Geometric integrators for Schrödinger equations

Philipp Bader

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Introduction

We study a variety of Schrödinger equations and propose efficient *geometric integrators* for their solution. A geometric integrator preserves some qualitative properties of the exact solution, e.g., norm (unitarity), Gauge-invariance, energy, etc.

- Time-dependent (with Blanes)

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

- Semi-classical (with Iserles, Kropielnicka, Singh)

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

- Stationary (with Blanes, Casas)

$$E\Psi(x) = (-\Delta + V(x))\,\Psi(x), \quad \Psi(x,t) = \Psi(x)e^{iEt}$$

- Nonlinear (with Blanes)

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left(-\Delta + V(x) + g|\Psi(x,t)|^2\right)\Psi(x,t), \quad \Psi(x,0) = \Psi_0(x)$$

Tools

The following concepts have been used in the derivation of new algorithms

- Lie-algebras
- Splitting

$$\dot y = A(y) + B(y) \Longrightarrow y(h) = \prod_{k=1}^{s} e^{hb_k B}e^{ha_k A}y_0 + \mathcal{O}\left(h^{p+1}\right).$$

- BCH formula

$$e^A e^B = e^{BCH(A,B)} = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}([A,[A,B]]-[B,[A,B]])+\cdots}$$

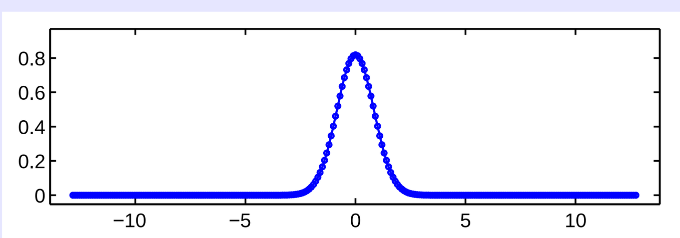
- Magnus expansion

$$\dot y = H(t)y \Longrightarrow y(h) = e^{\Omega_h}y_0,$$
$$\Omega_h = \int_0^h H(t_1)dt_1 + \frac{1}{2}\int_0^h\int_0^{t_2}[H(t_1),H(t_2)]dt_1\,dt_2 + \ldots$$

The Standard Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left(-\partial_x^2 + V(x,t)\right)\Psi(x,t), \quad \Psi(x,0) = \Psi_0(x)$$

Asymptotic boundary conditions



Splitting and Fourier transforms

$$\psi(x,h) = \prod_{k=1}^{s} e^{hb_i\tilde V_k}e^{ha_i T}\psi_0 + \mathcal{O}\left(h^{p+1}\right),$$

$\Rightarrow$ $T = -\partial_x^2$ is diagonal in Fourier space.

$\Rightarrow$ Magnus or evolve time with T, $\tilde V_k = V\left(\sum_j^k a_j\right)$.

Algebraic properties

$V = x^2$ or $V = f(t)x$ generate finite dimensional algebras:

$$\left\{p^2, x^2, px\right\}, \quad \left\{p^2, p, x, 1\right\}$$

Key ingredient: CM $\leftrightarrow$ QM as $\{\cdot,\cdot\} \leftrightarrow i[\cdot,\cdot]$

Example: Harmonic oscillator

$$e^{-ih(T+x^2)} = e^{-if(h)T}e^{-ig(h)x^2}e^{-if(h)T} = e^{-if(h)x^2}e^{-ig(h)T}e^{-if(h)x^2}$$

with $f(h) = \tan(h/2)$, $g(h) = \sin(h)$.

Generalizations

$$H = p_x^2 + p_y^2 + x^2 + y^2 + (yp_x - xp_y) + xp_x + yp_y + x + y.$$

Semi-classical Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left(-\varepsilon\partial_x^2 + \frac{1}{\varepsilon}V(x,t)\right)\Psi(x,t)$$

$\Rightarrow$ Highly oscillatory: $\varepsilon \sim \hbar$ vs. $\varepsilon \sim 1$

Key ingredients: sBCH, expansion $h \sim \varepsilon^\sigma$, derivatives

$$e^{h(X+Y)} = e^{h/2X}e^{sBCH(hX,hY)}e^{h/2X},$$

Example:

$$e^{-ihH} = e^{\mathcal{R}_0}e^{\mathcal{R}_1}e^{\mathcal{R}_2}e^{\mathcal{T}_3}e^{\mathcal{R}_2}e^{\mathcal{R}_1}e^{\mathcal{R}_0} + \mathcal{O}\left(\varepsilon^{7\sigma-1}\right)$$

where $\mathcal{R}_0 = \frac{1}{2}\tau\varepsilon\partial_x^2 \sim \varepsilon^{\sigma-1}$, $\mathcal{R}_1 = \frac{1}{2}\tau\varepsilon^{-1}V \sim \varepsilon^{\sigma-1}$, $\mathcal{R}_2 \sim \varepsilon^{3\sigma-1}$.

- Linear growth of no. of exp.
- separation of scales ($\sim \varepsilon^k$)

Generalization to $V(t)$ by Magnus expansion

Imaginary time Schrödinger equation

Eigenvalue problem

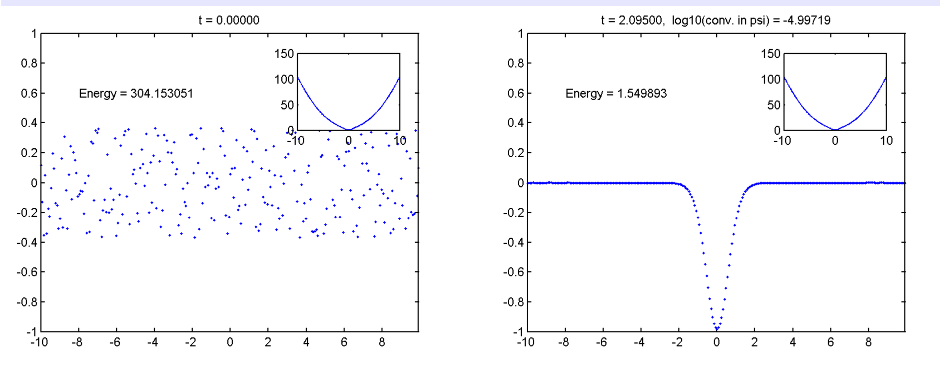
$$E\Psi(x) = (-\Delta + V(x))\,\Psi(x)$$

Expansion in eigenstates

$$\Psi(x,t) = e^{-itH}\Psi(x,0) = \sum_{n\in I} e^{-it\lambda_n}\langle\phi_n|\Psi_0\rangle\phi_n(x)$$

Imaginary time propagation, $t = -i\tau$:

$$\Psi(x,-i\tau) \to e^{-\tau\lambda_0}\langle\phi_0|\Psi_0\rangle\phi_0(x), \qquad (0 \le \lambda_i \le \lambda_{i+1} \le \ldots)$$



Splitting

- Parabolic equation $\to$ order restriction
- complex coefficient $\to$ higher order

Modified potentials [Koseleff]

Central observation:

$$[V,[V,\partial_x^2]] = -2(V'(x))^2$$

diagonal in coordinate space, thus

$$e^{-\tau H} = \prod e^{-a_i\tau\Delta}e^{-b_i\tau V - c_i\tau^3(V')^2} + \mathcal{O}\left(h^{p+1}\right)$$

$\to$ up to order 4 with positive real coefficients [Chin 2005].
(Higher order with complex time-step (pos. real part))

Gross-Pitaevskii equation

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

- Near-linear equation for $g \ll 1$, relevant terms

$$A = -\Delta + V, \; B = |\psi|^2 \quad \Longrightarrow \quad g\,[A,[A,B]], \; g\,[A,[A,[A,[A,B]]]]$$

- Real time: Real coeff. for Δ and $\partial_t|\Psi|^2 = 0$ or ($c = g/b_k$)

Norm: $\partial_t|\Psi|^2 = 2\Re(c)|\Psi|^4,$

Phase: $\partial_t \log(\Psi) = c|\Psi|^2$

- Imaginary time *(work in progress)*
  - $\Rightarrow$ real coefficients for B, complex coeff. for A
  - $\Rightarrow$ all complex (see above)
  - $\Rightarrow$ order reductions observed

References

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