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Operator splitting for semiclassical quantum dynamics

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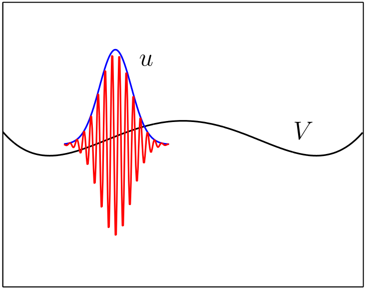
May 28, 2014

The semiclassical Schrödinger equation

$$\mathrm{i}\varepsilon u_t = -\frac{\varepsilon^2}{2}\Delta u + Vu, \qquad x \in \mathbb{R}^d, \quad t > 0.$$

A typical wave packet has width $\sim \sqrt{\varepsilon}$ and wavelength $\sim \varepsilon$.

The time and length scales of interest are $\mathcal{O}(1)$.



The Gaussian wave packet transform[1,2]

Idea: Factor out fast oscillations to leading order, solve for correction.

Introduce new spatial variable $\eta = \eta(x)$, and solve

$$\mathrm{i} w_t = -\frac{1}{2}\nabla_\eta \cdot M \nabla_\eta w + \frac{1}{2}\eta^T Q \eta w + V_{rem}\eta.$$

$$u(x,t) = w(\eta(x),t)\mathrm{e}^{\mathrm{i}\theta(x,t)/\varepsilon}, \text{ with}$$
$$\theta(x,t) = \gamma + p^T(x-q) + \frac{1}{2}(x-q)^T A (x-q).$$

[1] Russo and Smereka, *J. Comput. Phys.*, **233**:192–209, 2013.
[2] Russo and Smereka, *J. Comput. Phys.*, **257**:1022–1038, 2014.

Abstract framework

$$u' = Au + Bu, \qquad u(0) = u_0.$$

A, B generates strongly continuous (semi)groups of operators.

This roughly means $u(t) = \exp\big(t(A+B)\big)u_0$.

We consider force-gradient time-stepping schemes,

$$u_{n+1} = Su_n, \qquad S = \prod_{j=1}^{s} \exp\big(b_j hB + c_j h^3[B,[A,B]]\big)\exp\big(a_j hA\big).$$

When A is a differential and B a potential,
$[B,[A,B]]$ will also be a potential-like term.

Can construct 4th order method with five exponentials.

The main result[3]

Theorem

If the problem is reasonably regular and a force-gradient method is pth order accurate for a Hamiltonian ODE problem, it is pth order accurate also for the Schrödinger equation.

[3] K., *UU/IT Technical report*, **2014-004**, 2014.