

My research interest lies in kinetic approaches for multiscale physical systems including applications in seismic wave propagation and inversion, spin-transfer torque in micro-magnetics, and quantum tunneling in quantum chemistry and solid-state physics. The main tools that have been used in my research are the (frozen) Gaussian approximation, the Wigner transform and parallel computing. I will discuss these topics at a deeper depth in the following sections.

### Frozen Gaussian Approximation for 3-D Seismic Tomography

Three-dimensional (3-D) wave-equation-based seismic tomography is computationally challenging in large scales and high-frequency regime. We present a systematic introduction on applying frozen Gaussian approximation (FGA) to compute high-frequency sensitivity kernels for adjoint tomography in 3-D earth models. FGA approximates seismic wavefield by a summation of frozen (fixed-width) Gaussian wave-packets propagating along ray paths. One can use a relatively small number of Gaussians to get accurate approximations of high-frequency wavefield. Meanwhile, FGA algorithm can be perfectly parallelized, which speeds up the computation drastically with a high-performance computing station. In order to apply FGA to the computation of 3-D high-frequency seismic tomography, first, we reformulate the FGA so that one can efficiently compute the Green's functions whose convolutions with source time function produce wavefields needed for the construction of 3-D kernels; and second, we incorporate the Snell's law into the FGA formulation, and asymptotically derive reflection, transmission and free surface conditions for FGA to compute high-frequency seismic wave propagation in high contrast media. One paper in presenting these results has been published in *Geophys. J. Int.* [11].

The scalar wave equation arising from seismic wave propagation takes the form of

$$\partial_t^2 u - c^2(\mathbf{x})\Delta u = s^k(t)\delta(\mathbf{x} - \mathbf{x}_s), \quad (1)$$

where  $c(\mathbf{x})$  is sound speed,  $s^k$  is source time function to model an earthquake event,  $\delta$  is the Dirac delta function, and the wave number  $k \gg 1$  indicates that we are considering seismic wave propagation of high-frequency (corresponding to short wavelengths). The original FGA formulation is used to approximate the initial value problem of (1) in the homogeneous case ( $s^k \equiv 0$ ) by the following integral,

$$u_F^k(t, \mathbf{x}) = \sum_{\pm} \iint \frac{a_{\pm}}{(2\pi/k)^{9/2}} e^{ik\mathbf{P}_{\pm} \cdot (\mathbf{x} - \mathbf{Q}_{\pm}) - \frac{k}{2}|\mathbf{x} - \mathbf{Q}_{\pm}|^2} d\mathbf{q} d\mathbf{p}, \quad (2)$$

where we have used superscripts “+” and “-” to indicate two wave branches respectively, and the Gaussian center  $\mathbf{Q}_{\pm}(t, \mathbf{q}, \mathbf{p})$  and  $\mathbf{P}_{\pm}(t, \mathbf{q}, \mathbf{p})$  and the amplitude  $a_{\pm}(t)$  satisfy a system of uncoupled ODEs [16]. In practice, we should consider an inhomogeneous problem with a non-vanishing source time function. To achieve this we first get a finite frequency approximation  $G_F^k$  of the Green's function of (1) by solving (1) with initial conditions  $u(0, \mathbf{x}) = 0$  and  $\partial_t u(0, \mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_s)$  using FGA, and then we convolve  $G_F^k$  with the source time function  $s^k$  to get the approximation of the wavefields.

Development of efficient and accurate methods is constantly necessary to improve the modeling of seismic wave propagation in different situations, especially in complex media with high contrast heterogeneity. When waves hit the interface where the wave speed  $c(\mathbf{x})$  is discontinuous, proper interface conditions should be incorporated in the FGA formulation to capture reflected and transmitted waves. To overcome this difficulty we impose the reflection and transmission condition by applying the Snell's law and get the leading order terms in asymptotic expansion  $a^{\text{re}} = Ra^{\text{in}}$ , and  $a^{\text{in}} = Ta^{\text{in}}$ , with the reflection coefficient  $R$  and transmission coefficient  $T$  given by  $R = \frac{p_z^{\text{in}} - p_z^{\text{tr}}}{p_z^{\text{in}} + p_z^{\text{tr}}}$ , and  $T = \frac{2p_z^{\text{in}}}{p_z^{\text{in}} + p_z^{\text{tr}}}$ , where we have used in, re, and tr to indicate the incident, reflected, and transmitted waves respectively, and  $p^{\text{in/re/tr}}$  are velocities determined by Snell's law.

The derivation of the interface condition relies on the Eulerian formulation of frozen Gaussian approximation [16] and matching of the continuity conditions.

The embarrassingly parallel property, less limitation on the time steps in solving the uncoupled ODEs, and the interface conditions make FGA an efficient method for the large domain and high-frequency seismic wave simulation. We test the computational efficiency and accuracy of the FGA in comparison with the spectral element (SPE) method which is widely used in geographic physics. In Figure 1(a), we plot the one-step computational time with respect to different frequency number  $f$ , from which one can observe that the computational time spent by FGA increases more or less linearly in  $f$ , while that of the SPE increases like  $f^3$ . In Figure 1(b), to achieve a comparable accuracy as FGA, SPE needs 128 elements in each spatial direction, which requires an average computational three times longer than that of FGA. We then apply FGA in the computation of the seismic tomography [12]. As shown in Fig.2(a), we apply FGA to the computation of the sensitivity kernels in 3D seismic inversion in a three-layered cross-well setup. We also apply FGA in the local earthquake inversion using Landers source-receiver data, where the earthquake events are marked by red dots and the receivers are marked by blue triangles in Fig.2(b-d). The true velocity model is shown in Fig.2(d) and a full-waveform inversion result is shown in Fig.2(e).

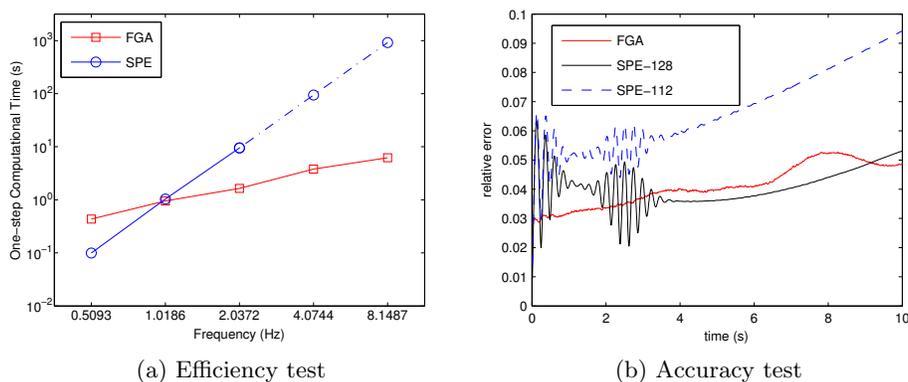


Figure 1

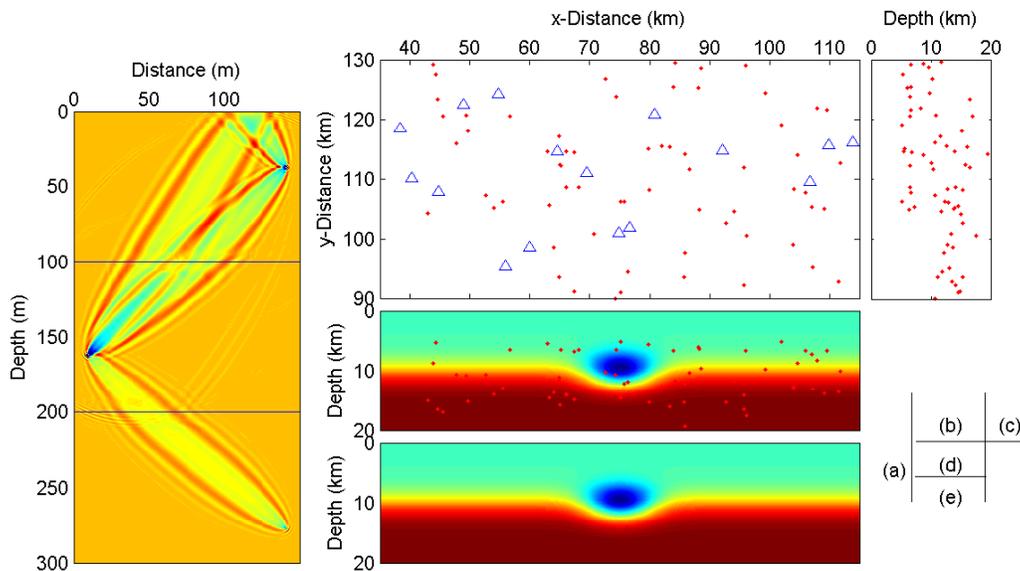


Figure 2

## Analysis of Semiclassical Limit for Spin-Magnetization Coupling

The spin-magnetization coupling plays a key role in the active control of domain-wall motion and magnetization reversal in magnetic multilayers, which are the core techniques used in magnetoresistance random access memories and race-track memories [4]. The Schrödinger-Poisson-Landau-Lifshitz-Gilbert (SPLLG) system is used to describe a mechanism known as spin-transfer torque that transfers the spin angular momentum to magnetization dynamics via spin-magnetization coupling, and was introduced in the seminal works of Slonczweski [18] and Berger [2].

The main goal of this research is to use a quantum-kinetic description and semiclassical analysis to set up a mathematical theory and foundation of spin polarized transport in ferromagnetic multilayers with strong orbit coupling from the most fundamental point of view, so that every important detail of trimming the model can be carefully analyzed. A paper to report these results is going to appear in *Arch. Ration. Mech. Anal.*, and specifically, we proved the following two theorems [6]:

**Theorem 1 (existence of weak solutions).** Consider the SPLLG system

$$\begin{aligned} i\varepsilon\partial_t\psi_j^\varepsilon &= -\frac{\varepsilon^2}{2}\Delta\psi_j^\varepsilon + V^\varepsilon\psi_j^\varepsilon - \frac{\varepsilon}{2}\mathbf{m}^\varepsilon \cdot \hat{\boldsymbol{\sigma}}\psi_j^\varepsilon, \text{ for } \mathbf{x} \in \mathbb{R}^3, j \in \mathbb{N}, \\ \partial_t\mathbf{m}^\varepsilon &= -\mathbf{m}^\varepsilon \times \mathbf{H}_{\text{eff}}^\varepsilon + \alpha\mathbf{m}^\varepsilon \times \partial_t\mathbf{m}^\varepsilon, \text{ for } \mathbf{x} \in \Omega \subset \mathbb{R}^3, \end{aligned} \quad (3)$$

where  $0 < \varepsilon \ll 1$  is the renormalized Planck constant in the semiclassical regime,  $\psi_j^\varepsilon \in \mathbb{R}^2$  stands for the  $j$ -th spinor,  $\mathbf{m}^\varepsilon \in \mathbb{R}^3$  is the magnetization, the potential  $V^\varepsilon = -N * \rho^\varepsilon$  is the Coulomb interaction, and the effective field  $\mathbf{H}_{\text{eff}}^\varepsilon = \Delta\mathbf{m}^\varepsilon + \mathbf{H}_s[\mathbf{m}^\varepsilon] + \frac{\varepsilon}{2}\mathbf{s}^\varepsilon$ , with  $\mathbf{H}_s[\mathbf{m}^\varepsilon] = -\nabla(\nabla N * \cdot \mathbf{m}^\varepsilon)$  being the self induced stray field, and  $N = 1/(4\pi|x|)$ . Then there exists  $\psi_j^\varepsilon \in L^\infty([0, \infty), H^1(\mathbb{R}^3))$  and  $\mathbf{m}^\varepsilon \in C([0, \infty), H^1(\Omega)) \cap H^1([0, T] \times \Omega)$  for all  $T > 0$ , such that  $(\psi_j^\varepsilon, \mathbf{m}^\varepsilon)$  is a weak solution to the SPLLG system (3).

**Theorem 2 (semiclassical limit).** Under certain assumptions on the initial conditions, there exists a sequence of solutions  $(\psi^\varepsilon, \mathbf{m}^\varepsilon)$  of the SPLLG system (3), and  $W^\varepsilon$  as the Wigner transform of  $\{\psi_j^\varepsilon\}$ , such that  $W^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} W$  in  $L^\infty((0, T), L^2(\mathbb{R}_x^3 \times \mathbb{R}_v^3))$  weak\*, and  $\mathbf{m}^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} \mathbf{m}$  in  $L^\infty((0, T), H^1(\Omega))$  weak\*, and  $(W, \mathbf{m})$  is a weak solution to the following VPLLG system,

$$\begin{aligned} \partial_t W &= -\mathbf{v} \cdot \nabla_x W + \nabla_x V \cdot \nabla_v W + \frac{i}{2}[\hat{\boldsymbol{\sigma}} \cdot \mathbf{m}, W], \\ \partial_t \mathbf{m} &= -\mathbf{m} \times \mathbf{H}_{\text{eff}} + \alpha\mathbf{m} \times \partial_t \mathbf{m}, \end{aligned}$$

where the potential  $V = -N * \rho$ , the density  $\rho = \int_{\mathbb{R}_v^3} W d\mathbf{v}$ , and the effective magnetic field  $\mathbf{H}_{\text{eff}} = \Delta\mathbf{m} + \mathbf{H}_s[\mathbf{m}]$ .

The coupling of the Schrödinger system and the LLG system bring us more difficulties, which include the non-wellposedness of regular solutions due to the nonlinear LLG system and the jump discontinuity of the magnetization across the boundary of the domain  $\Omega$ . The existence of the global regular solution of the LLG system is still an open problem, and for this reason we consider the weak solutions in  $H^1$  and prove the existence theorem. The jump discontinuity of the magnetization make the limit of the Wigner equation non-trivial when we try to estimate the remainder. We apply a mollifier in the intermediate step, successfully remove the discontinuity and obtain a uniform estimate, and then prove the semiclassical limit.

Then in  $\varepsilon \ll 1$  as the rescaled Knudsen number, we considered the s-wave form spin dynamics coupled with LLG system in the diffusion regime ,

$$\begin{aligned} \partial_t W^\varepsilon + \frac{1}{\varepsilon}(\mathbf{v} \cdot \nabla_x W^\varepsilon(\mathbf{x}, \mathbf{v}) - \nabla_x \phi(\mathbf{x}) \cdot \nabla_v W^\varepsilon(\mathbf{x}, \mathbf{v})) &= i[\hat{\boldsymbol{\sigma}} \cdot \mathbf{m}^\varepsilon, W^\varepsilon] + \frac{1}{\varepsilon^2}\mathcal{Q}(W^\varepsilon) + \mathcal{Q}_{\text{sf}}(W^\varepsilon), \\ \partial_t \mathbf{m}^\varepsilon &= -\gamma\mathbf{m}^\varepsilon \times (\Delta\mathbf{m}^\varepsilon + \mathbf{H}_s[\mathbf{m}^\varepsilon] + \mathbf{s}^\varepsilon) + \mathbf{m}^\varepsilon \times \partial_t \mathbf{m}^\varepsilon, \end{aligned} \quad (4)$$

with  $\varepsilon \ll 1$  as the rescaled Knudsen number, the BGK collision operator  $\mathcal{Q}$ , and the spin-flip operator  $Q_{\text{sf}}(W^\varepsilon) = \frac{I}{2} \text{Tr}_{\mathbb{C}^2} W^\varepsilon - W^\varepsilon$ . We studied the existence of solutions in a weighted  $L^2$  space, and rigorously proved the diffusion limit of the coupled system given by

$$\begin{aligned} \partial_t \rho - \nabla_{\mathbf{x}} \cdot (D \cdot (\nabla_{\mathbf{x}} \rho + \nabla_{\mathbf{x}} \phi \rho)) &= 0, \\ \partial_t \mathbf{s} - \nabla_{\mathbf{x}} \cdot (D \cdot (\nabla_{\mathbf{x}} \mathbf{s} + \nabla_{\mathbf{x}} \phi \mathbf{s})) &= -2\mathbf{m} \times \mathbf{s} - \mathbf{s}, \\ \partial_t \mathbf{m} &= -\gamma \mathbf{m} \times (\Delta \mathbf{m}^\varepsilon + \mathbf{H}_s[\mathbf{m}^\varepsilon] + \mathbf{s}) + \mathbf{m} \times \partial_t \mathbf{m}. \end{aligned} \quad (5)$$

The first term on the right hand side of (5) represents the precessional motion due to the sd interaction when the magnetization directions of the spin and the local moments are not parallel; the second term on the right hand side of (5) represents the spin-flip relaxation, which recover the diffusion model introduced in by Zhang, Levy and Fert (Nobel Prize, 2007) in [21]

### Semiclassical Models and Methods for Quantum Tunneling

My research works on inter-band tunneling studies the interaction between several coupled potential energy bands, *e.g.*, for crystal lattice, the Bloch bands may getting close to each other or even cross, in which cases particles may transit through the band gap to the other energy band. The study of such “quantum tunneling” is important in many applications, from quantum dynamics in chemical reaction [20], semiconductors to Bose-Einstein condensation [3]. In the first approach we considered the quantum system in phase-space using Wigner transform, and take the off-diagonal terms of the Wigner matrix into account to capture the tunneling. A paper presenting these results has been published in SIAM Journal on *Multiscale Model. Sim.* [8]. In the second approach [9] we studied the Schrödinger equation and propose a semiclassical-quantum hybrid numerical method. In the following I will take the Schrödinger equation with a lattice potential as examples and introduce these works in more detail.

**A semiclassical model using Wigner-Bloch theory.** We use the Wigner-Bloch theory to derive semiclassical models for the Schrödinger equation with periodic potentials that account for band-crossing [7]. Without band-crossing, the classical Vlasov limit can be obtained along each Bloch band [1, 13, 17], which only includes the diagonal entries of the Wigner-Bloch matrix and valid away from the crossing zone. In our semiclassical models we include the leading order of the off-diagonal entries, resulting in a coupled system

$$\partial_t \boldsymbol{\sigma} + A \partial_x \boldsymbol{\sigma} - \partial_x U \partial_p \boldsymbol{\sigma} = \partial_x U C \boldsymbol{\sigma} + \frac{iD}{\varepsilon} \boldsymbol{\sigma}. \quad (6)$$

Here,  $\boldsymbol{\sigma} = [\sigma_{11}, \sigma_{12}, \sigma_{21}, \sigma_{22}]^T$  represents the Wigner-Bloch components,  $A$ ,  $C$ , and  $D$  are  $4 \times 4$  matrices determined by the band structure. In particular, the entries of  $C$  are the *Berry connections*, and  $D = \text{diag}[0, E_2 - E_1, E_1 - E_2, 0]$  with  $E_m$  being the  $m$ -th Bloch band,  $m = 1, 2$ . In this system different bands are coupled together by  $C$  and inter-band transition happens. As  $\varepsilon$  goes to 0, the off-diagonal entries  $\sigma_{12}$  and  $\sigma_{21}$  go to 0 weakly, and the system goes to the classical Vlasov system

$$\partial_t \sigma_{mm} + \partial_p E_m \partial_x \sigma_{mm} - \partial_x U \partial_p \sigma_{mm} = 0. \quad (7)$$

The semiclassical Vlasov system (6) is defined in phase-space and contains a small parameter  $\varepsilon$ , so numerically solving it requires  $\Delta t, \Delta x < \varepsilon$ . In order to numerically solve the problem efficiently, we present a domain decomposition idea based on the asymptotic properties of the transition coefficients  $\sigma_{mn} (m \neq n)$ : In a  $\sqrt{\varepsilon}$  neighborhood of the crossing point, we solve the semiclassical Vlasov system (6) using a fine mesh with  $\Delta x$  and  $\Delta t$  less than  $\sqrt{\varepsilon}$ , and out of the neighborhood we solve the classical Vlasov system (7) using coarse mesh independent of  $\varepsilon$ .

**A Bloch decomposition based hybrid method.** In order to reduce the computational complexity, we develop a new Bloch decomposition-based Gaussian beam (BDGB) method in simulating the periodic Schrödinger equation in the momentum space away from the band-crossings. As an asymptotic solver, the BDGB method does not have the requirement on the  $\varepsilon$ -dependent mesh size and time step, and it reduces the original Schrödinger equation into a system of uncoupled ODEs, thus it can drastically speed up the computation. Moreover, the BDGB method in momentum space provides us a convenient way to combine it with the the Bloch decomposition-based time splitting (BDTS) method [14, 15] in order to capture the inter-band tunneling: Away from the crossing point, the use of the asymptotic Gaussian beam solution can reduce the computational cost efficiently; around the crossing point, the direct simulation of the Schrödinger equation by BDTS can capture the inter-band transitions, and one has to use fine spatial mesh and time steps of  $O(\varepsilon)$  to get the desired accuracy, but since one can suitably choose the size of computational region as  $O(\sqrt{\varepsilon})$  around the crossing point, the numerical cost of this part can also be reduced; and the exchange of data between different zones is achieved simply by Gaussian beam decomposition [19].

In Figure 3 we show the resulted Bloch coefficients in simulating the Schrödinger equation with a honeycomb lattice potential using the BDTS and BDGB hybrid method. The Schrödinger equation with a honeycomb lattice potential can be used to model the electron motion in a Graphene layer, and due to the existence of the Dirac point, inter-band transitions are very important in the simulations. But since this problem is defined in two dimensional space, when  $\varepsilon$  is small, to solve the Schrödinger equation using the BDTS method will be a huge challenge for the memory and cpu time. With the help of the hybrid method, this example can be done in one hour on a personal laptop. As it has been shown in Figure 3, the significant inter-band transition around the Dirac point can be captured clearly using the hybrid method.

### Ongoing and Future Research

**Seismic tomography.** Seismic tomography is one of the core methodologies for imaging the structural heterogeneity of the Earth’s interior. Our studies pave the way to directly apply wave-equation-based seismic tomography methods into real data around their dominant frequencies. We are currently working on the FGA for elastic wave equations in order to get a more reliable model in seismic tomography and apply it on real seismic data. On the other hand, though FGA could improve the efficiency, the adjoint tomography method is still very computational demanding in CPU time, memory and storage, since it is based on Born approximation and need to compute the sensitivity kernels. In order to overcome these difficulties, we are working on the global optimization method using *networks* and sparse parametrization techniques in order to make the most of the supper efficiency and parallelizability of FGA in simulating seismic wave equations.

**Spin-magnetization coupling in micro-magnetics.** The spin-magnetization coupling in ferromagnetic materials is definitely a multiscale problem. We have studied this problem in quantum, kinetic and fluid scalings [6, 5]. However, to study new models which can include more physical details is always interesting. For example, in our work on the diffusion limit, we didn’t include the self-induced electric field. We are thinking about to add a self-induced field in order to recover the physical phenomena such as the *linear response*. A self-induced field will make the analysis more difficult because then we don’t have the proper weighted  $L^2$  space and the associated conservation law as we did in [5]. The other model we have been working with is the spin dynamics governed by the Schrödinger-Maxwell system, and we want to analyze the semiclassical limit and coupling it with LLG. The main difficulty here is that we don’t have enough regularity of the magnetic field, so only some weakly coupling regime can be done so far. On the numerical side, to build efficient numerical solver, investigate the influences of the boundary layers, and construct the *asymptotic*

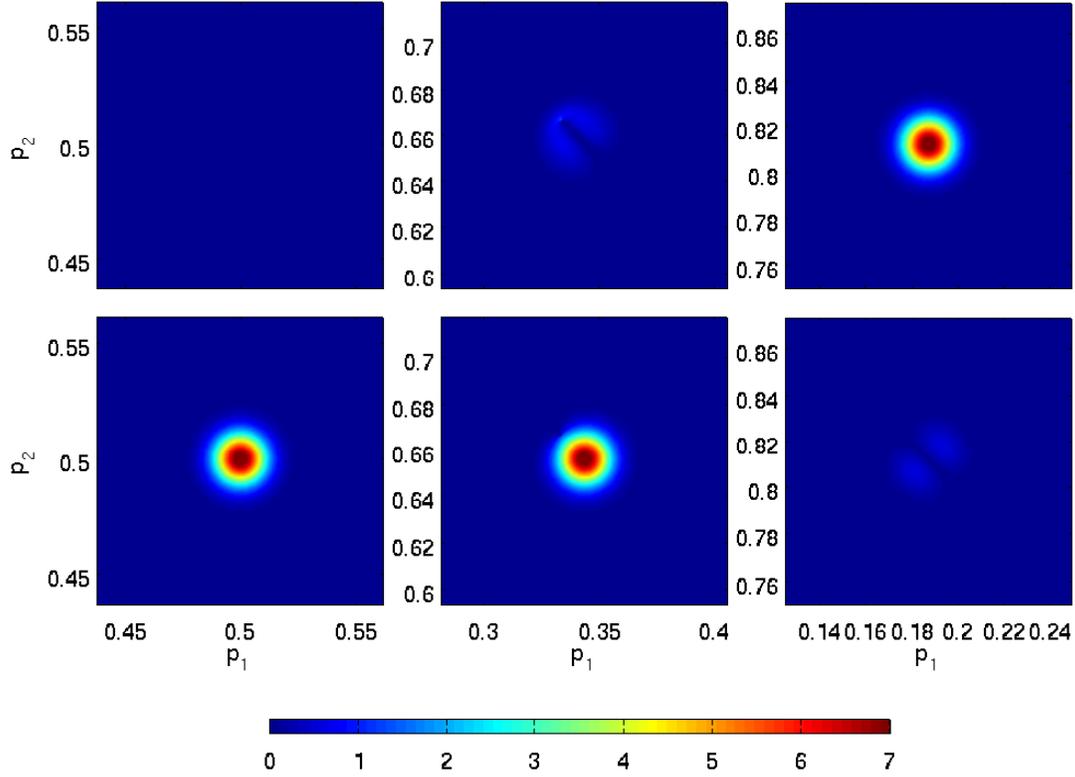


Figure 3: Solutions at different time by the hybrid method. Lower row: Bloch coefficient at the lower band; upper row: Bloch coefficient at the upper band. At time  $t = 0$  (left column), the wave is located at the first band and the second band is empty. At time  $t = 0.15625$  (middle column), the inter-band transition is happening at the Dirac point. At time  $t = 0.3125$  (right column), a large part of the population is on the upper band.

*preserving* scheme for coupling models in different scaling are delicate topics for me.

**Models and methods in quantum physics.** In the semiclassical method for quantum physics, the main difficulty is that to describe an essential quantum effect such as the tunneling by a semiclassical model, for which, we have developed non-diagonal systems and hybrid methods [7, 8, 9]. One interesting phenomena I have been thinking is the *Klein paradox* in the Graphene layer, for which the Schrödinger equation with a honeycomb lattice potential and a step potential is considered. The difficulty in simulating this problem using semiclassical method such as Gaussian beam method is from the jump discontinuity of the step potential, where quantum tunneling may happen. To overcome this difficulty, an interface condition over the discontinuity is considered to incorporate with the semiclassical dynamics. One another topic we are working on is the FGA for the 3-D Dirac equation and consider the semiclassical and non-relativity limits in different regime. The new nature in FGA brought by the Dirac equation is that we need consider the coupling dynamics in the two dimensional eigenspace due to the degeneracy of the eigenvalue of the Dirac Hamiltonian [10], and the *Berry connections* are included in the coupling. And we are going to investigate the limiting behavior for both the solution and FGA shall be considered in different regime.

## References

- [1] G. Bal, A. Fannjiang, G. Papanicolaou, and L. Ryzhik. Radiative transport in a periodic structure. *Journal of Statistical Physics*, 95(1):479–494, 1999.
- [2] L. Berger. Emission of spin waves by a magnetic multilayer traversed by a current. *Physical Review B*, 54(13):9353–9358, 1996.
- [3] A. Bohm, A. Mostafazadeh, H. Koizumi, Q. Niu, and J. Zwanziger. *The Geometric Phase in Quantum Systems: Foundations, Mathematical Concepts, and Applications in Molecular and Condensed Matter Physics*. Springer, 2012.
- [4] A. Brataas, A. Kent, and H. Ohno. Current-induced torques in magnetic materials. *Nat. Mater.*, 11:372–381, 2012.
- [5] L. Chai, C. J. García-Cervera, and X. Yang. Diffusion limit of the Wigner-Landau-Lifshitz-Gilbert system in ferromagnetic materials. *Submitted*.
- [6] L. Chai, C. J. García-Cervera, and X. Yang. Semiclassical limit of the Schrödinger-Poisson-Landau-Lifshitz-Gilbert system. *Archive for Rational Mechanics and Analysis*, to appear.
- [7] L. Chai, S. Jin, and Q. Li. Semi-classical models for the Schrödinger equation with periodic potentials and band crossings. *Kinetic and Related Models*, 6:505–532, 2013.
- [8] L. Chai, S. Jin, Q. Li, and O. Morandi. A multiband semiclassical model for surface hopping quantum dynamics. *Multiscale Modeling & Simulation*, 13(1):205–230, 2015.
- [9] L. Chai, S. Jin, and P. A. Markowich. A hybrid method for computing the Schrödinger equations with periodic potential with band-crossings in the momentum space. *Communications in Computational Physics, (a special issue in honor of the 80th birthday of Prof. Houde Han)*, to appear.
- [10] L. Chai, E. Lorin, and X. Yang. Frozen Gaussian approximation for 3-D Dirac equations. *In preparation*.
- [11] L. Chai, P. Tong, and X. Yang. Frozen gaussian approximation for 3-d seismic wave propagation. *Geophysical Journal International*, 208(1):59–74, 2017.
- [12] L. Chai, P. Tong, and X. Yang. Frozen Gaussian approximation for 3-D seismic tomography. *submitted*.
- [13] P. Gérard, P. Markowich, N. Mauser, and F. Poupaud. Homogenization limits and Wigner transforms. *Communications on Pure and Applied Mathematics*, 50(4):323–379, 1997.
- [14] Z. Huang, S. Jin, P. Markowich, and C. Sparber. A Bloch decomposition-based split-step pseudospectral method for quantum dynamics with periodic potentials. *SIAM Journal on Scientific Computing*, 29(2):515–538, 2008.

- [15] Z. Huang, S. Jin, P. A. Markowich, and C. Sparber. Numerical simulation of the nonlinear Schrödinger equation with multidimensional periodic potentials. *Multiscale Modeling & Simulation*, 7(2):539–564, 2008.
- [16] J. Lu and X. Yang. Convergence of frozen Gaussian approximation for high frequency wave propagation. *Communications on Pure and Applied Mathematics*, 65:759–789, 2012.
- [17] P. Markowich, N. Mauser, and F. Poupaud. A Wigner-function approach to (semi) classical limits: Electrons in a periodic potential. *Journal of Mathematical Physics*, 35:1066–1094, 1994.
- [18] J. C. Slonczewski. Current-driven excitation of magnetic multilayers. *Journal of Magnetism and Magnetic Materials*, 159(1):L1–L7, 1996.
- [19] N. M. Tanushev, B. Engquist, and R. Tsai. Gaussian beam decomposition of high frequency wave fields. *Journal of Computational Physics*, 228(23):8856–8871, 2009.
- [20] J. Tully and R. Preston. Trajectory surface hopping approach to nonadiabatic molecular collisions: the reaction of H with D. *The Journal of Chemical Physics*, 55:562–572, 1971.
- [21] S. Zhang, P. Levy, and A. Fert. Mechanisms of spin-polarized current-driven magnetization switching. *Physical review letters*, 88(23):236601, 2002.