One dimensional model systems in time-dependent density functional theory

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Outline

1. 1D model systems
2. Local density approximation
3. Rabi oscillations
4. Conclusions

Octopus code: www.tddft.org/programs/octopus

1D model systems

N particles in 1D

$$\sum_{j=1}^{N}\left[-\frac{d^2}{2dx_j^2}+v_{ext}(x_j)\right]+\frac{1}{2}\sum_{\substack{j,k=1\\j\neq k}}^{N}\frac{1}{\sqrt{(x_j-x_k)^2+1}}$$

- Equivalent to 1 particle in N dimensions
- Solve problem by exact diagonalization of Hamiltonian
- Fermionic symmetry enforced by projecting on Young diagrams

Local density approximation

- Parametrization of the correlation energy from Quantum Monte-Carlo calculations of 1D homogeneous electron gas

Linear response

Beryllium ions

$$v_{ext}(x,t) = -\frac{4}{\sqrt{x^2+1}} + \mathcal{E}_0\delta(t)$$

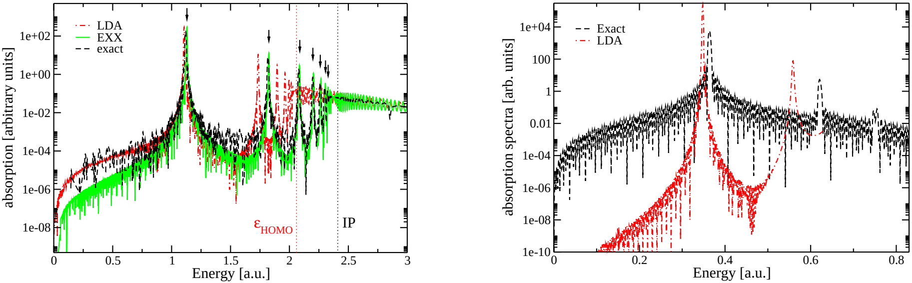
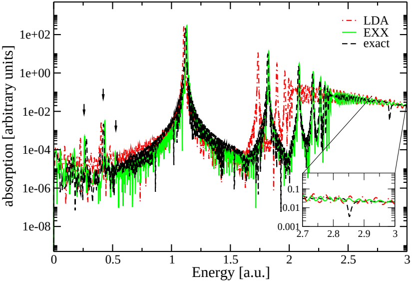


Fig. 1: Linear response spectra for Be^{2+} (left) and Be^{+} (right).

Nonlinear response

Increased amplitude $\mathcal{E}_0$

Second order response vanishes due to symmetry



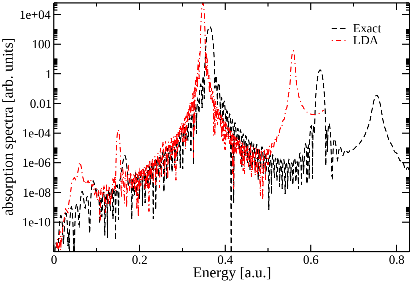


Fig. 2: Nonlinear response spectra for Be^{2+} (left) and Be^{+} (right).

Rabi oscillations

$$v_{ext}(x,t) = -\frac{2}{\sqrt{x^2+1}} + \mathcal{E}_0 \sin((\omega_0+\delta)t), \quad \omega_0 = 0.533\,\mathrm{Ha}$$

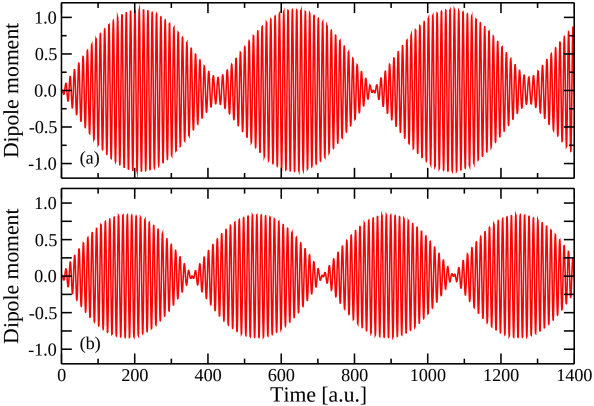


Fig. 3: Rabi oscillations with $\delta = 0.0006$ Ha and $\delta = 0.016$ Ha

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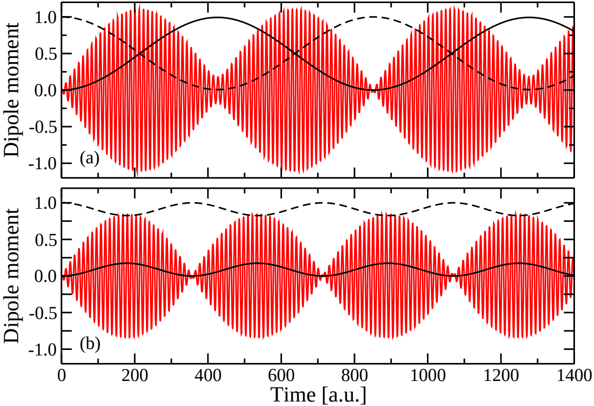

Fig. 3: Rabi oscillations with $\delta = 0.0006$ Ha and $\delta = 0.016$ Ha

Rabi oscillations in TDDFT

Excitation with resonant frequency from linear response

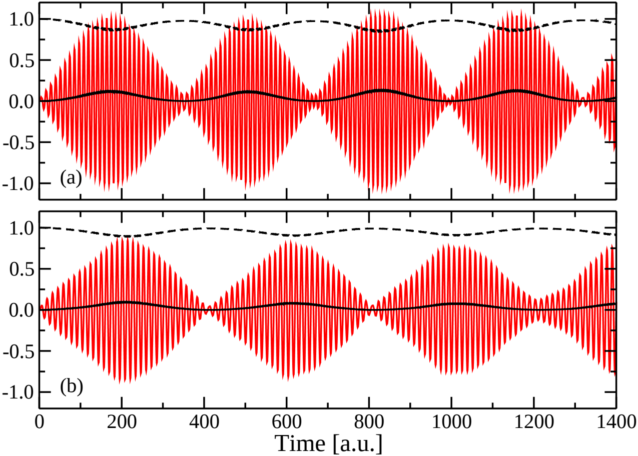

Fig. 4: Rabi oscillations in EXX (a) and LDA (b)

Theoretical analysis

Two level approximation

$$\begin{aligned}|\Psi(t)\rangle &= a_0(t)|\Psi_0\rangle + a_1(t)|\Psi_1\rangle \\ n_j(t) &= |a_j(t)|^2\end{aligned}$$

- Exact calculation

$$i\partial_t \begin{pmatrix} a_0(t) \\ a_1(t) \end{pmatrix} = \begin{pmatrix} \epsilon_0 & d_{10}\mathcal{E}(t) \\ d_{10}\mathcal{E}(t) & \epsilon_1 \end{pmatrix} \begin{pmatrix} a_0(t) \\ a_1(t) \end{pmatrix}$$

- DFT calculation

$$i\partial_t \begin{pmatrix} a_0^s(t) \\ a_1^s(t) \end{pmatrix} = \begin{pmatrix} \epsilon_0^s + \epsilon_0^{xc}(t) & d_{10}^s\mathcal{E}(t) + \mathcal{F}_{xc}(t) \\ d_{10}^s\mathcal{E}(t) + \mathcal{F}_{xc}^*(t) & \epsilon_1^s + \epsilon_1^{xc}(t) \end{pmatrix} \begin{pmatrix} a_0^s(t) \\ a_1^s(t) \end{pmatrix}$$

Theoretical model versus propagation

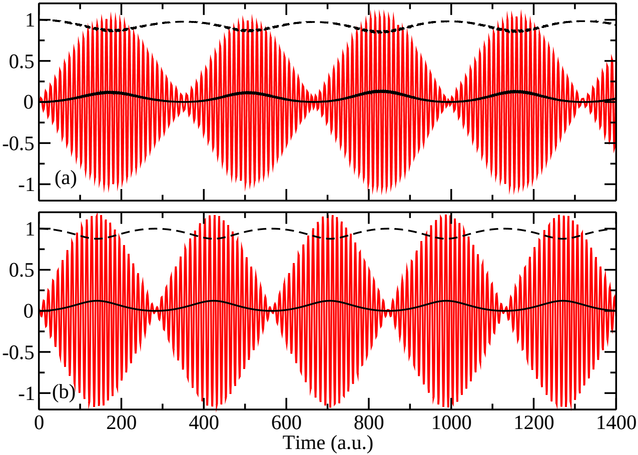

Fig. 5: Rabi oscillations from time propagation (a) and theoretical model (b) for the EXX functional

Conclusions and Outlook

- 1D LDA of the same quality as its 3D counterpart
- Good approximation for non-linear response
- Adiabatic approximations lead to detuning in Rabi oscillations
- Non-adiabatic approximations

References:

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arXiv:1101.2564 accepted in PRA

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