Fourier-Hermite methods for perturbed harmonic oscillator problems

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joint work with Sergio Blanes

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Structure

Different types of equations

Hamiltonian mechanics

$$H = \frac{1}{2}p^2 + V(q) \Longrightarrow \frac{d}{dt}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{Bmatrix} \nabla_p H \\ -\nabla_q H \end{Bmatrix}$$

Quantum mechanics - Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(x,t) = H\Psi(x,t) \equiv \left(-\frac{1}{2}\Delta + V(x)\right)\Psi(x,t)$$

Mean field nonlinear QM - Gross-Pitaevski equation

$$i\frac{\partial}{\partial t}\Phi(x,t) = \left(-\frac{1}{2}\Delta + V(x) + g|\Phi(x,t)|^2\right)\Phi(x,t)$$

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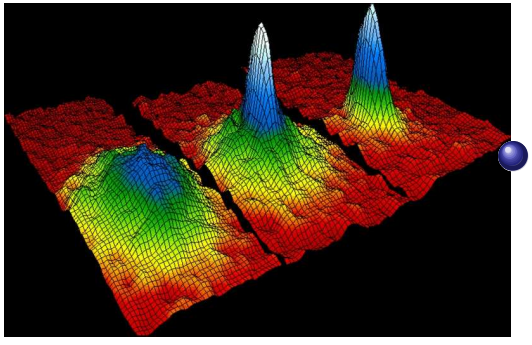
Motivation

Many physical potentials $V(x)$ allow Taylor expansions around their minimum

$$V(x) = \frac{1}{2}V''(0)x^2 + \frac{1}{6}V'''(0)x^3 + \dots$$

Often, we are only interested in the behaviour close to the minimum.



- Bose-Einstein-condensate (Nobel Prize 2001, Ketterle, Cornell, Wieman)

Schrödinger equation in units $\hbar = 1$

Consider the linear Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(x,t) = H\Psi(x,t) \equiv \left(-\frac{1}{2}\Delta + V(x)\right)\Psi(x,t), \quad \Psi(x,0) = \Psi_0(x) \tag{1}$$

with the solution (1-parameter family of unitary operators exists by self-adjointness of H, c.f. Stone's theorem)

$$\Psi(x,t) = e^{-itH}\Psi_0(x) \tag{2}$$

Spectral theorem

A self-adjoint compact operator on a Hilbert space with family of eigenvalues $(\lambda)_I$ and eigenfunctions $(\phi)_I$ yields an orthogonal basis on its domain

$$\Psi(x,t) = \sum_{n\in I} e^{-it\lambda_n}\langle\phi_n|\Psi_0\rangle\phi_n(x) \tag{3}$$

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The harmonic oscillator

Let H be a perturbed harmonic oscillator problems, for simplicity in $1D$

$$H = -\frac{1}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + \varepsilon V(x), \quad \varepsilon \ll 1 \tag{4}$$

The eigenfunctions of the (normalised) harmonic part are products of Gaussian exponentials with Hermite polynomials.

$$\lambda_n = \left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots, \tag{5}$$

$$\phi_n = \frac{1}{\pi^{1/4}}\frac{1}{\sqrt{2^n n!}} H_n(x) e^{-x^2/2} \tag{6}$$

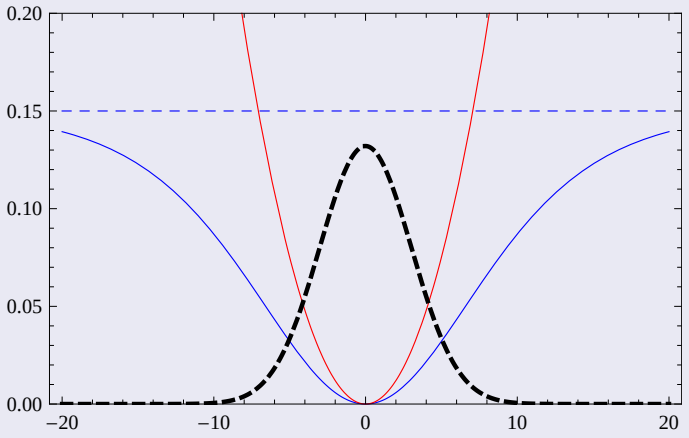
Hamilton operator H can be written

$$H = -\frac{1}{2}p^2 + \underbrace{\frac{1}{2}\omega^2 x^2}_{=:V_{HO}(x)} + \left(V(x,p) - \frac{1}{2}\omega^2 x^2\right) \tag{7}$$

For small residual potentials $V - V_{HO}$ around $x = 0$, Hamiltonian can be regarded as a perturbed harmonic oscillator.

Example

Pöschl-Teller potential $V(x) = -\frac{1}{2m}\alpha^2 \frac{\lambda(\lambda-1)}{\cosh^2 \alpha x}$



Hamiltonian of the form $H = \underbrace{T + V_{HO}}_{H_{HO}} + \varepsilon V(x)$

Hermite pseudo spectral method

Split as $H_{HO} + \varepsilon V$, evolution is

$$\Psi(x, h) = e^{-ihH}\Psi(x, 0) \overset{e.g.}{=} e^{-ihH_{HO}} e^{-ih\varepsilon V}\Psi(x, 0) + \mathcal{O}(h^2)$$

1. Rest potential V is already diagonal in coordinate space $\Rightarrow$ exponential of scalars
2. Use the spectral theorem to diagonalise harmonic part

Fourier pseudo spectral method

Split as $T + (V_{HO} + \varepsilon V)$

1. Potential is again diagonal
2. Use plane wave states to evolute kinetic part via FFT

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Structure

Definitions

A *Lie-algebra* $\mathfrak{g}$ is a vector space over some field F equipped with a *Lie-bracket*, that is a map $[\cdot,\cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ satisfying the following properties

- Bilinearity
- Alternating $\forall x \in \mathfrak{g}: \quad [x,x] = 0$
- Jacobi identity $[x,[y,z]] + [y,[z,x]] + [z,[x,y]] = 0 \forall x,y,z \in \mathfrak{g}$

Let X, Y be smooth vector fields on a manifold and f a smooth function

$$[X,Y](f) := (XY - YX)(f)$$

Poisson bracket for smooth functions in canonical coordinates (q,p) on the phase space

$$\{f,g\} = \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} \right)$$

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We begin with classical mechanical systems given by the Hamiltonian

$$H = \frac{1}{2} p^t M p + \frac{1}{2} q^t N q$$

with corresponding equations of motion

$$\frac{d}{dt} \begin{Bmatrix} q \\ p \end{Bmatrix} = J \nabla H = \begin{pmatrix} 0 & M \\ -N & 0 \end{pmatrix} \begin{Bmatrix} q \\ p \end{Bmatrix} \tag{8}$$

where J is the usual symplectic structur matrix.

Commutators of kinetic T and potential V terms (1D: $m = \omega = 1$)

$$\{T, V\} = -pq$$

and nested commutators

$$\{T, \{T, V\}\} = 2T \quad \text{and} \quad \{V, \{T, V\}\} = -2V$$

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or equivalently, with small m, n denoting the matrix elements of M, N,

$$H = -\frac{1}{2}\sum_{i,j} m_{ij}\frac{\partial^2}{\partial x_i \partial x_j} + \frac{1}{2}\sum_{ij} n_{ij} x_i x_j$$

Commutators of kinetic T and potential V terms (1D: $\hbar = m = \omega = 1$)

$$[T, V] = -i\frac{1}{2}(pq + qp)$$

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Structure

Exploit algebra isomorphism between the classical and quantum mechanical structure.

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2\right)\psi(x,t), \tag{9}$$

Let $A_1 \equiv -\frac{1}{2}\frac{\partial^2}{\partial x^2}$, $B_1 \equiv \frac{1}{2}x^2$, s.t. $e^{-ihA} = e^{-ih(A_1+B_1)}$.

Lemma

For $h < \pi$ the following property is satisfied

$$e^{-ihA} = e^{-if(h)A_1}\, e^{-ig(h)B_1}\, e^{-if(h)A_1} \tag{10}$$

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where

$$g(h) = \sin(h), \qquad f(h) = \tan(h/2). \tag{12}$$

Obtained by S.A. Chin et al. in a different way, PRE 72 (2005)

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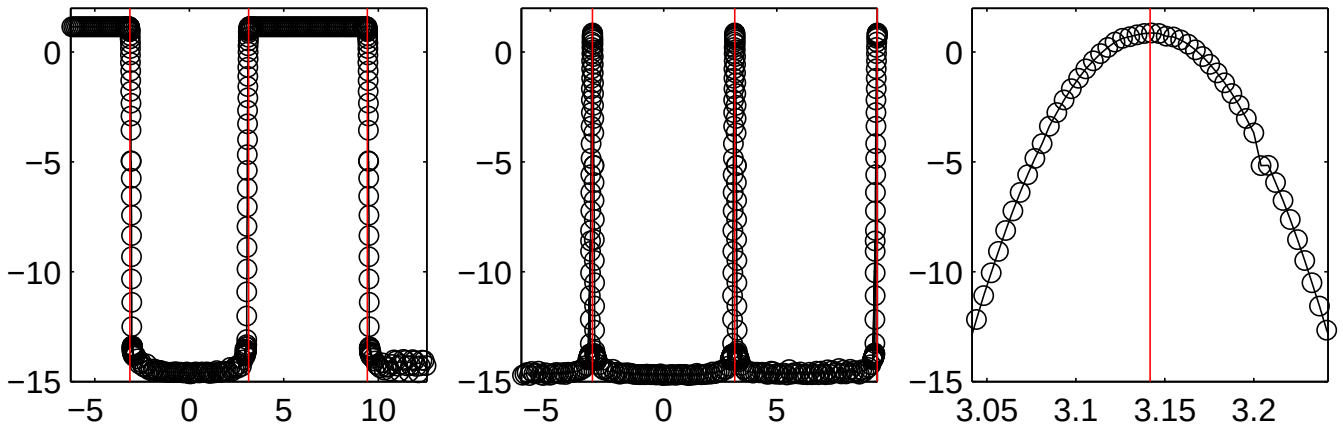
On the step-size limit



Error in logarithmic scale for the integration of the HO ground state using the Fourier-Hermite method

Explanation

Quantum ground state has non-zero energy $1/2$ (in appropriate units),

$$\Psi(x,t) = \sum_{n \in I} e^{-it(n+1/2)} \langle \phi_n | \Psi_0 \rangle \phi_n(x)$$

Proof

Algebra is generated by the two operators $T \equiv A$, $V \equiv B$, hence

$$\begin{aligned} e^{h/2V} e^{hT} e^{h/2V} &= e^{h(T+V) - \frac{h^3}{24}([V,[V,T]]+2[T,[V,T]])+\cdots} \\ &= e^{h(T+V) - \frac{h^3}{12}(-V+2T)+\cdots} \end{aligned}$$

Use matrix representation of classical HO algebra

$$T = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}, V = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

Easy to exponentiate and match with known solution

$$\begin{aligned} e^{f(h)V} e^{g(h)T} e^{f(h)V} &= \begin{pmatrix} 1 - g \cdot f & g \\ -2f + f \cdot g \cdot f & 1 - f \cdot g \end{pmatrix} \\ &\stackrel{!}{=} e^{h(T+V)} = \begin{pmatrix} \cos h & \sin h \\ -\sin h & \cos h \end{pmatrix} \end{aligned}$$

Exact decomposition - so what?

Suppose we split in harmonic part and rest $H = T + V_{HO} + \varepsilon V$, the method reads

$$\prod_j e^{-ia_j h \varepsilon V} e^{-ib_j h H_{HO}}$$

With the help of the lemma

$$\prod_j e^{-ia_j h \varepsilon V} e^{-if(b_j h) V_{HO}} e^{-ig(b_j h) T_{HO}} e^{-if(b_j h) V_{HO}}$$

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If we expand the product, we can group the commuting terms V_{HO} and V to reduce the number of exponentials (more: FSAL).

Summary

We can compute the main contribution H_{HO} exactly (cf. spatial discretisation) and quickly via FFT.

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Chosen methods

We compare different methods for the two splittings $(T + V_{HO}) + \varepsilon V$ and $T + (V_{HO} + \varepsilon V)$
Recall

$$\Phi_h^{[A+B]} = \prod_{i=1}^{s} \Phi_{a_i h}^{[A]} \circ \Phi_{b_i h}^{[B]} + \mathcal{O}\left(h^{p+1}\right)$$

- Runge-Kutta-Nyström-methods are particularly designed for the case $[B,[B,[B,A]]] = 0$, e.g. for Hamiltonians quadratic in kinetic energy
- Schemes for near-integrable systems, where $\varepsilon \ll 1$

  e.g. cancel $\varepsilon h^3 [A,[A,B]]$ but keep $h^3 \varepsilon^2 [B,[B,A]]$

  Composition $\tilde{\Phi}_h$ has order $(s_1, s_2, \ldots)$ if

  $$\tilde{\Phi}_h - \exp(h(A+\varepsilon B)) = \mathcal{O}\left(\sum \varepsilon^j h^{s_j+1}\right)$$

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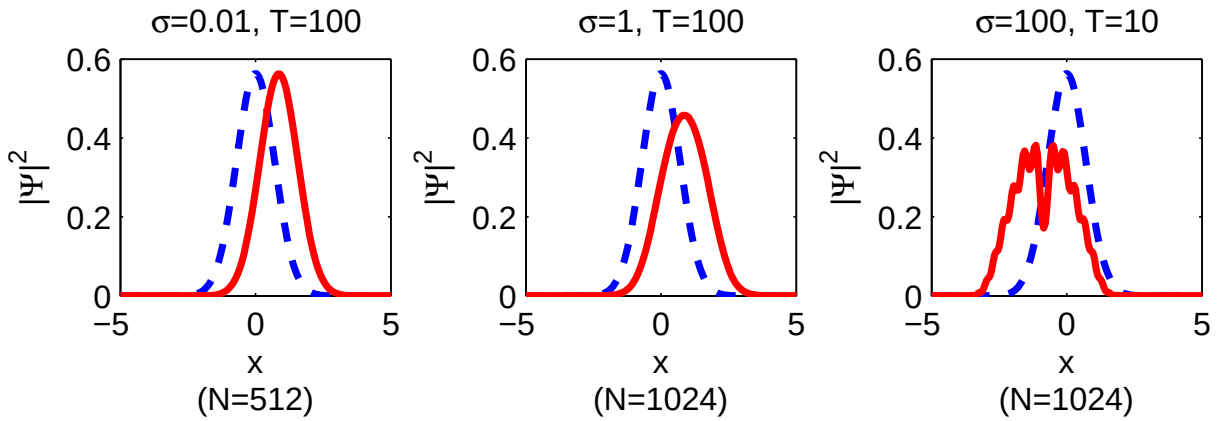
The Gross-Pitaevskii equation

Describes a Bose-Einstein condensate in a harmonic trap at zero temperature

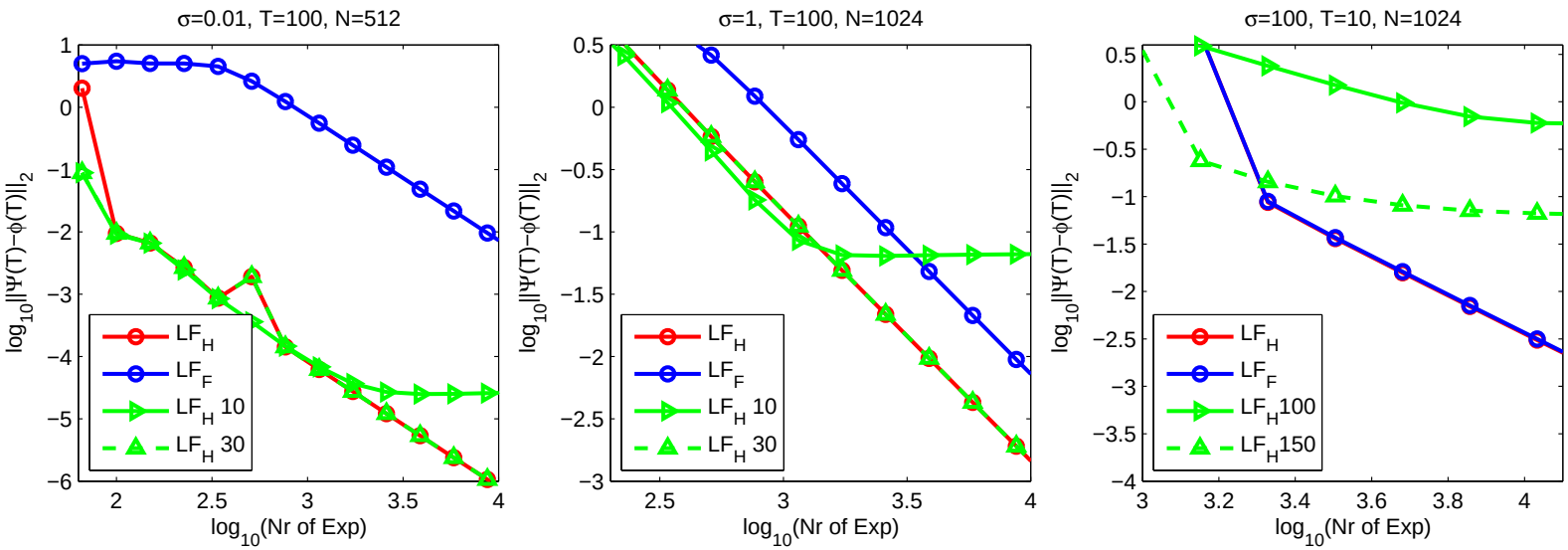
$$i\frac{\partial}{\partial t}\Phi(x,t) = \left(-\frac{1}{2m}\Delta + \frac{1}{2}m\omega^2 x^2 + g|\Phi(x,t)|^2\right)\Phi(x,t)$$

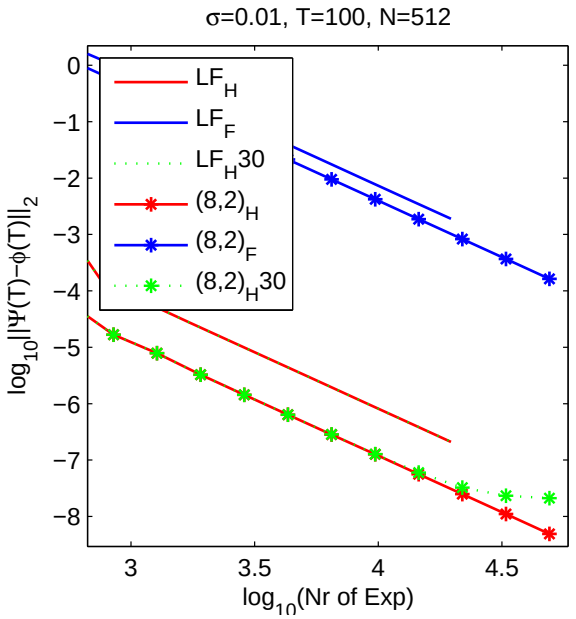
Norm preservation $|\Phi(x,t)|^2 = |\Phi(x,0)|^2$ allows for same splitting

(proof by derivation and plugging in of GPE and its complex conjugate)



Leapfrog method




σ=0.01, T=100, N=512
LF_H
LF_F
LF_H30
(8,2)_H
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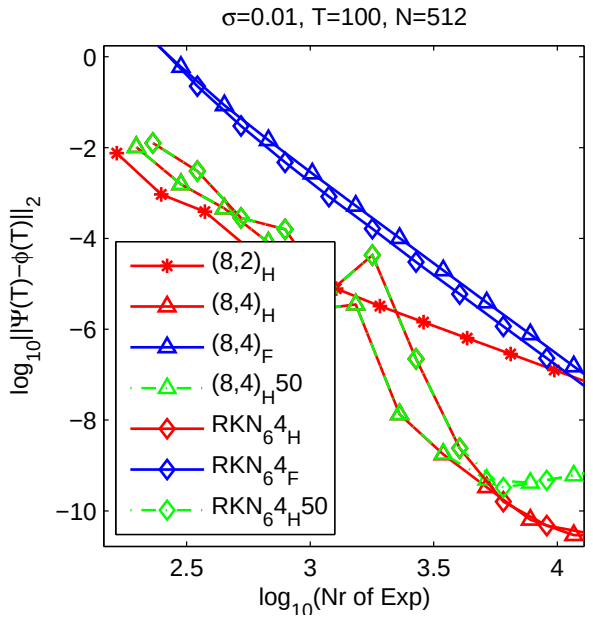
log10||Ψ(T)−φ(T)||2
log10(Nr of Exp)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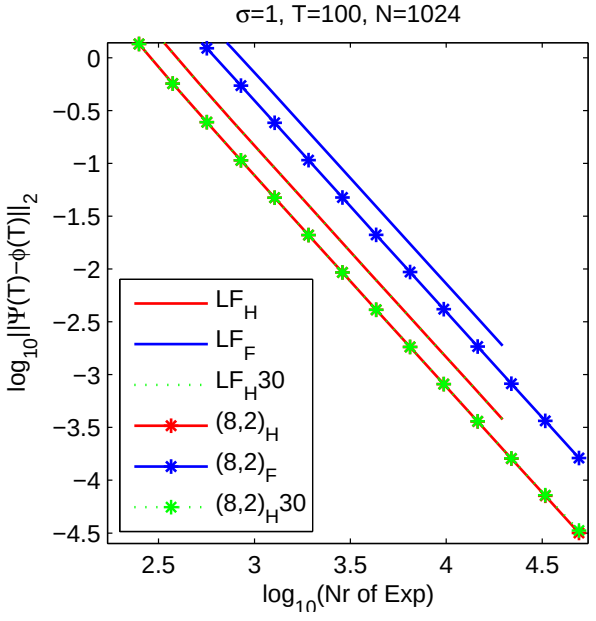
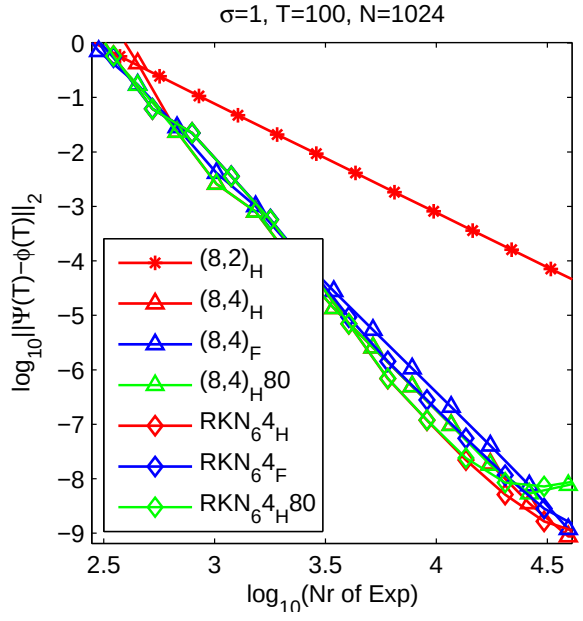
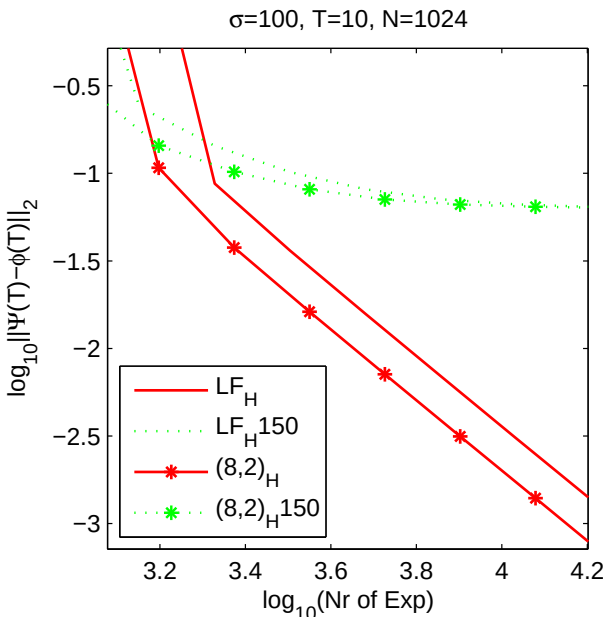
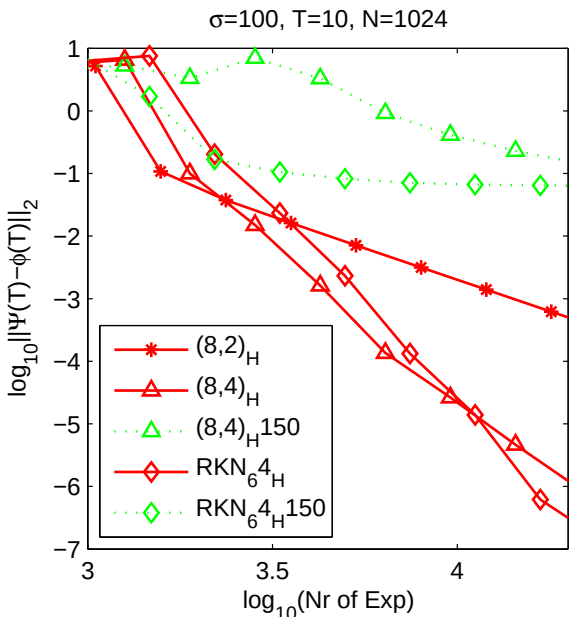
log10||Ψ(T)−φ(T)||2
log10(Nr of Exp)


σ=1, T=100, N=1024
LF_H
LF_F
LF_H30
(8,2)_H
(8,2)_F
(8,2)_H30
log10||Ψ(T)−φ(T)||2
log10(Nr of Exp)


σ=1, T=100, N=1024
(8,2)_H
(8,4)_H
(8,4)_F
(8,4)_H80
RKN_6 4_H
RKN_6 4_F
RKN_6 4_H80
log10||Ψ(T)−φ(T)||2
log10(Nr of Exp)





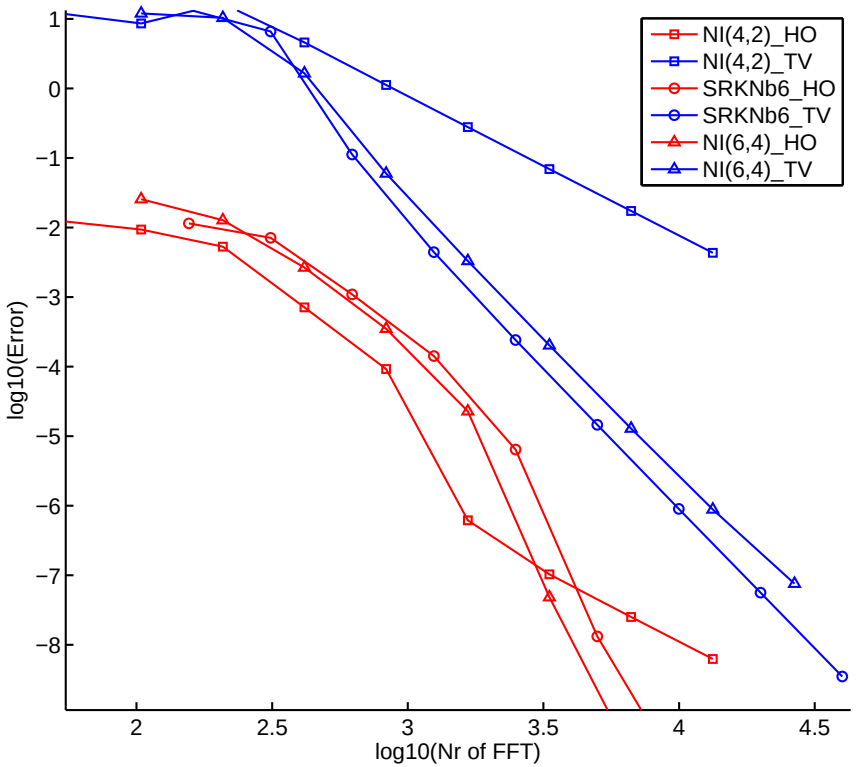
Fourier split omitted - coincides with Fourier-Hermite method

Quartic oscillator

Usual Schrödinger equation with potential

$$V = \frac{1}{2} m\omega^2 x^2 + \frac{1}{2}\beta x^4$$

where $\omega = 7$, $m = 5$, $\beta = \frac{1}{8} m^2 \left(\frac{\omega}{10}\right)^3 \approx 1.0719$,

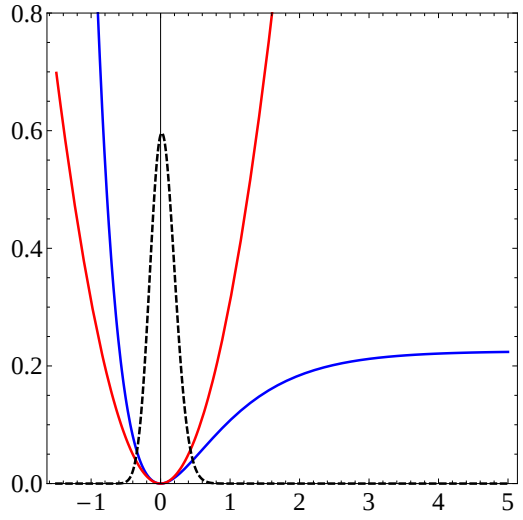


Morse potential

Approximation for the vibrational states of a diatomic molecule by

$$V(x) = D\left(1 - e^{-\alpha x}\right)^2 = D\alpha^2 x^2 + \mathcal{O}((\alpha x)^3)$$

(wavefunction not to scale)

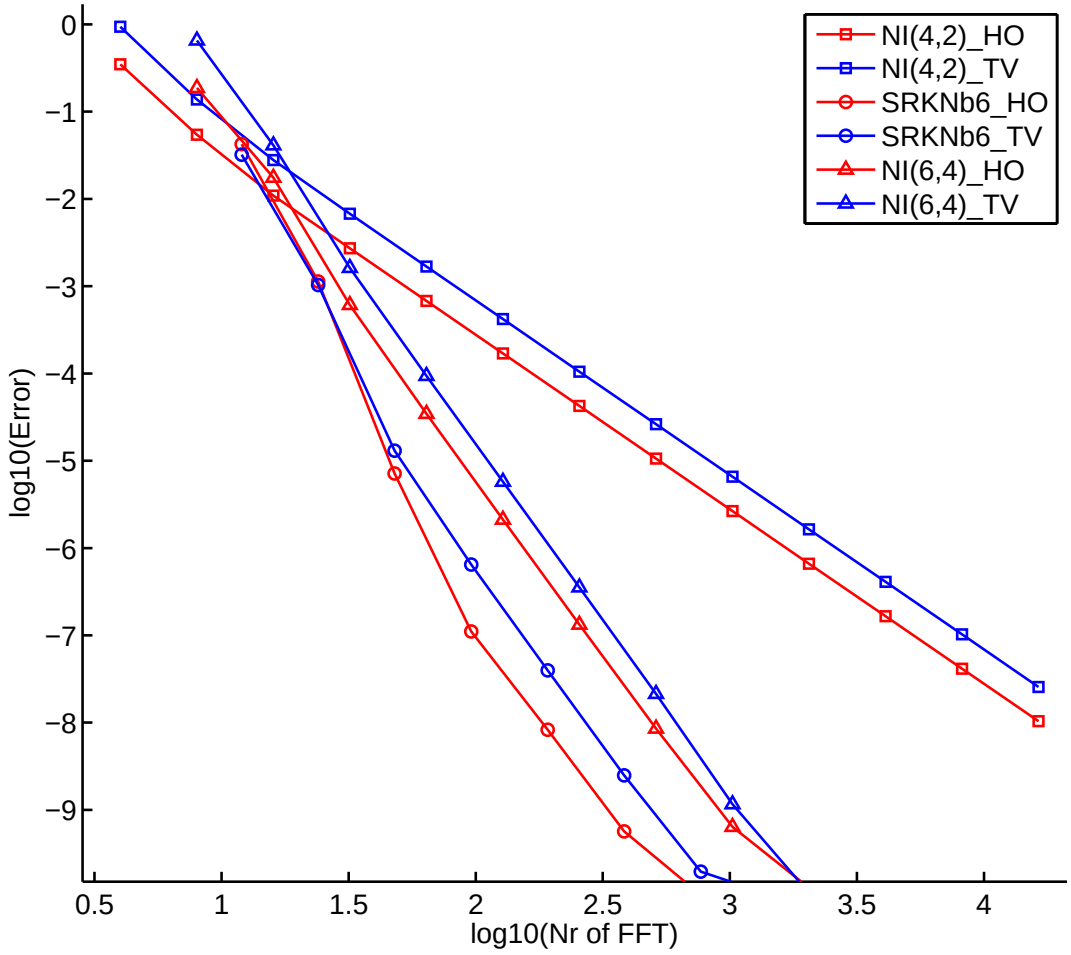


Parameters in a.u.	
mass	$\mu = 1745$
dissipation energy	$D = 0.2251$
length parameter	$\alpha = 1.1741$

2^8 grid points in $[-1.5, 5]$, $T = 100 + \pi$

Error for morse potential

Initial condition: slightly shifted exact ground state

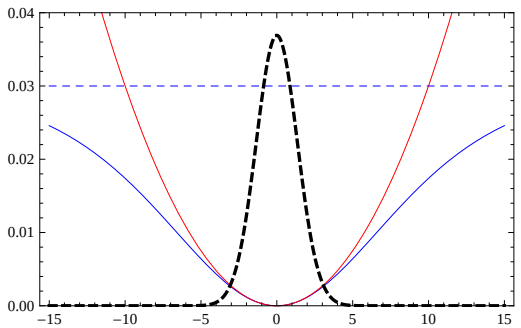


The potential reads

$$V(x) = -\frac{1}{2m}\alpha^2 \frac{\lambda(\lambda-1)}{\cosh^2 \alpha x} = \frac{\alpha^2}{2m}\left((\alpha x)^2 \lambda(\lambda-1)\right) + \mathcal{O}((\alpha x)^3)$$

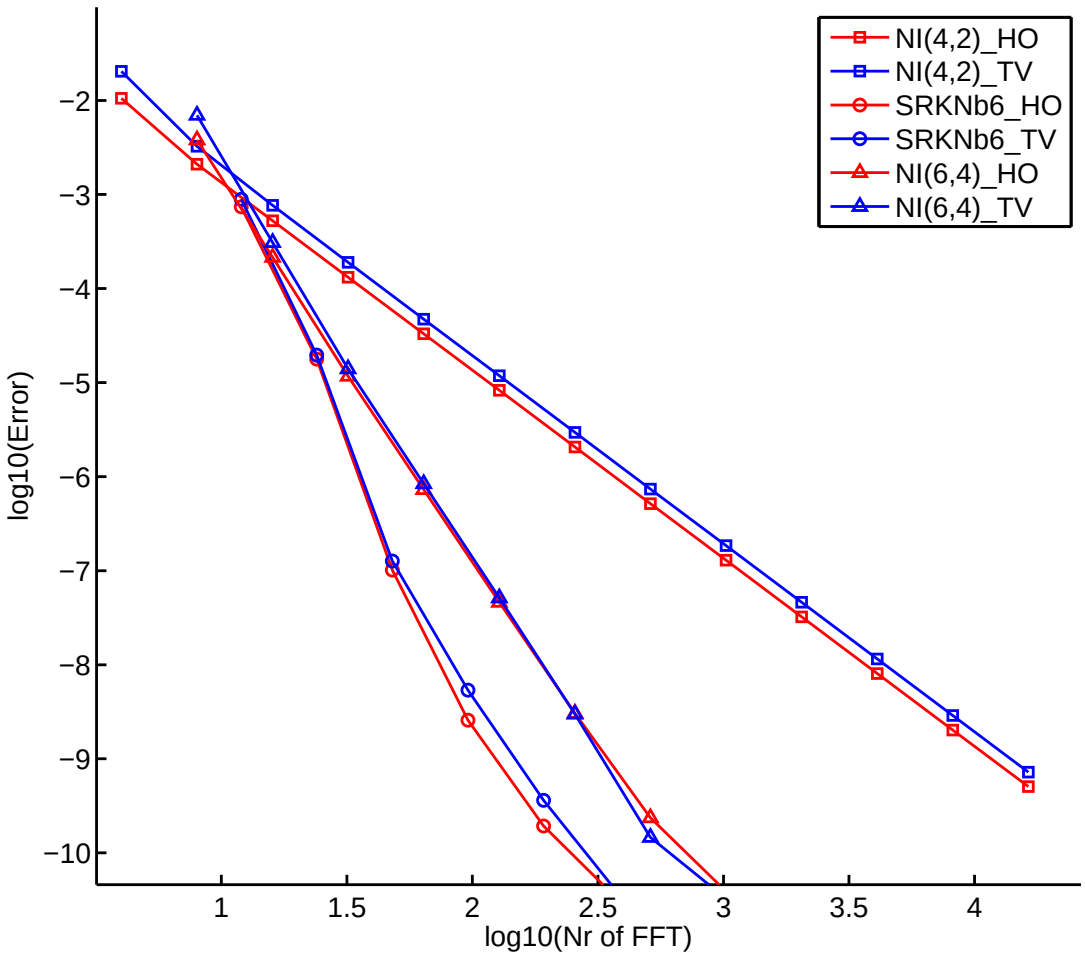
Parameters with $\hbar = 1$	
mass	$m = 5$
width	$\alpha = 0.1$
depth	$\lambda = 6$

(wavefunction not to scale)



Error for Pöschl-Teller potential

Initial condition: slightly shifted Gaussian



Structure

General case

$$i\frac{\partial}{\partial t}\psi(x,t) = \sum_{i,j}\left(-\frac{\alpha_{ij}}{2}\frac{\partial^2}{\partial x_i \partial x_j} + \frac{\beta_{ij}}{2}x_i x_j\right)\psi(x,t), \tag{13}$$

consider the classical problem

$$\frac{d}{dt}\begin{Bmatrix} q \\ p \end{Bmatrix} = \begin{pmatrix} 0 & M \\ -N & 0 \end{pmatrix}\begin{Bmatrix} q \\ p \end{Bmatrix} = (A+B)\begin{Bmatrix} q \\ p \end{Bmatrix} \tag{14}$$

with M, N matrices and

$$A \equiv \begin{pmatrix} 0 & M \\ 0 & 0 \end{pmatrix}, \qquad B \equiv \begin{pmatrix} 0 & 0 \\ -N & 0 \end{pmatrix}.$$

Shifted potentials and angular momentum

General linear inhomogeneous equation

$$\dot{\vec{x}} = A\vec{x} + \vec{b} \text{ has solution } \vec{x}(h) = e^{hA}\vec{x}_0 + A^{-1}\left(e^{hA} - I\right)\vec{b} \qquad (15)$$

Equations of motion of linearly extended Hamiltonian take form (18)

$$H = \frac{1}{2}p^T Mp + \frac{1}{2}q^T Nq + C^T p - D^T q$$

Added angular momentum

$$H = \frac{1}{2}p^T Mp + \frac{1}{2}q^T Nq + C^T p - D^T q + q^t Ep$$

non-symmetric composition necessary to separate momentum and space coordinates in the exponentials

Time dependent potentials

Consider time dependence in the trap frequency

$$V = \frac{1}{2}\omega(t)^2 x^2$$

or in the linear perturbation (phase)

$$V = \frac{1}{2}\omega^2 x^2 + \Omega(t)x$$

We expect simplifications through a careful study of the algebraic implications for a Magnus integrator.

Structure

References

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Preprint arXiv:1007.3470v1.

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Robert McLachlan
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BIT **35** (1995b).

Generalisation to higher dimensions

$$i\frac{\partial}{\partial t}\psi(x,t) = \sum_{i,j}\left(-\frac{\alpha_{ij}}{2}\frac{\partial^2}{\partial x_i \partial x_j} + \frac{\beta_{ij}}{2}x_i x_j\right)\psi(x,t), \tag{16}$$

is equivalent to consider the classical problem

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$$A \equiv \begin{pmatrix} 0 & M \\ 0 & 0 \end{pmatrix}, \qquad B \equiv \begin{pmatrix} 0 & 0 \\ -N & 0 \end{pmatrix}.$$

$$g(h,N,M) = M\sqrt{NM}^{-1}\sin\left(h\sqrt{NM}\right),$$

$$f(h,N,M) = \tan\left(\frac{h}{2}\sqrt{NM}\right)\sqrt{NM}M^{-1}.$$

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Extension to shifted potentials

General linear inhomogeneous equation

$$\dot{\vec{x}} = A\vec{x} + \vec{b} \text{ has solution } \vec{x}(h) = e^{hA}\vec{x}_0 + A^{-1}\left(e^{hA} - I\right)\vec{b} \qquad (18)$$

Equations of motion of linearly extended Hamiltonian take form (18)

$$H = \frac{1}{2}p^T M p + \frac{1}{2}q^T N q + C^T p - D^T q$$

Lemma

For M, N spd and simultanously diagonalisable, the following property is satsfied

$$e^{-ihH} = e^{-i\left(\frac{1}{2}q^T F_h q - D^T F_h q\right)} e^{-i\left(\frac{1}{2}p^T G_h p + C^T G_h p\right)} e^{-i\left(\frac{1}{2}q^T F_h q - D^T F_h q\right)}$$

where, as before,

$$G_h = M\sqrt{NM}^{-1}\sin\left(h\sqrt{NM}\right), \qquad F_h = \tan\left(\frac{h}{2}\sqrt{NM}\right)\sqrt{NM}M^{-1}.$$

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Proof

The generator of the Lie-algebra includes now more terms, for which we compute the composition in the associated Lie-group. As before, we split in easily solvable terms

$$H_A = \frac{1}{2}F_h q^2 + \alpha(h)q \quad \Rightarrow \begin{Bmatrix} q(h) \\ p(h) \end{Bmatrix} = \begin{Bmatrix} q_0 \\ p_0 - hF_h - h\alpha(h) \end{Bmatrix} \equiv \Phi_h^A(q_0, p_0)$$

$$H_B = \frac{1}{2}G_h p^2 + \beta(h)p \quad \Rightarrow \begin{Bmatrix} q(h) \\ p(h) \end{Bmatrix} = \begin{Bmatrix} q_0 + hG_h + h\beta(h) \\ p_0 \end{Bmatrix} \equiv \Phi_h^B(q_0, p_0)$$

and require the symmetric composition

$$\Psi_h(q_0, p_0) = \Phi_{h/2}^A \circ \Phi_h^B \circ \Phi_{h/2}^A(q_0, p_0) \tag{19}$$

to match the exact solution. Functions F, G, α, β have been added to account for the increased complexity of the algebraic structure. Computing (19) and matching the coefficients with the exact solution (18) yields the solution.

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Thank you for your attention