On the classical limit of a time-dependent self-consistent field system: analysis and computation

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Outline

The numerical simulation of many chemical, physical, and biochemical phenomena requires the direct simulation of dynamical processes within large systems involving quantum mechanical effects.

1. However, if the entire system is treated quantum mechanically...
   - curse of dimensionality
   - relatively short time scale, small model
2. Full classical approximation.
   - losing quantum mechanical information
3. Separating degrees of freedom:
   - slow-time scale (large spatial scale): effectively classical (e.g., nuclei);
   - fast-time scale: quantum mechanical (e.g., electrons).

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The studies on the separation of the whole system into a classical part and a quantum mechanical part often lead to what is called time-dependent self-consistent field equations (TDSCF).

One typically assumes that the total wave function of the system $\Psi(t, X)$, with $X = (x, y)$, can be approximated by

$$\Psi(X, t) \approx \psi(x, t) \times \varphi(y, t) \times \text{phase},$$

where x and y denote the degrees of freedom within a certain subsystem, only.
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In the following, we take $x \in \mathbb{R}^d$, $y \in \mathbb{R}^n$, with $d, n \in \mathbb{N}$. The total Hamiltonian of the system acting on $L^2(\mathbb{R}^{d+n})$ is assumed to be of the form

$$H = -\frac{\delta^2}{2}\Delta_x - \frac{\varepsilon^2}{2}\Delta_y + V(x, y), \tag{1}$$

where $V(x, y) \in \mathbb{R}$ is the real-valued potential.

- In (1), the Hamiltonian is in a dimensionless form;
- two (small) parameters $\varepsilon, \delta > 0$ remain, the dimensionless Planck's constants.

The TDSCF system at hand is then the following system of self-consistently coupled Schrödinger equations

$$\begin{cases} i\delta\partial_t\psi^{\varepsilon,\delta} = \left(-\dfrac{\delta^2}{2}\Delta_x + \langle\varphi^{\varepsilon,\delta}, V\varphi^{\varepsilon,\delta}\rangle_{L^2_y}\right)\psi^{\varepsilon,\delta}, \quad \psi^{\varepsilon,\delta}_{|t=0} = \psi^{\delta}_{\text{in}}(x), \\ i\varepsilon\partial_t\varphi^{\varepsilon,\delta} = \left(-\dfrac{\varepsilon^2}{2}\Delta_y + \langle\psi^{\varepsilon,\delta}, h^{\delta}\psi^{\varepsilon,\delta}\rangle_{L^2_x}\right)\varphi^{\varepsilon,\delta}, \quad \varphi^{\varepsilon,\delta}_{|t=0} = \varphi^{\varepsilon}_{\text{in}}(y), \end{cases} \tag{2}$$

where we denote by

$$h^{\delta} = -\frac{\delta^2}{2}\Delta_x + V(x,y), \tag{3}$$

the electronic Hamiltonian.

Coupling potentials

The coupling terms are explicitly given by

$$\langle \varphi^{\varepsilon,\delta}, V\varphi^{\varepsilon,\delta}\rangle_{L^2_y} = \int_{\mathbb{R}^n_y} V(x,y)|\varphi^{\varepsilon,\delta}(y,t)|^2\,dy =: \Upsilon^{\varepsilon,\delta}(x,t),$$

and after formally integrating by parts

$$\langle \psi^{\varepsilon,\delta}, h^\delta\psi^{\varepsilon,\delta}\rangle_{L^2_x} = \int_{\mathbb{R}^d_x} \frac{\delta^2}{2}|\nabla\psi^{\varepsilon,\delta}(x,t)|^2 + V(x,y)|\psi^{\varepsilon,\delta}(x,t)|^2\,dx =: \Lambda^{\varepsilon,\delta}(y,t).$$

Both $\Upsilon^{\varepsilon,\delta}$ and $\Lambda^{\varepsilon,\delta}$ are

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Mass conservation

The total masses of the system,

$$M^{\varepsilon,\delta}(t) := \|\psi^{\varepsilon,\delta}(\cdot,t)\|_{L_x^2}^2 + \|\varphi^{\varepsilon,\delta}(\cdot,t)\|_{L_y^2}^2 \equiv m_1^{\varepsilon,\delta}(t) + m_2^{\varepsilon,\delta}(t). \quad (4)$$

where $m_1^{\varepsilon,\delta}$, $m_2^{\varepsilon,\delta}$ denote the masses of the respective subsystem. We can prove that,

$$m_1^{\varepsilon,\delta}(t) = m_1^{\varepsilon,\delta}(0), \quad m_2^{\varepsilon,\delta}(t) = m_2^{\varepsilon,\delta}(0), \quad \forall\, t \in \mathbb{R}.$$

We shall, from now on assume that the initial data is normalized such that $m_1^{\varepsilon,\delta}(0) = m_2^{\varepsilon,\delta}(0) = 1$.

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Energy conservation

The total energy of the system can be written as

$$E^{\varepsilon,\delta}(t) := \frac{\delta^2}{2}\|\nabla\psi^{\varepsilon,\delta}(\cdot,t)\|_{L_x^2}^2 + \frac{\varepsilon^2}{2}\|\nabla\varphi^{\varepsilon,\delta}(\cdot,t)\|_{L_y^2}^2 + \iint_{\mathbb{R}^{d+n}} V(x,y)|\psi^{\varepsilon,\delta}(x,t)|^2|\varphi^{\varepsilon,\delta}(y,t)|^2\,dx\,dy. \tag{5}$$

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- We can also prove, with fixed ε and δ, the global existence of the solutions to the TDSCF system.
- However, as $\varepsilon \to 0$ and $\delta \to 0$, the highly oscillatory wave functions $\varphi^{\varepsilon,\delta}$ and $\psi^{\varepsilon,\delta}$ do not converge in a strong sense...
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  1. the physical observables (e.g., $\rho = |\psi|^2$);
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The semi-classical analysis: the Wigner transform

Previously, people have studied the classical limits of the TDSCF system by the classical WKB approximation, but we believe the Wigner transform is superior in many aspects:

1. the classical limit has global existence;
2. the convergence of the Wigner transform implies the convergence of physical observables.
3. it helps to design a better numerical scheme.

The Wigner transform

Denote by $\{f^\varepsilon\}_{0<\varepsilon\leqslant 1}$ a family of functions $f^\varepsilon \in L^2(\mathbb{R}^d)$, depending continuously on a small parameter $\varepsilon > 0$. The associated ε-scaled Wigner transform is then given by:

$$w^\varepsilon[f^\varepsilon](x,\xi) := \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} f^\varepsilon\left(x-\frac{\varepsilon}{2}z\right)\overline{f^\varepsilon}\left(x+\frac{\varepsilon}{2}z\right)e^{iz\cdot\xi}\,dz. \quad (6)$$

$$|f^\varepsilon(x)|^2 = \int_{\mathbb{R}^d} w^\varepsilon(x,\xi)\,d\xi. \quad \varepsilon \mathrm{Im}(\bar{f}^\varepsilon(x)\nabla f^\varepsilon(x)) = \int_{\mathbb{R}^d} \xi w^\varepsilon(x,\xi)\,d\xi.$$

For the expectation value of any Weyl-quantized operator $\mathrm{Op}^\varepsilon(a)$, corresponding to a classical symbol $a(x,\xi) \in \mathcal{S}(\mathbb{R}^d_x \times \mathbb{R}^d_\xi)$, one finds

$$\langle f^\varepsilon, \mathrm{Op}^\varepsilon(a) f^\varepsilon\rangle_{L^2_x} = \iint_{\mathbb{R}^{2d}} a(x,\xi) w^\varepsilon[f^\varepsilon](dx,d\xi),$$

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The Wigner measure

Under certain conditions,

$$w^\varepsilon[f^\varepsilon] \overset{\varepsilon\to 0_+}{\longrightarrow} \mu \quad \text{in } \mathcal{S}'(\mathbb{R}^d_x \times \mathbb{R}^d_\xi) \text{ weak}^*.$$

$$\lim_{\varepsilon\to 0_+} \langle f^\varepsilon, \mathrm{Op}^\varepsilon(a) f^\varepsilon\rangle_{L^2_x} = \iint_{\mathbb{R}^{2d}} a(x,p)\mu(dx,d\xi), \tag{7}$$

If $f^\varepsilon \in C_b(\mathbb{R}_t; L^2(\mathbb{R}^d))$ solves

$$i\varepsilon\partial_t f^\varepsilon = -\frac{\varepsilon^2}{2}\Delta f^\varepsilon + V(x) f^\varepsilon, \quad f^\varepsilon_{|t=0} = f^\varepsilon_{\mathrm{in}}(x),$$

then the Wigner measures μ solves

$$\partial_t \mu + \xi\cdot\nabla_x\mu - \nabla_x V(x)\cdot\nabla_\xi\mu = 0, \quad \mu_{|t=0} = \mu_{\mathrm{in}}(x,\xi), \tag{8}$$

in the sense of distributions $\mathcal{D}'(\mathbb{R}^d_x \times \mathbb{R}^d_\xi \times \mathbb{R}_t)$.

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Recall, the TDSCF equations

$$\begin{cases} i\delta\partial_t\psi^{\varepsilon,\delta} = \left(-\dfrac{\delta^2}{2}\Delta_x + \langle\varphi^{\varepsilon,\delta}, V\varphi^{\varepsilon,\delta}\rangle_{L^2_y}\right)\psi^{\varepsilon,\delta}, \quad \psi^{\varepsilon,\delta}_{|t=0} = \psi^{\delta}_{\text{in}}(x), \\ i\varepsilon\partial_t\varphi^{\varepsilon,\delta} = \left(-\dfrac{\varepsilon^2}{2}\Delta_y + \langle\psi^{\varepsilon,\delta}, h^{\delta}\psi^{\varepsilon,\delta}\rangle_{L^2_x}\right)\varphi^{\varepsilon,\delta}, \quad \varphi^{\varepsilon,\delta}_{|t=0} = \varphi^{\varepsilon}_{\text{in}}(y), \end{cases} \tag{9}$$

- Mixed quantum-classical limit: $\varepsilon \to 0_+$ with δ fixed.
- Full classical limit: $\varepsilon \to 0_+$, $\delta \to 0_+$.

Mixed quantum-classical limit

Under certain assumptions, for any $T > 0$, it holds

$$\psi^{\varepsilon,\delta} \overset{\varepsilon\to 0_+}{\longrightarrow} \psi^{\delta} \quad \text{in } L^\infty([0,T];L^2_y(\mathbb{R}^n)),$$

$$w^{\varepsilon}[\varphi^{\varepsilon,\delta}] \overset{\varepsilon\to 0_+}{\longrightarrow} \mu^{\delta} \quad \text{in } L^\infty([0,T];\mathcal{S}'(\mathbb{R}^n_y\times\mathbb{R}^n_\eta)) \text{ weak}^*,$$

where ψ^δ and μ^δ solve the mixed quantum-classical system

$$\begin{cases} i\delta\partial_t\psi^\delta = \left(-\dfrac{\delta^2}{2}\Delta_x + \Upsilon^\delta(x,t)\right)\psi^\delta\,, \quad \psi^\delta_{|t=0} = \psi^\delta_{\text{in}}(x), \\ \partial_t\mu^\delta + \eta\cdot\nabla_y\mu^\delta + F^\delta(y,t)\cdot\nabla_\eta\mu^\delta = 0\,, \quad \mu^\delta_{|t=0} = \mu_{\text{in}}(y,\eta). \end{cases} \tag{10}$$

Here μ_{in} is obtained as the weak* limit of $w^\varepsilon[\varphi^\varepsilon_{\text{in}}]$ and $\Upsilon^\delta(x,t) = \iint_{\mathbb{R}^{2n}} V(x,y)\mu^\delta(dy,d\eta,t)$, $F^\delta(y,t) = -\int_{\mathbb{R}^d}\nabla_y V(x,y)|\psi^\delta(x,t)|^2\,dx$.

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Connection to Ehrenfest method

In particular, if $\mu_0(y,\eta) = \delta(y - y_0, \eta - \eta_0)$, i.e. a delta distribution centered at $(y_0, \eta_0) \in \mathbb{R}^{2n}$, this yields $\mu^\delta(y,\eta,t) = \delta(y - y(t), \eta - \eta(t))$, for all times $t \in \mathbb{R}$.
The mixed quantum-classical system becomes (Ehrenfest model)

$$\begin{cases} i\delta\partial_t\psi^\delta = \left(-\dfrac{\delta^2}{2}\Delta_x + V(x,y(t))\right)\psi^\delta\,, \quad \psi^\delta_{|t=0} = \psi^\delta_{\text{in}}(x), \\ \ddot{y}(t) = -\displaystyle\int_{\mathbb{R}^d} \nabla_y V(x,y(t))|\psi^\delta(x,t)|^2\,dx, \quad y_{|t=0} = y_0,\ \dot{y}_{|t=0} = \eta_0, \end{cases} \tag{11}$$

Full classical limit

From the mixed quntum-classical limit: the Wigner transform

$$W^\delta \overset{\delta\to 0_+}{\longrightarrow} \nu \quad \text{in } L^\infty([0,T];\mathcal{S}'(\mathbb{R}^d_x\times\mathbb{R}^d_\xi))\,\text{weak}^*,$$

and the Wigner measure

$$\mu^\delta \overset{\delta\to 0_+}{\longrightarrow} \mu \quad \text{in } L^\infty([0,T];\mathcal{M}^+(\mathbb{R}^n_y\times\mathbb{R}^n_\eta))\,\text{weak}^*.$$

From TDSCF equation, $\delta=\varepsilon$, the associated limiting Wigner measures $\mu,\nu\in\mathcal{M}^+$, such that

$$w^\varepsilon[\varphi^\varepsilon] \overset{\varepsilon\to 0_+}{\longrightarrow} \mu \quad \text{in } L^\infty(\mathbb{R}_t;\mathcal{S}'(\mathbb{R}^d_y\times\mathbb{R}^d_\eta))\,\text{weak}^*,$$

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$\nu \in C(\mathbb{R}_t; \mathcal{M}^+(\mathbb{R}^d_x \times \mathbb{R}^d_\xi))$ and $\mu \in C(\mathbb{R}_t; \mathcal{M}^+(\mathbb{R}^n_y \times \mathbb{R}^n_\eta))$ solve the following coupled system of Vlasov-type equations

$$\begin{cases} \partial_t \nu + \xi \cdot \nabla_x \nu - \nabla_x \Upsilon(x,t) \cdot \nabla_\xi \nu = 0\,, \quad \nu_{|t=0} = \nu_{\text{in}}(x,\xi), \\ \partial_t \mu + \eta \cdot \nabla_y \mu - \nabla_x \Lambda(y,t) \cdot \nabla_\eta \mu = 0\,, \quad \mu_{|t=0} = \mu_{\text{in}}(y,\eta), \end{cases} \tag{12}$$

where

$$\Upsilon(x,t) = \iint_{\mathbb{R}^{2n}} V(x,y)\mu(dy,d\eta,t),$$

$$\Lambda(y,t) = \iint_{\mathbb{R}^{2d}} V(x,y)\nu(dx,d\xi,t).$$

Note that system (12) admits a special solution of the form

$$\nu(x,\xi,t)=\delta(x-x(t),\xi-\xi(t)),\quad \mu(y,\eta,t)=\delta(y-y(t),\eta-\eta(t)),$$

where $x(t),y(t),\xi(t),\eta(t)$ solve the following Hamiltonian system:

$$\begin{cases}\dot{x}(t)=\xi(t), & x(0)=x_0,\\ \dot{\xi}(t)=-\nabla_x V(x(t),y(t)), & \xi(0)=\xi_0,\\ \dot{y}(t)=\eta(t), & y(0)=y_0,\\ \dot{\eta}(t)=-\nabla_y V(x(t),y(t)), & \eta(0)=\eta_0.\end{cases}$$

Summary

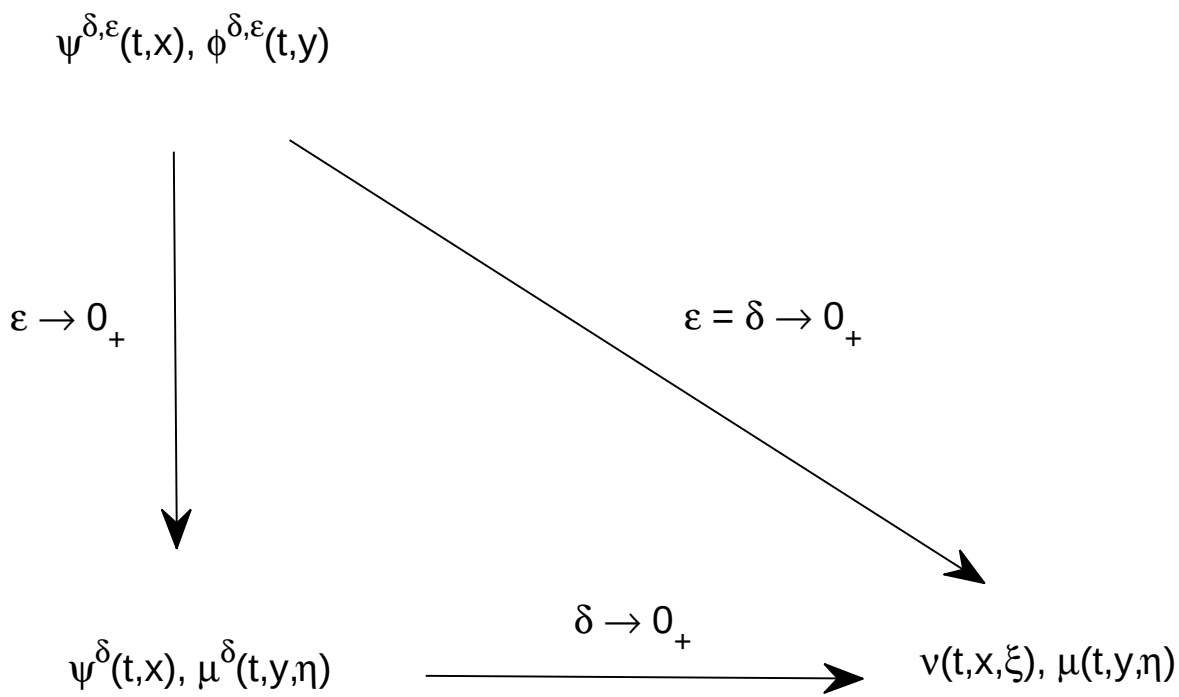

Figure: The diagram of semi-classical limits: the iterated limit and the classical limit.

In our numerical context, we will consider the semi-classically scaled TDSCF equations (9) where in one spatial dimension and subject to periodic boundary conditions, i.e.

$$\begin{cases} i\delta\partial_t\psi^{\varepsilon,\delta} = \left(-\dfrac{\delta^2}{2}\Delta_x + \Upsilon^{\varepsilon,\delta}(x,t)\right)\psi^{\varepsilon,\delta}, \quad a<x<b, \quad \psi^{\varepsilon,\delta}_{|t=0} = \psi^{\delta}_{\text{in}}(x), \\ i\varepsilon\partial_t\varphi^{\varepsilon,\delta} = \left(-\dfrac{\varepsilon^2}{2}\Delta_y + \Lambda^{\varepsilon,\delta}(y,t)\right)\varphi^{\varepsilon,\delta}, \quad a<y<b, \quad \varphi^{\varepsilon,\delta}_{|t=0} = \varphi^{\varepsilon}_{\text{in}}(y). \end{cases} \tag{13}$$

The numerical method SSP2

- work for all ε and δ, even if $\varepsilon \ll 1$ or $\delta \ll 1$,
- second order time in time, spectral accuracy in space,
- can still capture correct physical observables with $O(1)$ time steps,
- it can be naturally extended to the multi-dimensional case.

In our numerical context, we will consider the semi-classically scaled TDSCF equations (9) where in one spatial dimension and subject to periodic boundary conditions, i.e.

$$\begin{cases} i\delta\partial_t\psi^{\varepsilon,\delta} = \left(-\dfrac{\delta^2}{2}\Delta_x + \Upsilon^{\varepsilon,\delta}(x,t)\right)\psi^{\varepsilon,\delta}, \quad a < x < b, \quad \psi^{\varepsilon,\delta}_{|t=0} = \psi^{\delta}_{\text{in}}(x), \\ i\varepsilon\partial_t\varphi^{\varepsilon,\delta} = \left(-\dfrac{\varepsilon^2}{2}\Delta_y + \Lambda^{\varepsilon,\delta}(y,t)\right)\varphi^{\varepsilon,\delta}, \quad a < y < b, \quad \varphi^{\varepsilon,\delta}_{|t=0} = \varphi^{\varepsilon}_{\text{in}}(y). \end{cases} \tag{13}$$

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Semi-classical Schrödinger equation ($\varepsilon \ll 1$): oscillations both in space and time $O(\varepsilon)$.

Previously, (*2002 Bao, Jin and Markowich*) if $f^\varepsilon \in C_{\rm b}(\mathbb{R}_t; L^2(\mathbb{R}^d))$ solves

$$i\varepsilon\partial_t f^\varepsilon = -\frac{\varepsilon^2}{2}\Delta f^\varepsilon + V(x)f^\varepsilon, \quad f^\varepsilon_{|t=0} = f^\varepsilon_{\rm in}(x),$$

then by the time-splitting spectral method (TSSP),

- wave function: $\Delta x \sim O(\varepsilon)$ and $\Delta t = O(\varepsilon)$;
- physical observables: $\Delta x = O(\varepsilon)$ and $\Delta t = O(1)$.

The construction of our numerical method for (13) is based on the following operator splitting technique. For every time step $t \in [t^n, t^{n+1}]$, we solve the kinetic step

$$\begin{cases} i\delta\partial_t\psi^{\varepsilon,\delta} = -\dfrac{\delta^2}{2}\Delta_x\psi^{\varepsilon,\delta}, \\ i\varepsilon\partial_t\varphi^{\varepsilon,\delta} = -\dfrac{\varepsilon^2}{2}\Delta_y\varphi^{\varepsilon,\delta}; \end{cases} \tag{14}$$

and the potential step

$$\begin{cases} i\delta\partial_t\psi^{\varepsilon,\delta} = \Upsilon^{\varepsilon,\delta}(x,t)\psi^{\varepsilon,\delta}, \\ i\varepsilon\partial_t\varphi^{\varepsilon,\delta} = \Lambda^{\varepsilon,\delta}(y,t)\varphi^{\varepsilon,\delta}; \end{cases} \tag{15}$$

possibly for some fractional time steps in a specific order. (e.g., Strang splitting.)

The kinetic step

Let U_j^n be the numerical approximation of the wave functions at $x = x_j$ and $t = t_n$. Then, the kinetic step can be solved exactly in Fourier space via:

$$U_j^* = \frac{1}{N} \sum_{l=-N/2}^{N/2-1} e^{-i\delta(\varepsilon)\Delta t \mu_l^2/2} \hat{U}_l^n e^{i\mu_l(x_j-a)},$$

where $\hat{U}_l^n$ are the Fourier coefficients of U_j^n, defined by

$$\hat{U}_l^n = \sum_{j=0}^{N-1} U_j^n e^{-i\mu_l(x_j-a)}, \quad \mu_l = \frac{2\pi l}{b-a}, \quad l = -\frac{N}{2}, \cdots, \frac{N}{2}-1.$$

On the other hand, for the potential step (15) with $t_1 < t < t_2$, we formally find

$$\psi^{\varepsilon,\delta}(x, t_2) = \exp\left(-\frac{i}{\delta}\int_{t_1}^{t_2} \Upsilon^{\varepsilon,\delta}(x, s)\, ds\right) \psi^{\varepsilon,\delta}(x, t_1), \tag{16}$$

$$\varphi^{\varepsilon,\delta}(y, t_2) = \exp\left(-\frac{i}{\varepsilon}\int_{t_1}^{t_2} \Lambda^{\varepsilon,\delta}(y, s)\, ds\right) \varphi^{\varepsilon,\delta}(y, t_1), \tag{17}$$

where $0 < t_2 - t_1 \leq \Delta t$.

If we approximate the the time integrals by a quadrature rule:

- The discrete mass is conserved.
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- *It may result in an implicit scheme.*

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In the full dynamics, the coupling potentials $\Upsilon^{\varepsilon,\delta}$ and $\Lambda^{\varepsilon,\delta}$ are time dependent.

However, within the potential step,

$$\partial_t \Upsilon^{\varepsilon,\delta} = \frac{1}{i\varepsilon} \left\langle \varphi^{\varepsilon,\delta}, \left(V\Lambda^{\varepsilon,\delta} - \Lambda^{\varepsilon,\delta} V \right) \varphi^{\varepsilon,\delta} \right\rangle_{L^2_y} = 0.$$

$$\partial_t \Lambda^{\varepsilon,\delta} = \frac{1}{2} \left\langle \psi^{\varepsilon,\delta}, \nabla_x \Upsilon^{\varepsilon,\delta} \cdot (i\delta\nabla_x) \psi^{\varepsilon,\delta} \right\rangle_{L^2_x} + \frac{i\delta}{2} \left\langle \psi^{\varepsilon,\delta}, \Delta_x \Upsilon^{\varepsilon} \psi^{\varepsilon,\delta} \right\rangle_{L^2_x} = O(1).$$

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$$\psi^{\varepsilon,\delta}(x,t_2) = \exp\left(-\frac{i(t_1-t_2)}{\delta}\Upsilon^{\varepsilon,\delta}(x,t_1)\right)\psi^{\varepsilon,\delta}(x,t_1). \tag{18}$$

This is an *exact* solution formula for $\psi^{\varepsilon,\delta}$ at $t = t_2$.

$$\varphi^{\varepsilon,\delta}(y,t_2) \approx \exp\left(-\frac{i(\Lambda^{\varepsilon,\delta}(y,t_2)+\Lambda^{\varepsilon,\delta}(y,t_1))(t_1-t_2)}{2\varepsilon}\right)\varphi^{\varepsilon,\delta}(y,t_1). \tag{19}$$

This approximation introduces a phase error of order $O(\Delta t^2/\varepsilon)$.

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This numerical scheme has the following features:

1. discrete mass conserved.
2. second order in time, spectral accuracy in space.

We name this method method the Strang splitting spectral method (SSP2).

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- In the semi-classical regime, wave function: $\Delta x = O(\delta, \varepsilon)$, $\Delta t = O(\delta, \varepsilon)$.

Assume $\delta = \varepsilon \ll 1$, $\Lambda^\varepsilon(y,t)$, $t_1 < t < t_2$ is known. Consider,

$$i\varepsilon\partial_t\varphi^\varepsilon = \Lambda^\varepsilon(y,t)\varphi^\varepsilon, \quad t_1 < t < t_2,$$

where its Wigner transform $W^\varepsilon = w^\varepsilon[\varphi^\varepsilon]$ satisfies

$$\partial_t W^\varepsilon - \nabla_y \Lambda^\varepsilon(y,t)\cdot\nabla_\eta W^\varepsilon + O(\varepsilon) = 0.$$

The potential step for φ^ε can be viewed as the exact solution to

$$i\varepsilon\partial_t\tilde{\varphi}^\varepsilon = G^\varepsilon(y)\tilde{\varphi}^\varepsilon, \quad t_1 < t < t_2,$$

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$$G^\varepsilon(y) = \frac{1}{2}(\Lambda^\varepsilon(y,t_1) + \Lambda^\varepsilon(y,t_2)).$$

If one denotes the Wigner transform of $\tilde{\varphi}^{\varepsilon}(y,t)$ by $\tilde{w}^{\varepsilon}(y,\eta,t)$, then,

$$\partial_t \tilde{w}^{\varepsilon} - \nabla_y G^{\varepsilon} \cdot \nabla_\eta \tilde{w}^{\varepsilon} + O(\varepsilon) = 0. \tag{20}$$

By the method of characteristics, the discrepancy between W^{ε} and $\tilde{w}^{\varepsilon}$ at $t = t_2$ is clearly

$$W^{\varepsilon} - \tilde{w}^{\varepsilon} = O\left(\Delta t^3\right) + O\left(\varepsilon \Delta t\right).$$

- Thus, for fixed Δt, and as $\varepsilon \to 0_+$, this one-step error in computing the physical observables is dominated by $O(\Delta t^3)$, which is comparable to the operator splitting error.
- we consequently can take ε-*independent* time steps for accurately computing semi-classical behavior of physical observables: $\Delta x = O(\varepsilon)$, $\Delta t = O(1)$.

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- we consequently can take ε-*independent* time steps for accurately computing semi-classical behavior of physical observables: $\Delta x = O(\varepsilon)$, $\Delta t = O(1)$.

Consider a (semi-classical) Schrödinger equation coupled with Hamilton's equations for a classical point particle, i.e

$$\begin{cases} i\delta\partial_t\psi^\delta = \left(-\dfrac{\delta^2}{2}\Delta_x + V(x,y(t))\right)\psi^\delta\,, \quad a<x<b\,, \\ \dot{y}(t)=\eta(t), \quad \dot{\eta}(t) = -\displaystyle\int_{\mathbb{R}^d} \nabla_y V\left(x,y(t)\right)|\psi^\delta(x,t)|^2\,dx, \end{cases} \tag{21}$$

with initial conditions

$$\psi^\varepsilon_{|t=0} = \psi^\varepsilon_{\text{in}}(x), \quad y_{|t=0} = y_0, \quad \eta_{|t=0} = \eta_0,$$

and subject to periodic boundary conditions.
In a very similar fashion, we can design the SVSP2 method.

Numerical tests

The SSP2 method:

- spectral accuracy in space: $\Delta x = O(\delta)$, $\Delta y = O(\varepsilon)$.
- second order convergence in time.
- it allows large time steps to calculate correct physical observables.

Error tests:

- wave function: test l^2 norm.
- physical observables (e.g., $|\psi|^2$): test l^1 norm.

Spatial convergence test I

$\delta = 1, \varepsilon = \frac{1}{1024}$.

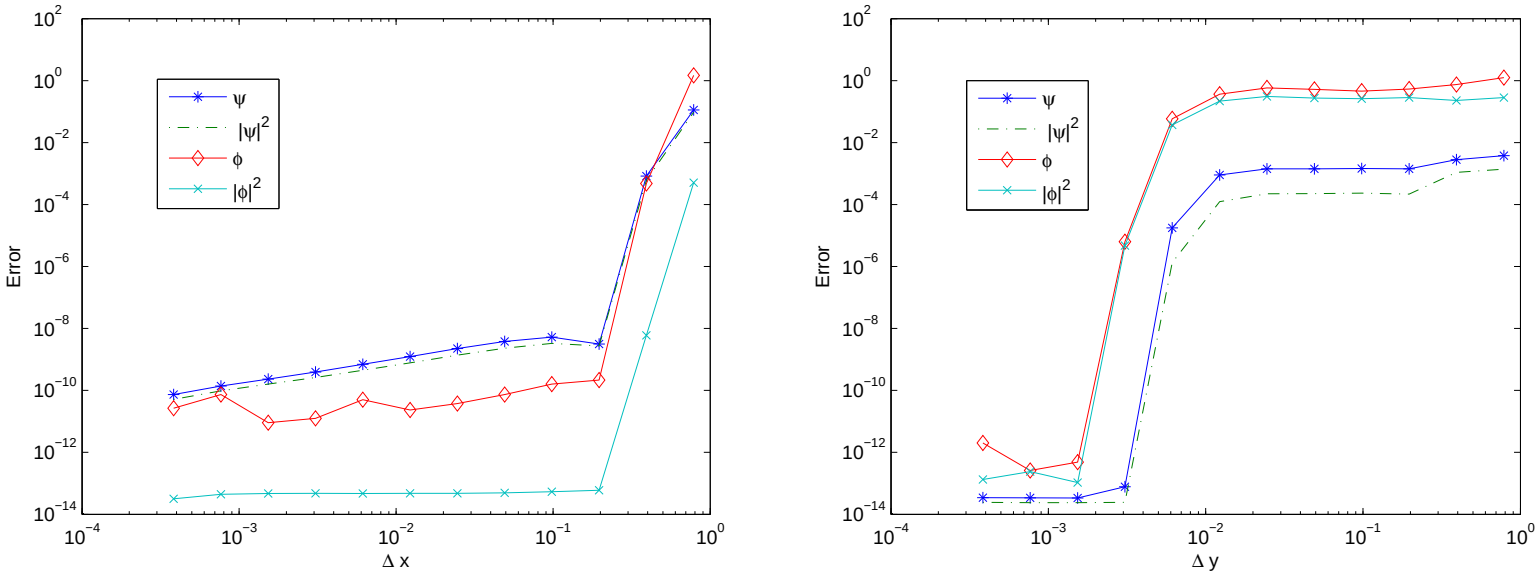

Figure: Reference solution: $\Delta x = \Delta y = \frac{2\pi}{32768}$ and $\Delta t = \frac{0.4}{4096}$. Upper picture: fix $\Delta y = \frac{2\pi}{32768}$ and $\Delta t = \frac{0.4}{4096}$, take $\Delta x = \frac{2\pi}{16384}, \frac{2\pi}{8192}, \frac{2\pi}{4096}, \frac{2\pi}{2048}, \frac{2\pi}{1024}, \frac{2\pi}{512}, \frac{2\pi}{256}, \frac{2\pi}{128}, \frac{2\pi}{64}, \frac{2\pi}{32}, \frac{2\pi}{16}, \frac{2\pi}{8}$. Lower Picture: fix $\Delta x = \frac{2\pi}{32768}$ and $\Delta t = \frac{0.4}{4096}$, take $\Delta y = \frac{2\pi}{16384}, \frac{2\pi}{8192}, \frac{2\pi}{4096}, \frac{2\pi}{2048}, \frac{2\pi}{1024}, \frac{2\pi}{512}, \frac{2\pi}{256}, \frac{2\pi}{128}, \frac{2\pi}{64}, \frac{2\pi}{32}, \frac{2\pi}{16}, \frac{2\pi}{8}$.

Spatial convergence test II

$$\delta = \varepsilon = \frac{1}{256},$$

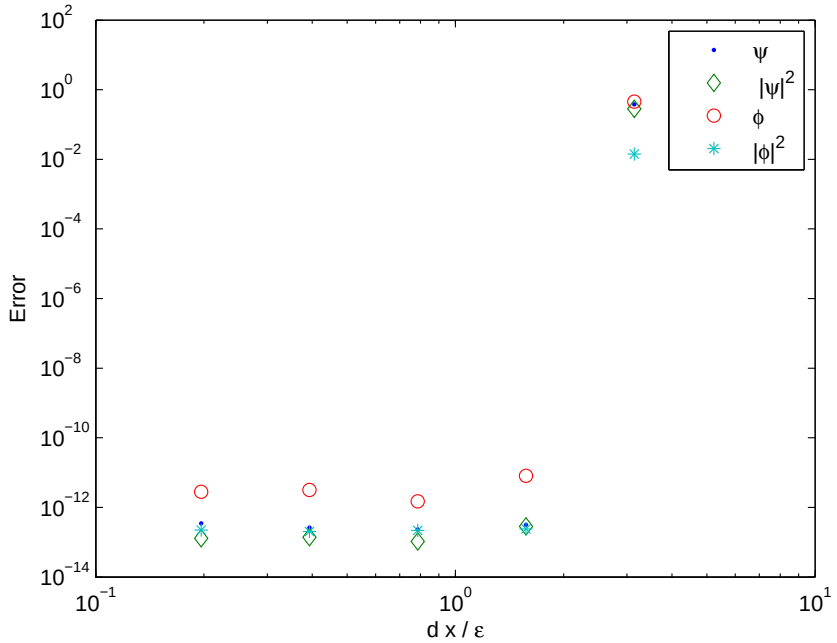

Figure: Fix $\varepsilon = \frac{1}{256}$ and $\Delta t = \frac{0.4\varepsilon}{16}$. Take $\Delta x = \frac{2\pi\varepsilon}{32}, \frac{2\pi\varepsilon}{16}, \frac{2\pi\varepsilon}{8}, \frac{2\pi\varepsilon}{4}, \frac{2\pi\varepsilon}{2}$ and $\frac{2\pi\varepsilon}{1}$ respectively. The reference solution is computed with the same Δt, but $\Delta x = \frac{2\pi\varepsilon}{64}$.

Time convergence test I

$\delta = 1, \varepsilon = \frac{1}{1024}$.

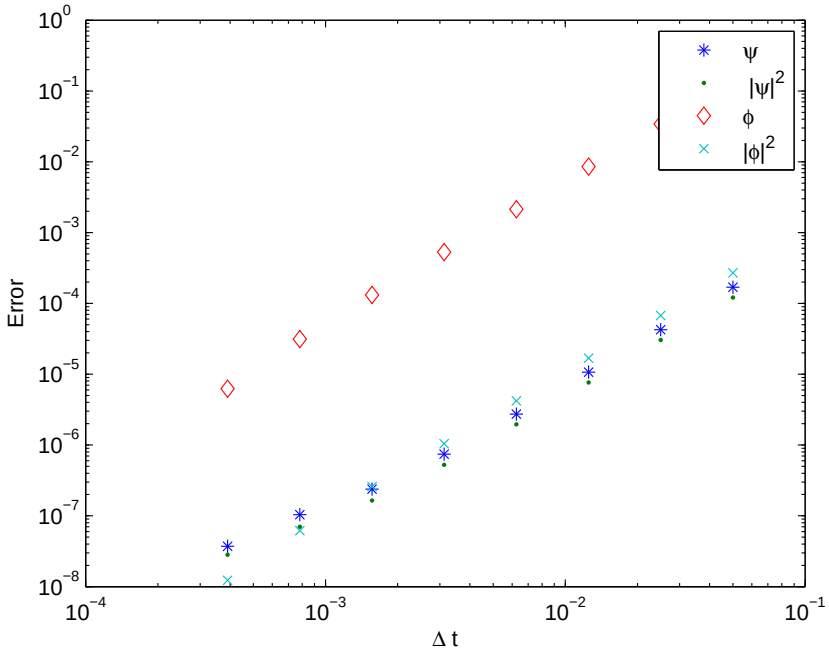

Figure: Reference solution: $\Delta x = \frac{2\pi}{512}$, $\Delta y = \frac{2\pi}{16348}$ and $\Delta t = \frac{0.4}{4096}$. SSP2: fix $\Delta x = \frac{2\pi}{512}$, $\Delta y = \frac{2\pi}{16348}$, take $\Delta t = \frac{0.4}{1024}, \frac{2\pi}{512}, \frac{2\pi}{256}, \frac{2\pi}{128}, \frac{2\pi}{64}, \frac{2\pi}{32}, \frac{2\pi}{16}, \frac{2\pi}{8}$

.

Time convergence test II

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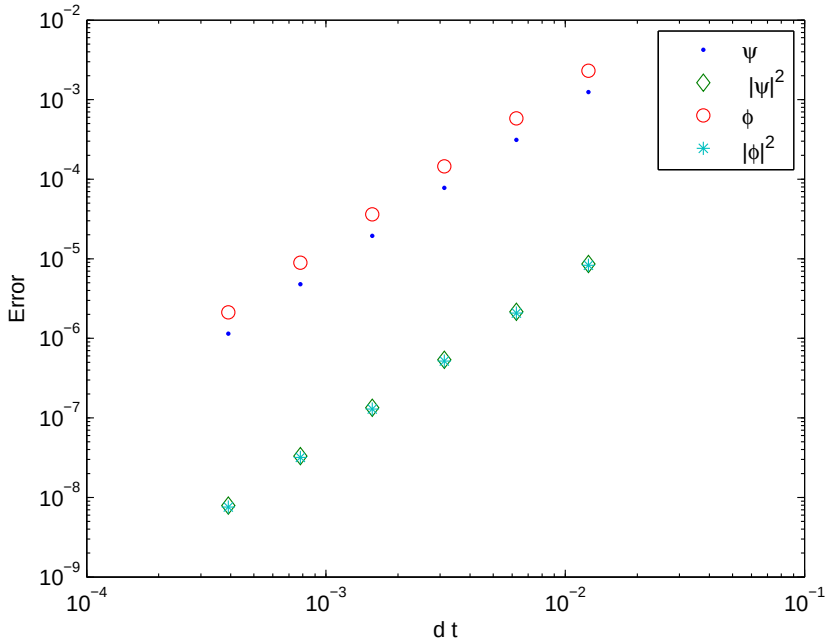

Figure: Fix $\varepsilon = \frac{1}{1024}$ and $\Delta x = \frac{2\pi}{16}$. Take $\Delta t = \frac{0.4}{32}, \frac{0.4}{64}, \frac{0.4}{128}, \frac{0.4}{256}, \frac{0.4}{512}$ and $\frac{0.4}{1024}$, respectively. The reference solution is computed with the same Δx, but $\Delta t = \frac{0.4}{8192}$.

Large time step test I

$\delta = 1$, various ε.

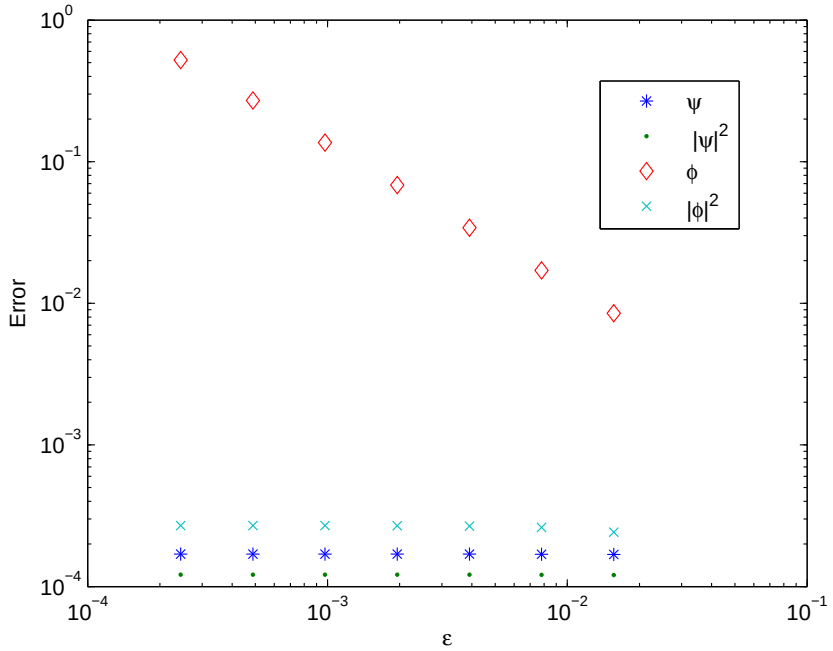

Figure: Fix $\Delta t = 0.05$. For $\varepsilon = 1/64, 1/128, 1/256, 1/512, 1/1024, 1/2048$ and $1/4096$, $\Delta x = 2\pi\varepsilon/16$, respectively. The reference solution is computed with the same Δx, but $\Delta t = \varepsilon/10$.

Large time step test II

$\delta = \varepsilon$.

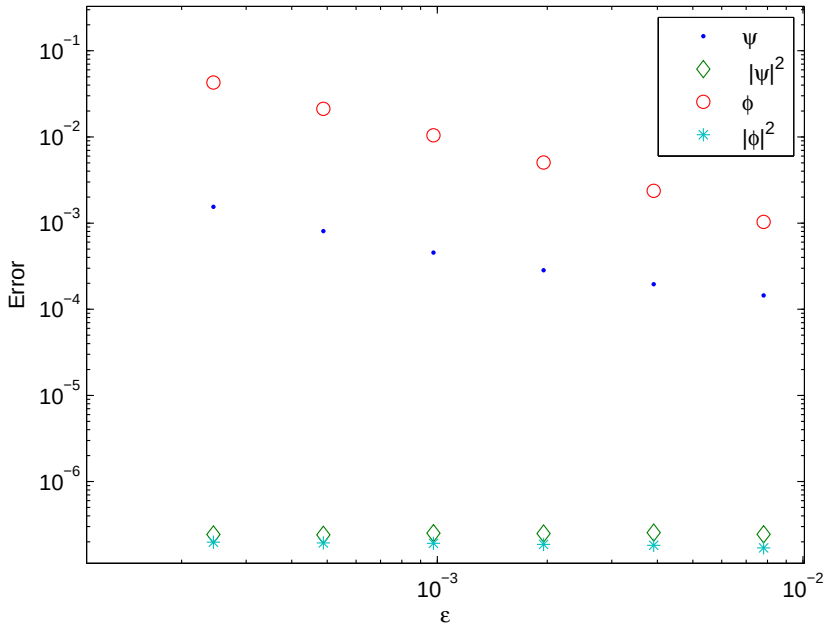

Figure: Fix Δ t=0.005. For $\varepsilon = \frac{1}{256}, \frac{1}{512}, \frac{1}{1024}, \frac{1}{2048}, \frac{1}{4096}$, $\Delta x = \frac{\varepsilon}{8}$, respectively. The reference solution is computed with the same Δx, but $\Delta t = \frac{0.54\varepsilon}{4}$.

Similar tests have been done by SVSP2 methods for the Ehrenfest model.

Thanks for your attention.
Please feel free to ask questions!

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