Supplementary Material: Time-step targeting time-dependent and dynamical density matrix renormalization group algorithms with ab initio Hamiltonians

Enrico Ronca,* Zhendong Li, Carlos A. Jimenez-Hoyos, and Garnet Kin-Lic Chan*

Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, USA

E-mail: enrico.r8729@gmail.com; gkc1000@gmail.com
1 Spin-Adaptation effects on td-DMRG LDOS

Figure 1: Effect of Spin-Adaptation on the Spectral Function of a 8 site Hubbard model calculated using td-DMRG. A potential energy $U = 0.1t$ and a broadening $\eta = 0.1$ a.u have been used. Spectral functions have been calculated at the first site of the chain.

2 Dependence of the LDOS accuracy from $\tau$

A careful optimization of the $\tau$ value is fundamental to get accurate simulations and, at the same time, to avoid wasting time in excessively long propagations. In figure 2 the spectral function for the 8 site Hubbard model has been calculated using different values of the time-step. All the propagations have been carried out, in this case, for the same total period of time ($T = 500$ a.u.) using the RK4 scheme. As expected, reducing the size of the time-step (in particular in the 0.3-0.05 a.u. range) we are able to improve the quality of the spectrum, providing better and better approximations of the exponential propagator. Looking at these
results we can estimate a \( \tau \approx 0.1 - 0.2 \) a.u. as the best compromise between accuracy and computational cost. When smaller (e.g. 0.01 a.u.) time-step values are used, the results deteriorate (see blue line in figure 2). This behaviour was already observed by Feiguin and White in Ref. 1 and is attributed to an increase of the truncation error when large numbers of propagation steps are performed.

3 Additional DOS of Hydrogen Chains
Figure 3: DMRG Spectral Functions of three equally spaced hydrogen chains (H$_{10}$ - red, H$_{20}$ - green, H$_{50}$ - blue) at $r = 2.4$ Bohr bond distance. All the LDOSs have been calculated on the central site of the chain. A broadening ($\eta$) equal to 0.05 a.u. has been used.

Figure 4: DMRG and HF Spectral Functions of a 10 atom hydrogen chain calculated at different inter-atomic distances. All the LDOSs have been calculated on the central site of the chain. A broadening ($\eta$) equal to 0.05 a.u. has been used.
Figure 5: DMRG and HF Spectral Functions of a 30 atom hydrogen chain calculated at different inter-atomic distances. All the LDOSs have been calculated on the central site of the chain. A broadening ($\eta$) equal to 0.05 a.u. has been used.

Figure 6: DMRG and HF Spectral Functions of a 50 atom hydrogen chain calculated at different inter-atomic distances. All the LDOSs have been calculated on the central site of the chain. A broadening ($\eta$) equal to 0.05 a.u. has been used.
References

(1) Feiguin, A. E.; White, S. R. Time-step targeting methods for real-time dynamics using the density matrix renormalization group. *Phys. Rev. B* **2005**, *72*, 020404.