Efficient Algorithms for Semiclassical Quantum Dynamics

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joint work with Caroline Lasser and Manfred Liebmann

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Time-dependent semiclassical Schrödinger equation

Goal: Find solution to

$$\mathrm{i}\,\varepsilon\,\frac{d}{dt}\psi(t) = -\frac{1}{2}\varepsilon^2 \triangle\,\psi(t) + V\,\psi(t)$$

with $\psi(0) = \psi_0 \in \mathrm{L}^2(\mathbb{R}^d)$, $\|\psi_0\|_{\mathrm{L}^2} = 1$ and $\varepsilon := \sqrt{\frac{m_e}{M_n}} \ll 1$.

Self-adjoint $\mathrm{H} := -\frac{1}{2}\varepsilon^2 \triangle + V$ generates U_t,

$$\psi(t) = \mathrm{U}_t\,\psi_0 = \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon} t\,\mathrm{H}}\psi_0$$

for all $t \in \mathbb{R}$.

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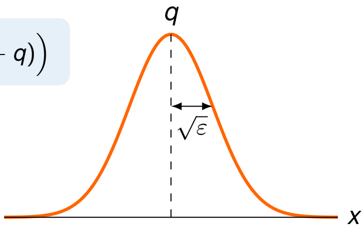
- high dimensional system
- small ε produces highly oscillatory solutions
- ...

Gaussian wave packets

$$g_z^\varepsilon(x) := (\pi\varepsilon)^{-\frac{d}{4}} \exp\left(-\frac{1}{2\varepsilon}|x-q|^2 + \frac{\mathrm{i}}{\varepsilon}\, p\cdot(x-q)\right)$$

$$z = \begin{pmatrix} q \\ p \end{pmatrix} \in \mathbb{R}^{2d}$$



$$\psi = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} g_z^\varepsilon \, \langle g_z^\varepsilon, \psi\rangle \, \mathrm{d}z \quad \text{for all } \psi \in \mathrm{L}^2(\mathbb{R}^d)$$

$$\mathrm{U}_t\psi = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} (\mathrm{U}_t g_z^\varepsilon) \, \langle g_z^\varepsilon, \psi\rangle \, \mathrm{d}z$$

Herman–Kluk Propagator

Definition (Herman & Kluk, 1984)

$$\mathcal{I}_t\psi := (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}}\left(u(t,z)\,\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}S(t,z)}g^{\varepsilon}_{\Phi^t(z)}\right)\langle g^{\varepsilon}_z,\psi\rangle\;\mathrm{d}z$$

depends on

- classical flow $\Phi^t = (X^t, \Xi^t) : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$,
- classical action integral $S(t,z) := \int_0^t \left(\frac{d}{d\tau}X^\tau(z)\cdot\Xi^\tau(z) - h(\Phi^\tau(z))\right)\,\mathrm{d}\tau$,
- Herman–Kluk factor $u(t,z)$

$$u(t,z) := \sqrt{2^{-d}\det(\partial_q X^t(z) + \partial_p \Xi^t(z) + \mathrm{i}\,(\partial_q \Xi^t(z) - \partial_p X^t(z)))}.$$

Herman–Kluk Propagator

$$\mathrm{U}_t\psi = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} \quad (\mathrm{U}_t g_z^\varepsilon) \quad \langle g_z^\varepsilon, \psi\rangle \; \mathrm{d}z$$

$$\mathcal{I}_t\psi = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} \left(u(t,z)\,\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}S(t,z)} g^\varepsilon_{\Phi^t(z)}\right)\langle g_z^\varepsilon, \psi\rangle \; \mathrm{d}z.$$

Theorem (Swart & Rousse, 2009)

$\mathcal{I}_t$ is a bounded operator on $\mathrm{L}^2(\mathbb{R}^d)$. For every $T > 0$, there exists $C > 0$ such that for all $\varepsilon > 0$

$$\sup_{t\in[0,T]} \|\mathcal{I}_t - \mathrm{U}_t\| \le C\,\varepsilon.$$

General strategy

1. High-dimensional quadrature

$$\mathcal{I}_t\psi = \int_{\mathbb{R}^{2d}} f(z)\,\mathrm{d}z \approx \frac{1}{M}\sum_{m=1}^{M} f(z_m).$$

2. Calculate $\Phi^t(z_m)$, $S(t, z_m)$, and $u(t, z_m)$ by solving a system of ODEs with a symplectic integrator.

Quadrature

Factorization

$$(2\pi\varepsilon)^{-d} \langle g_z^\varepsilon, \psi_0 \rangle =: r_0(z) \cdot \mu_0(z), \quad z \in \mathbb{R}^{2d}$$

where $\mu_0 : \mathbb{R}^{2d} \to \mathbb{R}$ is a probability distribution.

Rewrite $\mathcal{I}_t$ as weighted integral

$$\mathcal{I}_t \psi_0 = \int_{\mathbb{R}^{2d}} r_0(z)\, u(t,z)\, \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon} S(t,z)}\, g^\varepsilon_{\Phi^t(z)}\, \mathrm{d}\mu_0(z).$$

Quadrature

Define $\psi_M(t) \in \mathrm{L}^2(\mathbb{R}^d)$ by

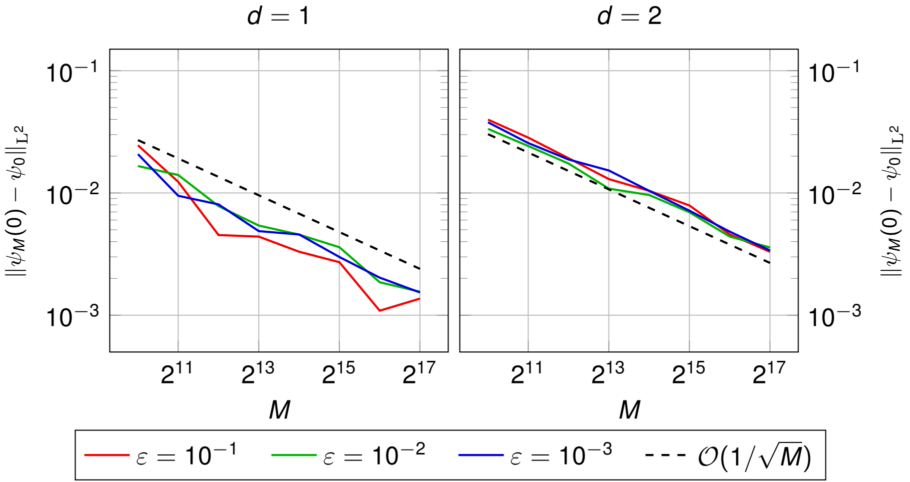
$$\psi_M(t) := \frac{1}{M} \sum_{m=1}^{M} r_0(z_m)\, u(t, z_m)\, \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon} S(t,z_m)} g^{\varepsilon}_{\Phi^t(z_m)}$$

with $z_1, \ldots, z_M \in \mathbb{R}^{2d}$ chosen as

- independent samples of μ_0 (Monte Carlo quadrature),

  or
- low μ_0-discrepancy points (quasi-Monte Carlo quadrature).

Monte Carlo quadrature



Time discretization

$\Phi^t(z_m)$ is solution to

$$\dot{z}(t) = J\,\nabla h(z(t)), \quad z(0) = z_m. \qquad (\mathbb{R}^{2d})$$

$S(t, z_m)$ is solution to

$$\dot{S}(t, z_m) = \tfrac{1}{2}|\Xi^t(z_m)|^2 - V(X^t(z_m)), \quad S(0, z_m) = 0. \qquad (\mathbb{R})$$

$$u(t, z_m) = \sqrt{2^{-d}\det(\partial_q X^t(z_m) + \partial_p \Xi^t(z_m) + \mathrm{i}(\partial_q \Xi^t(z_m) - \partial_p X^t(z_m)))}$$

is calculated from

$$\tfrac{d}{dt}\mathrm{D}\Phi^t(z_m) = J \cdot \nabla^2 h(\Phi^t(z_m)) \cdot \mathrm{D}\Phi^t(z_m). \qquad (\mathbb{R}^{2d\times 2d})$$

Time discretization

Theorem

Calculate $\tilde{\Phi}^t$, $\tilde{S}$ and $\tilde{u}$ with symplectic method of order $\gamma \in \mathbb{N}$. Set

$$\tilde{\mathcal{I}}_t \psi := (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \tilde{u}(t,z)\, \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\tilde{S}(t,z)} g^{\varepsilon}_{\tilde{\Phi}^t(z)} \langle g^{\varepsilon}_z, \psi \rangle \,\mathrm{d}z.$$

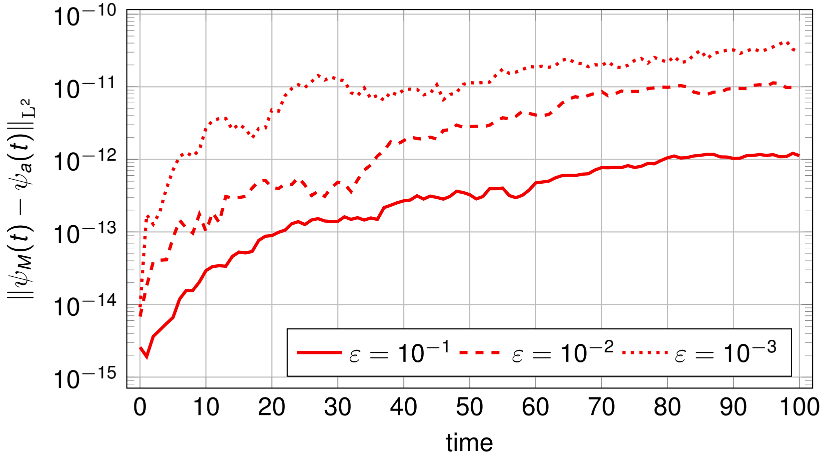
For all $t > 0$ there exist $c_0, c_1, c_2 > 0$ such that for all $\varepsilon > 0$

$$\left\| \tilde{\mathcal{I}}_t - \mathrm{U}_t \right\| \leq \varepsilon\, c_0 + \frac{\tau^\gamma}{\varepsilon}\, c_1 + \tau^\gamma\, c_2 + \mathcal{O}(\tau^{\gamma+2})$$

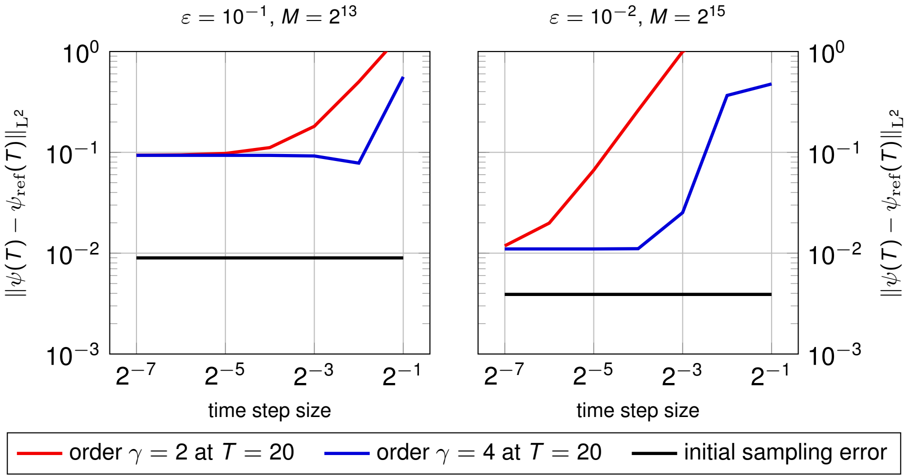
where $\tau > 0$ is the time step size.

Time evolution of error

for harmonic potential



Dependence on time step size



Efficient implementation

Idea: Solve

$$\dot{\mathcal{Z}}(t, z_m) = F\left(\mathcal{Z}(t, z_m)\right) \in \mathbb{R}^{4d^2+2d+2}$$

independently for all z_m

- (MPI and OpenMP) parallelisation + (SSE/AVX) vectorisation
- Automated C++ code generation by computer algebra system

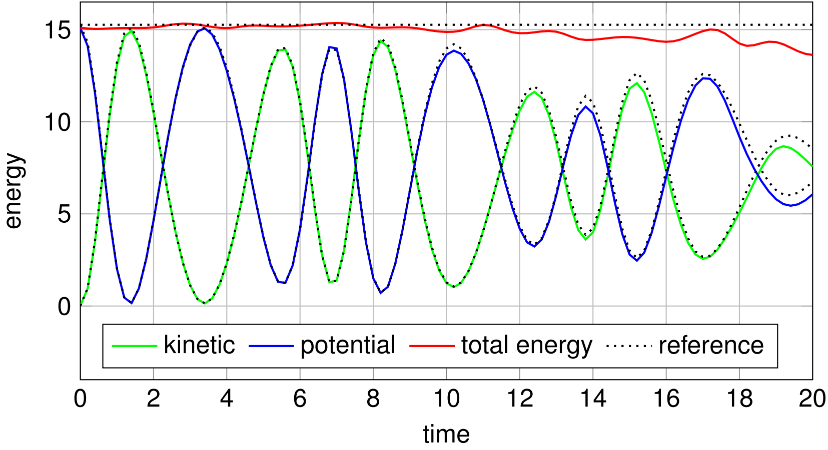
Example: Henon–Heiles potential for $d = 6$

$$V(x) = \sum_{k=1}^{6} \frac{1}{2} x_k^2 + \sigma \sum_{k=1}^{5} \left(x_k x_{k+1}^2 - \frac{1}{3} x_k^3 \right) + \frac{\sigma^2}{16} \sum_{k=1}^{5} \left(x_k^2 + x_{k+1}^2 \right)^2$$

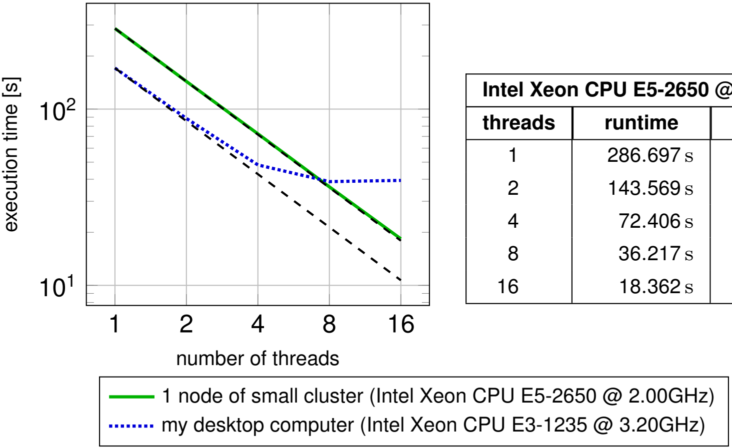
- $M = 2^{22}$ sampling points resulting in 331,350,016 scalar ODEs
- 200 time steps

Example

Henon–Heiles potential for $d = 6$, $\varepsilon = 10^{-2}$, $\tau = 0.1$, $\sigma = \frac{1}{\sqrt{80}}$, $\psi_0 = g^{\varepsilon}_{(2,\dots,2,0,\dots,0)}$

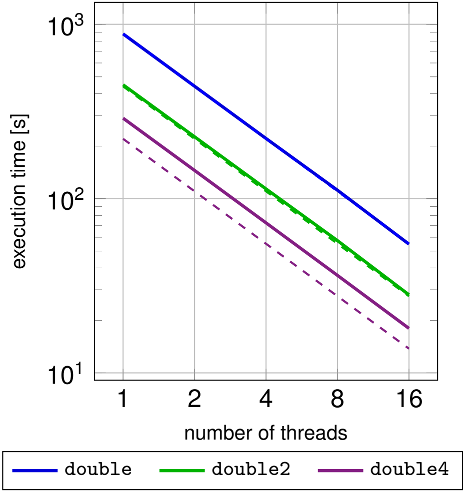


Parallelization



Intel Xeon CPU E5-2650 @ 2.00GHz		
threads	**runtime**	**speedup**
1	286.697 s	
2	143.569 s	1.997
4	72.406 s	3.960
8	36.217 s	7.916
16	18.362 s	15.614

Parallelization + Vectorization



threads	`double` (64 bit)	speedup
1	881.14 s	
2	441.31 s	2.00
4	221.23 s	3.98
8	111.65 s	7.89
16	54.78 s	16.09

threads	`double2` (128 bit)	speedup
1	449.78 s	1.96
2	226.34 s	3.89
4	113.61 s	7.76
8	57.38 s	15.36
16	28.05 s	31.41

threads	`double4` (256 bit)	speedup
1	289.34 s	3.05
2	145.16 s	6.07
4	72.58 s	12.14
8	36.25 s	24.31
16	18.00 s	48.95

Expectation values

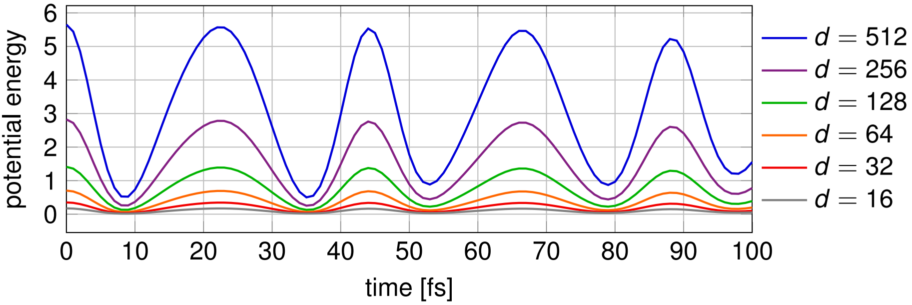
Egorov's Theorem / LSC - IVR

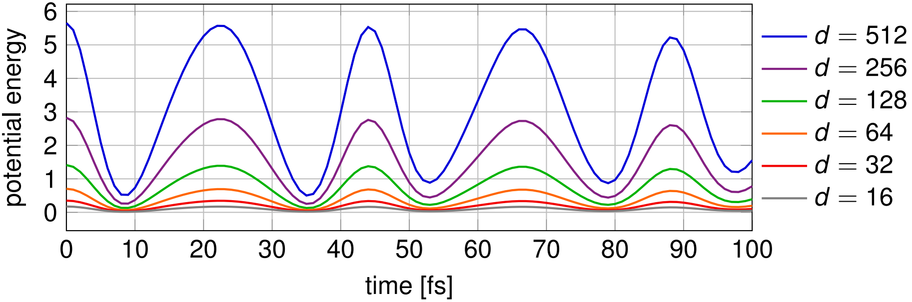
$$\langle \psi(t) | \mathrm{A} | \psi(t) \rangle - \int_{\mathbb{R}^{2d}} (a \circ \Phi^t)(z) \, W(\psi_0)(z) \, \mathrm{d}z = \mathcal{O}(\varepsilon^2)$$

Example: Henon–Heiles potential

$$V(x) = \frac{1}{2}\sum_{k=1}^{d} x_k^2 + 1.8436 \sum_{k=1}^{d-1}\left(x_k x_{k+1}^2 - \frac{1}{3}x_k^3\right) + 0.4 \sum_{k=1}^{d-1}\left(x_k^2 + x_{k+1}^2\right)^2$$

with $\varepsilon = 0.0037$.





dim	2 $\times$ Intel Xeon E5-2650	1 $\times$ Nvidia Tesla K20	speedup
16	4.260 s	0.641 s	6.646
32	10.386 s	1.180 s	8.802
64	24.793 s	4.412 s	5.619
128	109.393 s	29.266 s	3.738
256	219.183 s	71.980 s	3.045
512	454.614 s	155.915 s	2.916

Thank you for your attention!