Semi-classical Dynamics in Schrödinger Equations: Convergence and Computation

Hailiang Liu

Department of Mathematics Iowa State University–USA http://orion.math.iastate.edu/hliu

Collaborators: Christof Sparber(Cambridge) Zhongming Wang(ISU)

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- Mathematical description of BECs
- Semiclassical convergence for nonlinear GPE
- Level set method for computation of semiclassical limit
- Numerical examples

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- BECs play important roles in present-day physics. Understanding BECs' behavior is of fundamental importance.
- Dynamical phenomena: Rotation and quantized vortices are connected to superfluidity
- Experimentation set-up: rotational trapping potential
- Mathematical description: celebrated Gross-Pitaevskii equation (GPE):

$$i\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \Delta \psi + V(x)\psi + \kappa |\psi|^2 \psi + i\Omega x^{\perp} \cdot \nabla_x \psi, \quad (1)$$

where $x^{\perp} = (x_2, -x_1, 0)^{\top}$ in d = 3 spatial dimensions.

[N. Ben Abdallah, W. Bao, Q. Du, D. Jaksch, T.-C. Lin, P. Markowich, C. Sparber, ...]

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Questions of physical interest:

- Nucleation mechanisms (analysis?)
- Observation of density and phase (how to compute);
- Stability, decay, precession (analysis?)
- Shape and dynamics of a single vortex (simulation).
- Formation and dynamics of vortex lattices (analysis?)
- Fast rotating condensates and giant vortices (simulation)
- Coreless vortices and textures in spinor condensates (visualization)
- interaction with thermal atoms, solitons, surface modes.
- Vortex rings, vortex-antivortex pairs, etc.

▶ ...

In semi-classical regime the dynamics is presumably well described by the *hydrodynamical equations for rotating super-fluids*:

$$\begin{cases} \partial_t \rho + \nabla_x \cdot \left(\rho(\mathbf{v} - \Omega x^{\perp}) \right) = 0, \\ \partial_t \mathbf{v} + \nabla_x \left(\frac{|\mathbf{v}|^2}{2} - \Omega x^{\perp} \cdot \mathbf{v} + V_0 + f(\rho) \right) = 0, \end{cases}$$
(2)

where $\rho := |\psi|^2$ denotes the particle density, $f(\rho) = \rho$, and **v** the corresponding superfluid velocity defined by

$$\mathbf{v} := \frac{\hbar}{m} \frac{\operatorname{Im}\left(\overline{\psi} \, \nabla_{\mathsf{x}} \psi\right)}{|\psi|^2}.$$

The passage from (1) to (2) is usually explained by using the classical *Madelung transformation* of the wave function

$$\psi(t,x) = \sqrt{\rho(t,x)} \exp(i\Phi(t,x)/\hbar),$$

and consequently identifies $\boldsymbol{v}:=\nabla_{\boldsymbol{x}}\boldsymbol{\Phi}\text{-}irrotational$ velocity field

- ▶ Semiclassical convergence: equation (2) approximates (1) when $\hbar \rightarrow 0$ (for smooth solutions)?
- Can one use (2) as a computational model for computing semiclassical limit of (1)?

[Madelung E. Z. Phys. 40, 322 (1927)]

$$\begin{cases} i\epsilon \,\partial_t \psi^\epsilon = -\frac{\epsilon^2}{2} \Delta \psi^\epsilon + V(x) \psi^\epsilon + f(|\psi^\epsilon|^2) \psi^\epsilon + i\epsilon \,\Omega x^\perp \cdot \nabla_x \psi^\epsilon \\ \psi^\epsilon|_{t=0} = \psi^\epsilon_{\rm in}(x) = a^\epsilon_{\rm in}(x) \, e^{i\Phi_{\rm in}(x)/\epsilon}, \end{cases}$$
(3)

where
$$t \in \mathbb{R}$$
, $x \in \mathbb{R}^d$, for $d = 2, 3$, and $\Omega \ge 0$

Assumptions:

(i) The nonlinearity $f \in C^{\infty}(\mathbb{R})$ and f' > 0.

(ii) The potential V quadratic

(iii) Initial amplitude a_{in}^{ϵ} is complex-valued whereas $\Phi_{in}(x)$ is cindenendent, real-valued, and sub-guadratic

 $\epsilon\text{-independent, real-valued, and sub-quadratic.}$

We aim

(i) to give a rigorous justification of (2) as limit of (3).(ii) to describe the dynamical features of rotational BECs from the semi-classical point of view.

- Classical Madelung transformation is not suited Re: Grenier(98), Liu and Tadmor(02), Carles(07)
- The modified WKB

$$\psi^{\epsilon}(t,x) = a^{\epsilon}(t,x)e^{i\Phi^{\epsilon}(t,x)/\epsilon}, \qquad (4)$$

where from now on the "amplitude" a^{ϵ} is allowed to be complex-valued. Moreover a^{ϵ} and (real-valued) phase Φ^{ϵ} are assumed to admit an asymptotic expansion of the form

$$a^{\epsilon} \sim a + \epsilon a_1 + \epsilon^2 a_2 + \cdots, \quad \Phi^{\epsilon} \sim \Phi + \epsilon \Phi_1 + \epsilon^2 \Phi_2 + \cdots.$$
 (5)

The main gain: it yields a separation of scales within the appearing fast, i.e. ε-oscillatory, phases and slowly varying phases.

Equivalent equations

1) Schrödinger equation

$$\begin{cases} \partial_t \Phi^{\epsilon} + \frac{1}{2} |\nabla_x \Phi^{\epsilon}|^2 + V(x) - \Omega x^{\perp} \cdot \nabla_x \Phi^{\epsilon} + f(|a^{\epsilon}|^2) = 0, \\ \partial_t a^{\epsilon} + \nabla_x \Phi^{\epsilon} \cdot \nabla_x a^{\epsilon} + \frac{1}{2} a^{\epsilon} \Delta \Phi^{\epsilon} - \Omega x^{\perp} \cdot \nabla_x a^{\epsilon} = \frac{i\epsilon}{2} \Delta a^{\epsilon}. \end{cases}$$

ii) Hydrodynamic equation

$$\begin{cases} \partial_t \Phi + \frac{1}{2} |\nabla_x \Phi|^2 + V(x) - \Omega x^{\perp} \cdot \nabla_x \Phi + f(|a|^2) = 0, \\ \partial_t a + \nabla_x \Phi \cdot \nabla_x a + \frac{1}{2} a \Delta \Phi - \Omega x^{\perp} \cdot \nabla_x a = 0. \end{cases}$$

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Decompose the phase Φ^ϵ into

$$\Phi^{\epsilon} = \varphi^{\epsilon} + S, \tag{6}$$

where S is the smooth phase function satisfying the classical *rotational* Hamilton-Jacobi equation (HJ)

$$\partial_t S + \frac{1}{2} |\nabla_x S|^2 + V(x) - \Omega x^{\perp} \cdot \nabla_x S = 0.$$
 (7)

Lemma

If $S_{in}(x) \in C^{\infty}(\mathbb{R}^d)$ is sub-quadratic, then there exists a $\tau > 0$ such that (7) admits a unique smooth solution for $t \in [0, \tau)$. Moreover, the phase S(t, x) remains sub-quadratic in x, for all $t \in [0, \tau)$.

$$\begin{cases} \partial_t \varphi^{\epsilon} + \nabla_x S \cdot \nabla_x \varphi^{\epsilon} + \frac{1}{2} |\nabla_x \varphi^{\epsilon}|^2 - \Omega x^{\perp} \cdot \nabla_x \varphi^{\epsilon} + f(|a^{\epsilon}|^2) = 0, \\ \partial_t a^{\epsilon} + \nabla_x (S + \varphi^{\epsilon}) \cdot \nabla_x a^{\epsilon} + \frac{a^{\epsilon}}{2} \Delta (S + \varphi^{\epsilon}) - \Omega x^{\perp} \cdot \nabla_x a^{\epsilon} = \frac{i\epsilon}{2} \Delta_x a^{\epsilon}. \end{cases}$$
(8)

The system is written as a hyperbolic system

$$\partial_t U^{\epsilon} + \sum_{j=1}^d \left(A_j(U^{\epsilon}) + B_j(w)\right) \partial_{x_j} U^{\epsilon} + M(\nabla_x w) U^{\epsilon} = \frac{\epsilon}{2} L U^{\epsilon},$$

where $w := \nabla_x S - \Omega x^{\perp}$ is sub-linear and

$$U^{\epsilon} := (\operatorname{\mathsf{Re}} a^{\epsilon}, \operatorname{\mathsf{Im}} a^{\epsilon}, \partial_{x_1} \varphi^{\epsilon}, \dots, \partial_{x_d} \varphi^{\epsilon})^{\top},$$

Analysis is done relying on the following norm

$$\mathcal{N}[U^{\epsilon}(t]) := \| U^{\epsilon}(t) \|_{s} + \| |x| U^{\epsilon}(t) \|_{s-1}.$$
(9)

Local convergence

If $U_{in}^{\epsilon} \in H^{s}(\mathbb{R}^{d})$ and $|x|U_{in}^{\epsilon} \in H^{s-1}(\mathbb{R}^{d})$, for s > 2 + d/2. Then there exists a time $T_{\epsilon} \in (0, \tau)$, and a unique solution of the following form

$$\psi^{\epsilon}(t,x) = a^{\epsilon}(t,x)e^{i\Phi^{\epsilon}(t,x)/\epsilon}, \quad \text{for } 0 \leq t \leq T_{\epsilon}.$$

Convergence rates

Suppose that $\|a_{in}^{\epsilon} - a_{in}\|_{s} = O(\epsilon)$. Let $U := (\operatorname{Re} a, \operatorname{Im} a, \partial_{x_{1}}\varphi, \dots, \partial_{x_{d}}\varphi)^{\top}$ be the smooth solution in $(0, T^{*})$ to the limit equation corresponding to the initial data (Φ_{in}, a_{in}) , then there exists ϵ_{0} and $C_{*} > 0$, such that for $\epsilon \leq \epsilon_{0}$ we have

$$\|a^{\epsilon}(t) - a(t)\|_{s} \leq C_{*}\epsilon, \quad \|\Phi^{\epsilon}(t) - \Phi(t)\|_{s} \leq C_{*}\epsilon t,$$

for all $t \in [0, \min\{T^*, T^\epsilon\})$.

- A generic global convergence result
 The semi-classical convergence holds true globally in time if the super-fluid model admits global smooth solution.
- Mathematical description
 Under the same assumptions as before and for any C₁ satisfying

 $\mathcal{N}[U_0^\epsilon] \leq C_0 < C_1, \quad \mathcal{N}[U^\epsilon(t)] \leq C_1 < C, \quad \text{for } t \in [0, \min\{T^*, T^\epsilon\}),$

it holds $T^{\epsilon}(C_1) > T^*$ for $\epsilon > 0$ sufficiently small.

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Rotational dynamics of semi-classical super-fluids

► The expectation value of the angular momentum:

$$m^{\epsilon}(t) := i\epsilon \int_{\mathbb{R}^d} \overline{\psi^{\epsilon}}(t, x) x^{\perp} \cdot \nabla_x \psi^{\epsilon}(t, x) \, dx, \qquad (10)$$

 $m^{\epsilon}(t) \neq 0$ signifies the *vortex nucleation* in BEC experiments.

► This quantity is dominated by the classical rotational effect; In contrast, for ε = O(1) this quantity remains unchanged, as shown by Bao, Du and Zhang (2006).

Corollary

Let f(z) = z and impose the same assumptions as before. Then, as $\epsilon \to 0$ it holds

$$m^{\epsilon}(t)=m(0)+rac{\Omega}{2}\left(\langle|x|^{2}
angle_{
ho(t)}-\langle|x|^{2}
angle_{
ho_{\mathrm{in}}}
ight)+O(\epsilon).$$

Moreover we have

$$rac{\mathrm{d}}{\mathrm{d}t}m^{\epsilon}(t)=\Omega\langle x\cdot \mathbf{v}
angle_{
ho(t)}+rac{\delta}{2\omega_{\perp}^{2}}\langle x_{1}x_{2}
angle_{
ho(t)}+O(\epsilon),$$

where $\delta = \frac{\omega_1^2 - \omega_2^2}{\omega_1^2 + \omega_2^2}$ denotes the trap deformation and $\omega_{\perp}^2 = \frac{1}{2}(\omega_1^2 + \omega_2^2)$ the radial frequency.

Outline:

- Background
- Jet/phase space based level set method
 - -The Schrödinger equation with an external potential
- Field space based level set method
 - The Schrödinger equation with a self-consistent potential
- Bloch-band based level set method
 - The Schrödinger equation with a periodic potential

Consider the re-scaled Schrödinger equation of the form

$$i\epsilon\partial_t\psi = -rac{\epsilon^2}{2}\Delta\psi + W\psi,$$

with

$$W = \{V_e(x), V_p, V(\frac{x}{\epsilon})\}.$$

⊙ Its role in quantum mechanics for microscopic particles (such as electrons, atomic nuclei, etc.) is analogous to Newton's second law in classical mechanics for macroscopic particles.

 \odot Semiclassical approximation—a high frequency approximation ($\epsilon \downarrow 0$) that is used to approximate quantum mechanics.

⊙ Goals:

- Efficient numerical methods for capturing semi-classical field statistics
- Evaluation of physical observables
- Reconstruction of the wave field
- Tools and methods:
 - Asymptotic methods to obtain effective equations
 - Level set method for capturing semi-classical field statistics
 - Projection for evaluation of physical observables

- Semiclassical approximation of Schrödinger equations
- High frequency wave propagation in: geometrical optics, seismology, medical imaging, ...
- Math Theory: semiclassical analysis, Lagrangian path integral, wave dynamics in nonlinear PDEs ...

Computational challenge: when wave field is highly oscillatory, direct numerical simulation of the wave dynamics can be very costly and approximate models for wave propagation must be used. The effective equation is often nonlinear, and classical entropy solutions are inadequate

The WKB system

► The WKB method applied to a linear wave equation typically results in a weakly coupled system of an eikonal equation for phase S and a transport equation for position density ρ = |A|² respectively:

$$\begin{aligned} \partial_t S + H(\mathbf{x}, \nabla S) &= 0, \quad (t, \mathbf{x}) \in R^+ \times R^n, \\ \partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho \nabla_{\mathbf{k}} H(\mathbf{x}, \nabla_{\mathbf{x}} S)) &= 0. \end{aligned}$$

► The semiclassical limit of the Schrödinger equations:

$$H = \frac{1}{2} |\mathbf{k}|^2 + V(\mathbf{x}) - \Omega x^{\perp} \cdot \mathbf{k}.$$

▶ 1D free motion with $u = S_x$ is governed by the Burgers' equation

$$u_t + uu_x = 0.$$

Advantage and disadvantage: ε-free, superposition principle lost ...

- u must be a gradient of phase S;
- we must allow S to be a multi-valued function, otherwise a singularity would appear in

$$\nabla_{\mathsf{x}}\psi^{\epsilon} = (\nabla A/A + i\nabla S/\epsilon)\psi^{\epsilon}$$

 (enforce quantization) In order for the wave field to remain single valued, one needs to impose

$$\oint_L u \cdot dl = 2\pi j, \quad j \in Z.$$

- phase shift, Keller-Maslov index.

Ray tracing (rays, characteristics), ODE based;

 Hamilton-Jacobi Methods—nonlinear PDE based [Fatemi-Engquist-Osher], [Benamou], [Abgrall], [Symes-Qian] ...

Kinetic Methods — linear PDE based

(i)<u>Wave front methods:</u>

[Engquist-Tornberg], [Runborg], [Formel-Sethian],

[Osher-Cheng-Kang-Shim and Tsai] ...

(ii) Moment closure methods:

[Brenier-Corrias], [Engquist-Runborg], [Gosse], [Jin-Li]...

Configuration space based level set method

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Collaborators: L.T. Cheng(UCSD), S. Jin(Wisconsin-Madison), S. Osher(UCLA), R. Tsai(Texas-Austin) and Z.-M. Wang (ISU).

- Level set methods for WKB system [L.T. Cheng, H.-L. Liu and S. Osher (03)][Jin and Osher (03)]
- Level set methods for computing physical observables [Jin, Liu, Osher and Tsai (05)]
- Level set framework for general first order equation [Liu-Cheng-Osher (06)].
- A review article at CICP [H. Liu, S. osher and R. Tsai (06)].
- ► Field-space based level set method for Euler-Poisson equations [H. Liu and Z.M. Wang (06)]
- ▶ Bloch-band based level set method [H. Liu and Z.M. Wang (07)]

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▶ 1-D Burgers' equation

$$\partial_t u + u \partial_x u = 0, \quad u(x,0) = u_0(x).$$

Characteristic method gives $u = u_0(\alpha)$, $X = \alpha + u_0(\alpha)t$

- ► In physical space (t, x): $u(t, x) = u_0(x u(t, x)t)$.
- ▶ In the space (t, x, y) (graph evolution)

$$\phi(t,x,y)=0, \quad \phi(t,x,y)=y-u_0(x-yt),$$

with $\phi(t, x, y)$ satisfying

$$\partial_t \phi + y \partial_x \phi = 0, \quad \phi(0, x, y) = y - u_0(x).$$

Consider the HJ equation

$$\partial_t S + H(x, \nabla_x S) = 0, \quad H(x, k) = \frac{1}{2}|k|^2 + V(x).$$

For this equation the graph evolution is not enough to unfold the singularity since *H* is also nonlinear in $\nabla_x S$.

Our strategy:

- ▶ to choose the **Jet space** (x, k, z) with z = S(x, t) and $k = \nabla_x S$;
- to select and evolve an implicit representative of the solution manifold.

Characteristic dynamics and the level set equation

Characteristic equation: In the jet space (x, k, z) the HJ equation is governed by a closed ODE system

$$\begin{aligned} \frac{dx}{dt} &= k, \quad x(0,\alpha) = \alpha, \\ \frac{dk}{dt} &= -\nabla_x V, \quad k(0,\alpha) = \nabla_x S_0(\alpha), \\ \frac{dz}{dt} &= |k|^2/2 - V(x), \quad z(0,\alpha) = S_0(\alpha). \end{aligned}$$

- Level set function \simeq global invariants of the above ODEs.
- Level set equation for $\phi \in R^{n+1}$

$$\partial_t \phi + k \cdot \nabla_x \phi - \nabla_x V \cdot \nabla_k \phi + \left(\frac{|k|^2}{2} - V(x)\right) \partial_z \phi = 0.$$

► **Hamitonian dynamics**: If one just wants to capture the velocity $k = \nabla_x S$ or to track the wave front, *z* direction is unnecessary.

$$\frac{dx}{dt} = \nabla_k H(x, k), \quad x(0, \alpha) = \alpha,$$

$$\frac{dk}{dt} = -\nabla_x H(x, k), \quad k(0, \alpha) = \nabla_x S_0(\alpha).$$

Liouville equation

$$\partial_t \phi + k \cdot \partial_x \phi - \nabla_x V(x) \cdot \nabla_k \phi = 0, \quad \phi \in \mathbb{R}^n.$$

Note here ϕ is a geometric object — level set function, instead of the distribution function.

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The multi-valued velocity is realized by

$$u(x,t) \in \{\mathbf{k}, \phi(t,x,\mathbf{k})=0\}.$$

► We evaluate the density in physical space by projecting its value in phase space (x, k) onto the manifold φ = 0, i.e., for any x we compute

$$\bar{
ho}(\mathbf{x},t) = \int_{R^{\mathbf{k}}} f(t,\mathbf{x},\mathbf{k}) \delta(\phi) d\mathbf{k},$$

where $f := \tilde{\rho}(t, \mathbf{x}, \mathbf{k}) |J(t, \mathbf{x}, \mathbf{k})|$ and $J := \det(\nabla_{\mathbf{k}} \phi)$.

It is shown that

$$f(t, \mathbf{x}, \mathbf{k}) := \widetilde{
ho}(t, \mathbf{x}, \mathbf{k}) |J(t, \mathbf{x}, \mathbf{k})|$$

solves again the Liouville equation

$$\partial_t f + \nabla_{\mathbf{k}} H \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} H \cdot \nabla_{\mathbf{k}} f = 0, \quad f_0 = \rho_0 |J_0|.$$

Post-processing

$$ar{
ho}(x,t) = \int f(t,x,k)\delta(\phi)dk,$$

 $ar{u}(x,t) = \int kf(t,x,k)\delta(\phi)dk/ar{
ho}.$

 $\delta(\phi) := \prod_{j=1}^{n} \delta(\phi_j)$ with ϕ_j being the *j*-th component of ϕ . O(nlogn) minimal effort, local level set method.

Multi-valued density and superposition

Let u_i be multi-valued velocity given by

$$u_i \in \{k | \quad \phi(t, x, k) = 0\}.$$

Superposition principle (w/Wang (2006))

$$\int fg(x,k)\delta(\phi)dk = \sum_{i=1}^{N}g(x,u_i)\rho_i(t,x).$$

Level set approach

$$\rho_i \in \left\{ \frac{f}{\left|\det\left(\frac{\partial \phi}{\partial k}\right)\right|} \middle| \phi = \mathbf{0} \right\},\label{eq:rho_i}$$

where ϕ is the vector level set function used to determine the multi-valued velocity, and f solves the same level set equation in phase space (x, p), subject to the given initial density ρ_0 .

B. The self-consistent potential (w/Wang (06))

The re-scaled Schrödinger-Poisson equation

$$i\epsilon\psi^{\epsilon}_t = -rac{\epsilon^2}{2}\Delta_x\psi^{\epsilon} + \mathcal{K}V\psi^{\epsilon}, \quad -\Delta_xV = |\psi^{\epsilon}|^2 - c(x).$$

▶ In semi-classical approximation of Schrödinger-Poisson equation via $\psi^{\epsilon} = \sqrt{\rho^{\epsilon}} e^{iS^{\epsilon}/\epsilon}$, one arrives at a Quantum Euler-Poisson system

$$\begin{split} \rho_t^{\epsilon} &+ (\rho^{\epsilon} u^{\epsilon})_x = 0, \\ u_t^{\epsilon} &+ u^{\epsilon} u_x^{\epsilon} = \mathcal{K} \mathcal{E} + \frac{\epsilon^2}{2} \{ \cdots \}, \\ \mathcal{E}_x &= \rho^{\epsilon} - c(x), \quad \mathcal{E} = -V_x. \end{split}$$

 Fluid equations: We shall compute multi-valued solutions to 1D Euler-Poisson equations

$$egin{array}{lll} \rho_t + (
ho u)_{ imes} &= 0, \ u_t + u u_{ imes} &= KE, \ E_{ imes} &=
ho - c(x), \end{array}$$

where K is a physical constant indicating the property of forcing, i.e. repulsive when K > 0 and attractive when K < 0

Applications:

Plasma dynamics

Beam propagation in Klystons

Semi-classical approximation of Schrödinger-Poisson equations ...

Kinetic approach (Vlasov-Poisson)

$$\begin{split} f_t + \xi \omega_x + \mathcal{K} E(t,x) f_{\xi} &= 0 \\ E_x &= \int_{\mathbb{R}} f(t,x,\xi) d\xi - c. \end{split}$$

However, this description is inadequate where the electric field E(t, x) also becomes multi-valued.

- Lagrangian approach may be applied to handle the multi-valued electric field [Gosse-Mauser (06)].
- We shall adopt a geometric point of view...

Consider an augmented field space,

(x, p, q),

with

$$p = u(t, x),$$
$$q = E(t, x),$$

so that

$$(u, E) \in \{(p, q), \quad \Phi(t, x, p, q) = 0\}.$$

A key equation for deriving the level set dynamics is

$$E_t + uE_x = -cu.$$

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Level set formulation for u and E

Let u(t, x) and E(t, x) be any solution of the EP system and be determined by

$$\Phi(t,x,u(t,x),E(t,x))=0, \quad \Phi=(\phi_1,\phi_2)^T\in\mathbb{R}^2.$$

The level set equation reads

$$\Phi_t + p\phi_x + Kq\Phi_p - cp\Phi_q = 0, \quad \Phi \in \mathbb{R}^2.$$
(11)

Initialization:

•
$$\phi_1(0, x, p, q) = p - u_0(x),$$

- $\bullet \ \phi_2(0,x,p,q) = q E_0(x), \quad E_0 \leftarrow \rho_0.$
- The projection of common zeros of Φ onto the physical space gives multi-values of u and E.

By projection of a density representative $\tilde{\rho}(t, x, p, q)$ onto the manifold

$$M = \{(p,q) | \phi_1 = 0, \phi_2 = 0\},\$$

the density $\overline{\rho}(t, x)$ can be evaluated by

$$\overline{\rho}(t,x) = \int f(t,x,p,q)\delta(\phi_1)\delta(\phi_2)dpdq,$$

where

$$f_t + pf_x + Kqf_p - cpf_q = 0, \quad f(0, x, p, q) = \rho_0(x).$$

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One could also compute the density $\bar{\rho}$ by solving the field transport equation

$$\partial_t \eta + p \partial_x \eta + K q \partial_p \eta - c(x) p \partial_q \eta = 0,$$

subject to initial data involving delta functions,

$$\eta(0, x, p, q) = \rho_0(x)\delta(p - u_0(x))\delta(q - E_0(x)).$$

The density is then evaluated by

$$ar{
ho} = \int \eta d
ho d
ho dq.$$

Level set method

$$\rho_i \in \left\{ \frac{f}{\left| \det \left(\frac{\partial(\phi_1, \phi_2)}{\partial(p, q)} \right) \right|} \middle| \phi_1 = 0, \phi_2 = 0 \right\},\$$

where ϕ_1, ϕ_2 are two level set functions needed to determine both multi-valued velocity u and electric field E, and f solves the same level set equation in field space (x, p, q), subject to the given initial density ρ_0 .

Superposition principle

$$\bar{\rho}(t,x) = \sum_{i=1}^{N} \rho_i(t,x).$$

C. Periodic structure

The re-scaled Schrödinger equation

$$\begin{split} i\epsilon\partial_t\psi &= -\frac{\epsilon^2}{2}\partial_x\left(a\left(\frac{x}{\epsilon}\right)\partial_x\psi\right) + V\left(\frac{x}{\epsilon}\right)\psi + V_e(x)\psi,\\ \psi(0,x) &= \exp\left(\frac{iS_0}{\epsilon}\right)f\left(x,\frac{x}{\epsilon}\right), \end{split}$$

where the lattice potential V and a > 0 are 2π - periodic functions and V_e is a given smooth function.

Scale separation leads to a shifted cell problem

$$A(k, y)Z_n(y) = E_n(k)Z_n(y), \quad Z \in H^1(0, 2\pi).$$

The wave field can be then decomposed (Bloch waves) as

$$\psi^{\epsilon} = \sum_{j} a_{j}(t, x) Z_{j}(k, y) e^{iS_{j}(t, x)/\epsilon}, \quad y = \frac{x}{\epsilon}, \quad k = \nabla_{x} S_{j}.$$

► In each Bloch band associated with E_n , one solves a WKB system with Hamiltonian $H_n(k, x) = E_n(k) + V_e(x)$

$$\partial_t S + E_n(\nabla_x S) + V_e(x) = 0.$$

Our aim: (1) to develop a level set method to capture the field statistics in each band.

(2) to reconstruct the wave field from the obtained field statistics in each band

- This work is in progress ...
- Ref: [1] Bensoussan, Lions and Papanicolaou (1978)(before caustics)[2] L.Gosse and P.A. Markowich (2004) (computing multi-valued solutions).

- Optical waves
- Superposition of multi-valued solutions
- Euler-Poisson equations

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Contracting ellipse in 2D



Contracting ellipse in 2D



SUPERPOSITION IN HIGH FREQUENCY WAVE DYNAMICS



FIGURE 7. Example 4, at t = 0.3515. Sub-figures, from up left, are velocity, $g = 1, g = \nabla_p H$ and g = H with $\tilde{\epsilon} = 0.01$ and $\epsilon = 2h$. Circle and solid line represent the results from integration and superposition.

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FIGURE 9. Example 2, at t = 1.00700. Sub-figures, from up left, are velocity, $g = 1, g = \nabla_p H$ and g = H with $\tilde{\epsilon} = 0.01$ and $\epsilon = h$. Circle and solid line represent the results from integration and superposition.

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$$c = 0$$
, $K = 0.01$, $u(0, x) = \sin^3(x)$, $\rho(0, x) = \frac{1}{\pi}e^{-(x-\pi)^2}$



In this figure and what follows, solid blue line is the exact solution while red dots are numerical results.

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density profile

 ρ



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$$c = 0$$
, $K = -1$, $u(0, x) = 0.01$, $\rho(0, x) = \frac{1}{\pi}e^{-(x-\pi)^2}$



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density ρ

$$c = 0$$
, $K = -1$, $u(0, x) = 0.01$, $\rho(0, x) = \frac{1}{\pi}e^{-(x-\pi)^2}$



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$$c = 1$$
, $K = 1$, $u(0, x) = 2\sin^4 x$, $\rho(0, x) = 1$



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density profile ρ

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, $K = 1$, $u(0, x) = 2\sin^4 x$, $\rho(0, x) = 1$



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We have presented

- A rigorous derivation of the rotational super-fluid model as a semiclassical limit of the GPE;
- Several configuration space based level set methods for capturing semi-classical limit in Schrödinger equations with different potentials
 - The level set equation is derived from the WKB approximation, independent of the Wigner approach;
 - The geometric solution set captured by the level set method gives much more information than the kinetic formulation; In particular, the jet space method offers the multi-valued phase.
 - The techniques discussed here are naturally geometrical and well suited for handling multi-valued solutions, arising in a large class of highly oscillatory problems.