A Poisson integrator for Gaussian wavepacket dynamics

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Time-dependent Schrödinger equation in quantum MD

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

- Wave function $\psi = \psi(x,t)$, $x = (x_1, \ldots, x_N)$ 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

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

This amounts to

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

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

- Applications :Time-dependent Hartree, Hatree-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

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

Finite dimensional complex submanifold parametrized by

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

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

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

$c_k = \gamma_k + i\delta_k$ complex phase parameter, and ϕ a real phase.

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

GWP equations

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

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

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

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 $u = \chi(y)$, $y = (q_k, p_k, \ldots)$ 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 $\varepsilon \longrightarrow 0$ 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

$$u^{n+1} = \varphi^V_{\Delta t/2} \circ \varphi^T_{\Delta t} \circ \varphi^V_{\Delta t/2}(u^n)$$

- $u(t) = \varphi^V_t(u_0)$ is the solution of

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

- $u(t) = \varphi^T_t(u_0)$ is the solution of

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

Projection of the Strang or symmetric Trotter splitting algorithm.

The T-magic

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

GWP $\quad (N = 1)$:

$$
\begin{aligned}
\dot{q} &= \frac{p}{m} \\
\dot{p} &= -\langle\, u \,|\, \nabla_x V \,|\, u \,\rangle \\
\dot{a} &= -\frac{2a^2}{m} - \frac{1}{2d}\langle\, u \,|\, \Delta_x V \,|\, u \,\rangle \\
\dot{c} &= \frac{i\varepsilon d a}{m} + \frac{\varepsilon}{8\beta}\langle\, u \,|\, \Delta_x V \,|\, u \,\rangle \\
\dot{\phi} &= \frac{|p|^2}{2m} - \langle\, u \,|\, V \,|\, u \,\rangle
\end{aligned}
$$

The T-magic

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

$$\varphi^T_{\Delta t}: \quad \begin{aligned} \dot{q} &= \frac{p}{m} \\ \dot{p} &= 0 \\ \dot{a} &= -\frac{2a^2}{m} \\ \dot{c} &= \frac{i\varepsilon da}{m} \\ \dot{\phi} &= \frac{|p|^2}{2m} \end{aligned}$$

The T-magic

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

$$\varphi^T_{\Delta t}: \quad \begin{aligned} q^1 &= q^0 + \frac{\Delta t}{m} p^0 \\ p^1 &= p^0 \\ a^1 &= a^0 \Big/ \Big(1 + 2\frac{\Delta t}{m} a^0\Big) \\ c^1 &= c^0 + \frac{i\varepsilon d}{2} \log\Big(1 + 2\frac{\Delta t}{m} a^0\Big). \\ \phi^1 &= \phi^0 + \Delta t \frac{|p^0|^2}{2m} \end{aligned}$$

The flow $\varphi^T_{\Delta t}$ can be computed exactly.

The V-magic

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

GWP :

$$
\begin{aligned}
\dot{q} &= \frac{p}{m} \\
\dot{p} &= -\langle\, u \,|\, \nabla_x V \,|\, u \,\rangle \\
\dot{a} &= -\frac{2a^2}{m} - \frac{1}{2d}\langle\, u \,|\, \Delta_x V \,|\, u \,\rangle \\
\dot{c} &= \frac{i\varepsilon d a}{m} + \frac{\varepsilon}{8\beta}\langle\, u \,|\, \Delta_x V \,|\, u \,\rangle \\
\dot{\phi} &= \frac{|p|^2}{2m} - \langle\, u \,|\, V \,|\, u \,\rangle
\end{aligned}
$$

The V-magic

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

$$\varphi^V_{\Delta t}: \quad \begin{aligned} \dot{q} &= 0 \\ \dot{p} &= -\langle\, u \,|\, \nabla_x V \,|\, u \,\rangle \\ \dot{a} &= -\tfrac{1}{2d}\langle\, u \,|\, \Delta_x V \,|\, u \,\rangle \in \mathbb{R} \\ \dot{c} &= \frac{\varepsilon}{8\beta}\langle\, u \,|\, \Delta_x V \,|\, u \,\rangle \in \mathbb{R} \\ \dot{\phi} &= -\langle\, u \,|\, V \,|\, u \,\rangle \end{aligned}$$

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

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

The V-magic

Computation of $u_1 = \varphi^V_{\Delta t}(u_0)$, 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,

$$\varphi^V_{\Delta t} : \quad \begin{aligned} q^1 &= q^0 \\ p^1 &= p^0 - \Delta t \langle\, u_0 \,|\, \nabla_x V \,|\, u_0 \,\rangle \\ \alpha^1 &= \alpha^0 - \tfrac{\Delta t}{2d} \langle\, u_0 \,|\, \Delta_x V \,|\, u_0 \,\rangle \\ \beta^1 &= \beta^0 \\ \gamma^1 &= \gamma^0 + \frac{\Delta t\, \varepsilon}{8\beta^0} \langle\, u_0 \,|\, \Delta_x V \,|\, u_0 \,\rangle \\ \delta^1 &= \delta^0 \\ \phi^1 &= \phi^0 - \Delta t \langle\, u_0 \,|\, V \,|\, u_0 \,\rangle \end{aligned}$$

The flow $\varphi^V_{\Delta t}$ can be computed exactly.

Properties

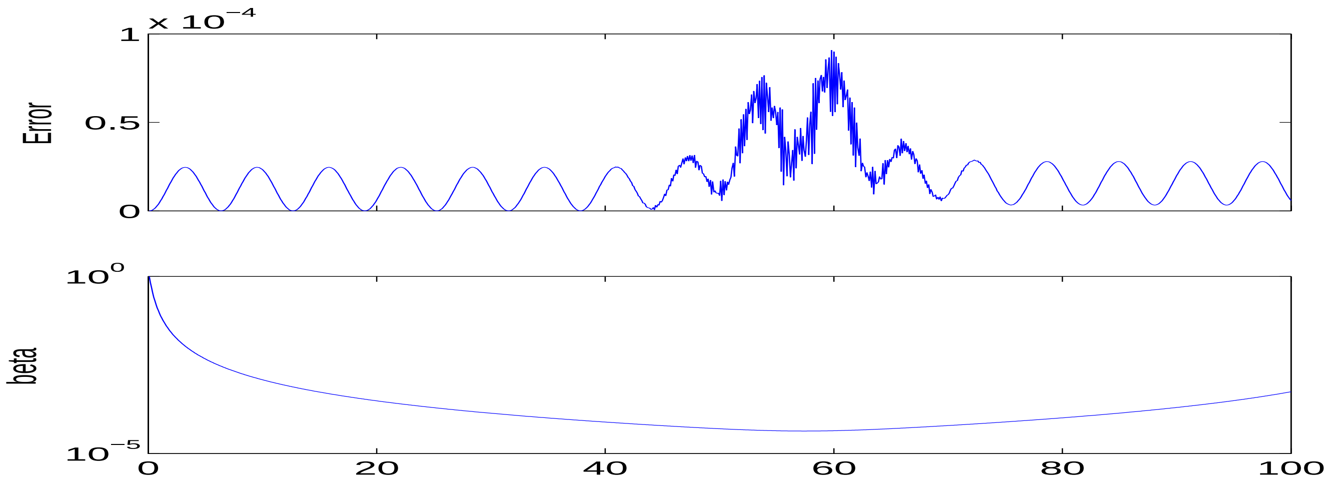
- Poisson integrator that preserve the L^2 norm, and the linear and angulum momentum.
- Order 2 : $\left\| |u^n|^2 - |u(t^n)|^2 \right\| = O(\Delta t^2)$, but $\|u^n - u(t^n)\| = O(\Delta t^2/\varepsilon)$.
- Energy conservation : if the q_k are bounded and if $\beta_k \geq c_0\varepsilon$

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

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 :

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

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

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

where $B_k = \mathrm{Im}\, A_k$ and $\nabla^2_{x_k} V$ 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.