

A Poisson integrator for Gaussian wavepacket dynamics

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Time-dependent Schrödinger equation in quantum MD

$$i\varepsilon \frac{\partial \psi}{\partial t} = H\psi, \quad \psi(x, 0) = \psi_0(x).$$

- Wave function $\psi = \psi(x, t)$, $x = (x_1, \dots, x_N)$ with $x_k \in \mathbb{R}^d$ ($d = 1$ or 3) and time $t \in \mathbb{R}$.
- Hamiltonian $H = T + V$ with the kinetic and potential energy operators

$$T = - \sum_{k=1}^N \frac{\varepsilon^2}{2m_k} \Delta_{x_k} \quad \text{and} \quad V = V(x),$$

Particle mass : $m_k > 0$. Laplace operator Δ_{x_k} . Real potential $V(x)$.

- ε is a (small) positive number representing the scaled Planck constant.

Dirac-Frenkel-McLachlan Principle

- $\mathcal{M} \subset L^2$ an approximation manifold.
- $T_u\mathcal{M}$ the tangent space at $u \in \mathcal{M}$ (the space of admissible variations).
- $t \mapsto u(t)$ solution of

$$\operatorname{Re} \left\langle \delta u, \frac{\partial u}{\partial t} - \frac{1}{i} H u \right\rangle = 0 \quad \text{for all } \delta u \in T_u\mathcal{M}.$$

This amounts to

$$\frac{\partial u}{\partial t} = P(u) \frac{1}{i} H u.$$

with the orthogonal projection $P(u) : \mathcal{H} \rightarrow T_u\mathcal{M}$

- **Applications** : Time-dependent Hartree, Hartree-Fock, MCTDH, Gaussian wave packets, etc...

Gaussian wave packets

\mathcal{M} made of functions of the form $u(x, t) = e^{i\phi(t)/\varepsilon} \prod_{k=1}^N \varphi_k(x_k, t)$ with

$$\varphi_k(x_k, t) = \exp\left(\frac{i}{\varepsilon} (a_k(t) |x_k - q_k(t)|^2 + p_k(t) \cdot (x_k - q_k(t)) + c_k(t))\right),$$

Finite dimensional complex submanifold parametrized by

$$q_k = \langle u | x_k | u \rangle \in \mathbb{R}^d \text{ position average}$$

$$p_k = \langle u | -i\varepsilon \nabla_{x_k} | u \rangle \in \mathbb{R}^d \text{ momentum average}$$

$$a_k = \alpha_k + i\beta_k \text{ (with } \beta_k > 0 \text{) complex width parameter,}$$

$$c_k = \gamma_k + i\delta_k \text{ complex phase parameter, and } \phi \text{ a real phase.}$$

Heller (75), Lee & Heller (82), Coalson & Karplus (90)

GWP equations

$$\begin{aligned}\dot{q}_k &= \frac{p_k}{m_k} \\ \dot{p}_k &= -\langle u | \nabla_{x_k} V | u \rangle \\ \dot{a}_k &= -\frac{2a_k^2}{m_k} - \frac{1}{2d} \langle u | \Delta_{x_k} V | u \rangle \\ \dot{c}_k &= \frac{i\varepsilon da_k}{m_k} + \frac{\varepsilon}{8\beta_k} \langle u | \Delta_{x_k} V | u \rangle \\ \dot{\phi} &= \sum_{k=1}^N \frac{|p_k|^2}{2m_k} - \langle u | V | u \rangle\end{aligned}$$

where $(a_k = \alpha_k + i\beta_k$ and $c_k = \gamma_k + i\delta_k)$

$$\langle u | W | u \rangle = \int_{\mathbb{R}^N} W(x) \prod_{j=1}^N \exp\left(-\frac{2}{\varepsilon}(\beta_j |x_j - q_j|^2 + \delta_j)\right) dx.$$

This average depends only on the parameters q_j , β_j , and δ_j .

Poisson structure

- The GWP system has a Poisson structure $\dot{y} = B(y)\nabla K(y)$ where $u = \chi(y)$, $y = (q_k, p_k, \dots)$ inherited from the symplectic structure of the Schrödinger equation.
- Conservation of the energy $K(y) = \langle u | H | u \rangle$:

$$\langle u | H | u \rangle = \|u\|^2 \sum_{k=1}^N \left(\frac{|p_k|^2}{2m_k} + \frac{\varepsilon d}{2m_k} \frac{\alpha_k^2 + \beta_k^2}{\beta_k} \right) + \langle u | V | u \rangle.$$

As $\varepsilon \rightarrow 0$ and $\|u\| = 1$, the energy tends to the classical one.

- Conservation of the L^2 -norm and of the linear and angular momentum.

Variational splitting

The decomposition $H = T + V$ induces the symmetric splitting scheme

$$u^{n+1} = \varphi_{\Delta t/2}^V \circ \varphi_{\Delta t}^T \circ \varphi_{\Delta t/2}^V(u^n)$$

- $u(t) = \varphi_t^V(u_0)$ is the solution of

$$\langle \delta u, i\varepsilon \dot{u} - Vu \rangle = 0 \quad \text{for all } \delta u \in T_u \mathcal{M}, \quad u(0) = u_0$$

- $u(t) = \varphi_t^T(u_0)$ is the solution of

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Projection of the Strang or symmetric Trotter splitting algorithm.

The T-magic

Computation of $u_1 = \varphi_{\Delta t}^T(u_0)$, where u_0 is represented by $(q^0, p^0, a^0, c^0, \phi^0)$:

$$\dot{q} = \frac{p}{m}$$

$$\dot{p} = -\langle u | \nabla_x V | u \rangle$$

$$\text{GWP } (N = 1) : \quad \dot{a} = -\frac{2a^2}{m} - \frac{1}{2d} \langle u | \Delta_x V | u \rangle$$

$$\dot{c} = \frac{i\varepsilon da}{m} + \frac{\varepsilon}{8\beta} \langle u | \Delta_x V | u \rangle$$

$$\dot{\phi} = \frac{|p|^2}{2m} - \langle u | V | u \rangle$$

The T-magic

Computation of $u_1 = \varphi_{\Delta t}^T(u_0)$, where u_0 is represented by $(q^0, p^0, a^0, c^0, \phi^0)$:

$$\dot{q} = \frac{p}{m}$$

$$\dot{p} = 0$$

$$\varphi_{\Delta t}^T : \quad \dot{a} = -\frac{2a^2}{m}$$

$$\dot{c} = \frac{i\epsilon da}{m}$$

$$\dot{\phi} = \frac{|p|^2}{2m}$$

The T-magic

Computation of $u_1 = \varphi_{\Delta t}^T(u_0)$, where u_0 is represented by $(q^0, p^0, a^0, c^0, \phi^0)$:

$$q^1 = q^0 + \frac{\Delta t}{m} p^0$$

$$p^1 = p^0$$

$$\varphi_{\Delta t}^T : a^1 = a^0 / \left(1 + 2 \frac{\Delta t}{m} a^0\right)$$

$$c^1 = c^0 + \frac{i\varepsilon d}{2} \log\left(1 + 2 \frac{\Delta t}{m} a^0\right).$$

$$\phi^1 = \phi^0 + \Delta t \frac{|p^0|^2}{2m}$$

The flow $\varphi_{\Delta t}^T$ can be computed exactly.

The V-magic

Computation of $u_1 = \varphi_{\Delta t}^V(u_0)$, where u_0 is represented by $(q^0, p^0, a^0, c^0, \phi^0)$:

$$\dot{q} = \frac{p}{m}$$

$$\dot{p} = -\langle u | \nabla_x V | u \rangle$$

$$\text{GWP : } \dot{a} = -\frac{2a^2}{m} - \frac{1}{2d} \langle u | \Delta_x V | u \rangle$$

$$\dot{c} = \frac{i\varepsilon da}{m} + \frac{\varepsilon}{8\beta} \langle u | \Delta_x V | u \rangle$$

$$\dot{\phi} = \frac{|p|^2}{2m} - \langle u | V | u \rangle$$

The V-magic

Computation of $u_1 = \varphi_{\Delta t}^V(u_0)$, where u_0 is represented by $(q^0, p^0, a^0, c^0, \phi^0)$:

$$\dot{q} = 0$$

$$\dot{p} = -\langle u | \nabla_x V | u \rangle$$

$$\varphi_{\Delta t}^V : \quad \dot{a} = -\frac{1}{2d} \langle u | \Delta_x V | u \rangle \in \mathbb{R}$$

$$\dot{c} = \frac{\varepsilon}{8\beta} \langle u | \Delta_x V | u \rangle \in \mathbb{R}$$

$$\dot{\phi} = -\langle u | V | u \rangle$$

$$\implies \quad \dot{q} = 0, \dot{\beta} = 0, \dot{\delta} = 0.$$

$$(a = \alpha + i\beta \text{ and } c = \gamma + i\delta)$$

The V-magic

Computation of $u_1 = \varphi_{\Delta t}^V(u_0)$, where u_0 is represented by $(q^0, p^0, a^0, c^0, \phi^0)$:

As $\langle u_0 | W | u_0 \rangle$ depends only on q^0, β^0 and δ^0 ,

$$q^1 = q^0$$

$$p^1 = p^0 - \Delta t \langle u_0 | \nabla_x V | u_0 \rangle$$

$$\alpha^1 = \alpha^0 - \frac{\Delta t}{2d} \langle u_0 | \Delta_x V | u_0 \rangle$$

$$\varphi_{\Delta t}^V : \beta^1 = \beta^0$$

$$\gamma^1 = \gamma^0 + \frac{\Delta t \varepsilon}{8\beta^0} \langle u_0 | \Delta_x V | u_0 \rangle$$

$$\delta^1 = \delta^0$$

$$\phi^1 = \phi^0 - \Delta t \langle u_0 | V | u_0 \rangle$$

The flow $\varphi_{\Delta t}^V$ can be computed exactly.

Properties

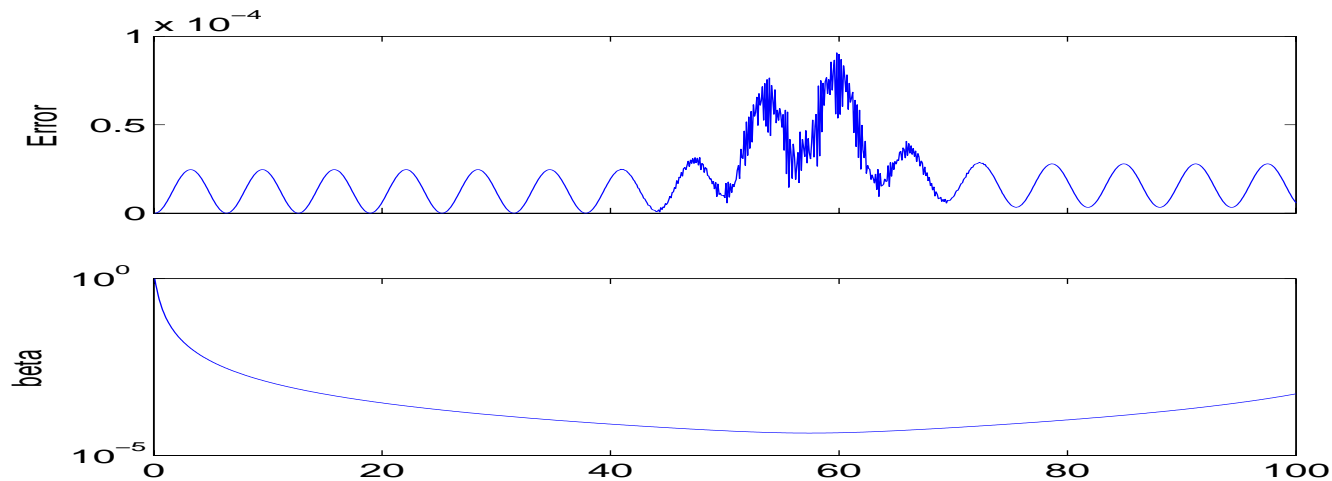
- **Poisson integrator** that preserve the L^2 norm, and the linear and angular momentum.
- Order 2 : $\left| \|u^n\|^2 - \|u(t^n)\|^2 \right| = O(\Delta t^2)$, but $\|u^n - u(t^n)\| = O(\Delta t^2/\varepsilon)$.
- Energy conservation : if the q_k are bounded and if $\beta_k \geq c_0\varepsilon$

$$\left| \langle u^n | H | u^n \rangle - \langle u^0 | H | u^0 \rangle \right| \leq C\Delta t^2 \quad \text{for } n\Delta t \leq \exp(c/\Delta t)$$

where c and C are positive constants that are independent of Δt , and ε .

Kepler 3D potential

$N = 1$, $d = 3$ and $V(q) = -1/|q|$. $p^0 = (1, 0, 0)^T$, $q^0 = (0, 1, 0)^T$, $\alpha^0 = 1$, $\beta^0 = 1$, $\gamma^0 = 0$, $\phi^0 = 0$, and $\delta^0 = -\frac{3}{4}\varepsilon \log(2\beta^0\pi^{-1}\varepsilon^{-1})$ to ensure unit norm of the wavepacket. $\Delta t = 0.1$, $\varepsilon = 10^{-4}$. **Energy error :**



Extensions

Non-spherical GWP :

$$\varphi_k(x_k) = \exp\left(\frac{i}{\varepsilon}\left((x_k - q_k)^T A_k (x_k - q_k) + p_k \cdot (x_k - q_k) + c_k\right)\right)$$

with a $d_k \times d_k$ complex matrix A_k with symmetric positive definite imaginary part.

Denoting by M_k the mass matrix for the (one or several) particles with the coordinates $x_k \in \mathbb{R}^{d_k}$, the equations of motion for A_k and c_k become

$$\begin{aligned}\dot{A}_k &= -2A_k M_k^{-1} A_k - \frac{1}{2} \langle u | \nabla_{x_k}^2 V | u \rangle \\ \dot{c}_k &= i\varepsilon \operatorname{tr}(M_k^{-1} A_k) + \frac{\varepsilon}{8} \langle u | \operatorname{tr}(B_k^{-1} \nabla_{x_k}^2 V) | u \rangle\end{aligned}$$

where $B_k = \operatorname{Im} A_k$ and $\nabla_{x_k}^2 V$ is the Hessian matrix of V with respect to the variables x_k . These equations admit the same splitting as previously which still can be solved explicitly by a straightforward adaptation of the previous formulas.