynomial degrees) made independent of the wave length
- The method works for oscillatory source term or oscillatory initial data, not both
- If one needs more details of quantum transition near the crossing zone one should use smaller mesh size near the crossing zone: local mesh refinement. Since the scheme is uniformly accurate in ε, this can be done quite easily
- To recover the oscillations, one can use different coarse mesh points in different—but parallel—runs and then rebuild the oscillatory curve—this makes highly oscillatory computations possible
- Same approach works for crossing of Bloch band for Schrodinger equation with periodic potentials and graphene modeling
- More theoretical study and numerical experiments are needed but so far the preliminary results look very promising