Symplectic methods for the time integration of the Schrödinger equation

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When investigating the dynamical behavior of quantum systems of low to moderate dimension, very often it is necessary to solve numerically the time dependent Schrödinger equation. After a spatial discretisation, one has to solve a linear differential equation

$$i\frac{d}{dt}u(t) = Hu(t), \qquad u(0) = u_0 \in \mathbb{C}^N, \tag{1}$$

where $u(t)$ represents a discretized version of the wave function at the space grid points. H is an Hermitian matrix associated to the Hamiltonian, and then the problem can be seen as a system of N coupled harmonic oscillators with "unknown" frequencies, $\lambda_1, \ldots, \lambda_N$. However, in general, one can know upper and lower bounds to the extreme eigenvalues of H, say E_{min} and E_{max}, such that $E_{min} \leq \lambda_i \leq E_{max}, \ \ \forall i$.

We look for approximate solutions, $\tilde{u}$, to $u(t_f) = e^{-it_f H}\, u_0$ which only uses products of vectors with the matrix H, i.e. polynomial approximations. Given a tolerance, tol, the goal is to look for an efficient scheme which provides $\tilde{u}$ such that $\|\tilde{u} - u(t_f)\| < tol$ with the smaller amount of vector-matrix multiplications and storage requirements.

Among the most employed numerical schemes in the literature within this class are the Chebyshev methods, being in general about twice faster than Taylor methods. However, the analysis of the simple scalar harmonic oscillator (from the perspective of the analysis, optimization, algebra and geometric structure) allows us to build new symplectic methods with better geometric properties which at the same time provide the desired solution between 50% faster and twice faster.

The algorithm contains a subroutine with a set of symplectic methods, each one optimized for different problems which can be used as a black box for the user.