Decompositions of Ordered Operator Exponentials for Computational Quantum Physics

Gradient symplectic

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ARTICLES

Gradient symplectic algorithms for solving the Schrödinger equation with time-dependent potentials

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For $H(t)$ a time-dependent operator, the evolution equation,

$$\frac{\partial}{\partial t}\psi(t)=H(t)\psi(t), \tag{1}$$

has the operator solution

$$\psi(t+\Delta t)=T\left(\exp\int_t^{t+\Delta t}H(s)ds\right)\psi(t). \tag{2}$$

The time-ordered exponential not only has the conventional expansion,

$$T\left(\exp\int_t^{t+\Delta t}H(s)ds\right)=1+\int_t^{t+\Delta t}H(s_1)ds_1+\int_t^{t+\Delta t}ds_1\int_t^{s_1}ds_2H(s_1)H(s_2)+\cdots, \tag{3}$$

but also the more intuitive interpretation

$$T\left(\exp\int_t^{t+\Delta t}H(s)ds\right)=\lim_{n\to\infty}T(e^{(\Delta t/n)\Sigma_{i=1}^{n}H(t+i(\Delta t/n))}),$$
$$=\lim_{n\to\infty}e^{(\Delta t/n)H(t+\Delta t)}\cdots e^{(\Delta t/n)H(t+2\Delta t/n)}\times e^{(\Delta t/n)H(t+\Delta t/n)}. \tag{4}$$

as time zero. Thus, the two second order algorithms for solving the Schrödinger equation with step size Δt can be denoted simply as

second-order

$$\mathcal{T}_A^{(2)}(\epsilon)=e^{\frac{1}{2}\epsilon T}e^{\epsilon V(\epsilon/2)}e^{\frac{1}{2}\epsilon T},$$

$$\mathcal{T}_B^{(2)}(\epsilon)=e^{\frac{1}{2}\epsilon V(\epsilon)}e^{\epsilon T}e^{\frac{1}{2}\epsilon V(0)}.$$

fourth-order

$$\mathcal{T}_C^{(4)}(\epsilon)\equiv e^{\frac{1}{6}\epsilon T}e^{\frac{3}{8}\epsilon V(5\epsilon/6)}e^{\frac{1}{3}\epsilon T}e^{\frac{1}{4}\epsilon\tilde{V}(\epsilon/2)}\times e^{\frac{1}{3}\epsilon T}e^{\frac{3}{8}\epsilon V(\epsilon/6)}e^{\frac{1}{6}\epsilon T},$$

$$\mathcal{T}_D^{(4)}(\epsilon)\equiv e^{\frac{1}{8}\epsilon\tilde{V}(\epsilon)}e^{\frac{1}{3}\epsilon T}e^{\frac{3}{8}\epsilon V(2\epsilon/3)}e^{\frac{1}{3}\epsilon T}\times e^{\frac{3}{8}\epsilon V(\epsilon/3)}e^{\frac{1}{3}\epsilon T}e^{\frac{1}{8}\epsilon\tilde{V}(0)},$$

Thus, for $H(t)=T+V(t)$, the effect of time ordering is to increment the time dependence of each potential operator $V(t)$ by the sum of the time steps of all the T operators to its right.

Suzuki-Trotter

Finding Exponential Product Formulas of Higher Orders

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In the actual application of the approximant, we divide the parameter x into n slices in the form

$$\left(e^{\frac{x}{n}A}e^{\frac{x}{n}B}\right)^n=\left[e^{\frac{x}{n}(A+B)+\frac{1}{2}\left(\frac{x}{n}\right)^2[A,B]+O\left(\left(\frac{x}{n}\right)^3\right)}\right]^n=e^{x(A+B)+\frac{1}{2}\frac{x^2}{n}[A,B]+O\left(\frac{x^3}{n^2}\right)}. \tag{21}$$

Thus the correction term vanishes in the limit $n\to\infty$. We refer to the integer n as the Trotter number.

Now we discuss as to why we should be interested in generalizing the Trotter approximation. The Trotter approximant (1) and the generalized one (3), in fact, have a remarkable advantage over other approximants such as the frequently used one

$$e^{x(A+B)}=I+x(A+B)+O(x^2). \tag{22}$$

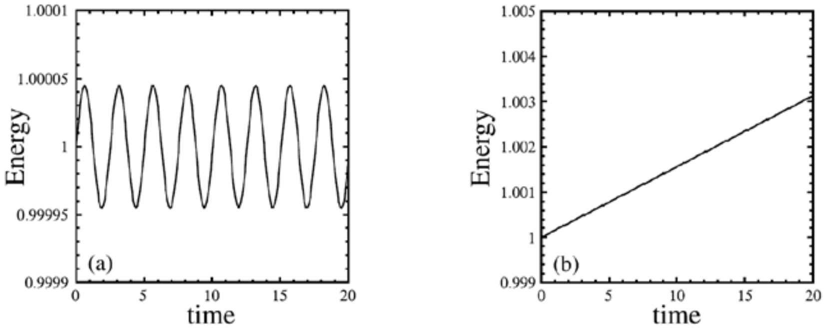

Figure 1: The energy deviation due to the approximations given by (a) the Trotter approximant (29) and (b) the perturbational approximant (30). In both calculations, we put $\Gamma=3/4$ and $\Delta t=0.0001$. The initial state is the one in Eq. (27) with the energy expectation $\langle\mathcal{H}\rangle=1$.

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Fourth-order factorization of the evolution operator for time-dependent potentials

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$$U(t+\Delta t,t)=\exp\left\{-i\int_t^{t+\Delta t}dt_1\,H(t_1)-\frac{1}{2}\int_t^{t+\Delta t}dt_1\int_t^{t_1}dt_2\left[H(t_1),H(t_2)\right]+O(\Delta t^5)\right\}.$$

$$U=e^{-i\frac{1}{6}\Delta t W_1+i\Delta t^2W_2}e^{-i\frac{1}{2}\Delta t H_0}e^{-i\frac{2}{3}\Delta t\tilde{W}_1}e^{-i\frac{1}{2}\Delta t H_0}\times e^{-i\frac{1}{6}\Delta t W_1-i\Delta t^2W_2}+O(\Delta t^5). \tag{10}$$

In Eq. (10), the modified operator reads

$$\tilde{W}_1=W_1-\frac{1}{48}\Delta t^2[W_1,[H_0,W_1]]=W_1-\frac{1}{48m}\Delta t^2(\nabla W_1)^2. \tag{11}$$

$$W_1(t)=\frac{1}{6}\left[V(t)+4V\left(t+\frac{1}{2}\Delta t\right)+V(t+\Delta t)\right]+O(\Delta t^4) \tag{12}$$

and

$$W_2(t)=\frac{1}{12\Delta t}[V(t)-V(t+\Delta t)]+O(\Delta t^2). \tag{13}$$

With the help of Eqs. (10) to (13), an algorithm of order Δt^5 is obtained. It contains five exponentials in place of three in Eq. (2).

The same principle should provide approximations of at least order Δt^7. However, the factorization involves at least nine exponentials and some terms are significantly more complicated. It is not obvious that these expressions would be more efficient than expressions (10) to (13).