Note

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1 Time evolution

Consider time $t = N\Delta t$. Δt is the numerical integration step length. In the first place we choose Taylor expansion to deal with it:

$$e^{\mathrm{i}tH} = \sum_{n=0}^{\infty} \frac{(\mathrm{i}tH)^n}{n!}. \tag{1}$$

Of cousre we cannot compute to the infinite order practically thus we shall determine the order n_c to be cut off. Factorial grows faster than the exponential with a constant base. Here we define the cut-off criterion as

$$\epsilon = \langle\psi|\frac{(tH)^{n_c}}{n_c!}|\psi\rangle \leq 10^{-15}. \tag{2}$$

Alternatively, we can integrate step by step as

$$|\psi(t)\rangle = \left(e^{-\mathrm{i}\Delta tH}\right)^N |\psi(0)\rangle, \quad |\psi_{n+1}\rangle \simeq (1 - \mathrm{i}\Delta tH)|\psi_n\rangle. \tag{3}$$

Askar proposed another method in terms of the differentiation between $|\psi_{n+1}\rangle$ and $|\psi_{n-1}\rangle$

$$|\psi_{n+1}\rangle - |\psi_{n-1}\rangle = \left(e^{-\mathrm{i}\Delta tH} - e^{\mathrm{i}\Delta tH}\right)|\psi_n\rangle \simeq -2\mathrm{i}\Delta tH|\psi_n\rangle. \tag{4}$$

While this scheme is still not unitary. Goldberg proposed to replace the step approximation by a unitary one

$$e^{-\mathrm{i}\Delta tH} \simeq \frac{1 - \frac{1}{2}\mathrm{i}\Delta tH}{1 + \frac{1}{2}\mathrm{i}\Delta tH} \tag{5}$$

and one can obtain an improved version of Askar method

$$|\psi_{n+1}\rangle \simeq |\psi_{n-1}\rangle - \frac{2\mathrm{i}\Delta tH}{1 + \frac{1}{4}\Delta t^2H^2} \simeq |\psi_{n-1}\rangle - 2\mathrm{i}\Delta tH\left(1 - \frac{1}{4}\Delta t^2H^2\right)|\psi_n\rangle. \tag{6}$$