A Comparison of Methods for Simulating Quantum Dot Dynamics

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24th September 2024, University of Tsukuba

Jonas Boym Flaten

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Preliminaries

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- quantum dot = spatially localised quantum system
- simulating dynamics => time evolution
- comparison of methods => numerical study
- **Work in progress!**

Outline

- System
- Methods
- Results
- Outlook

System

- **3-dimensional harmonic oscillator:**

$$\mathbf{H} = \sum_{i}^{N} \left(\frac{\vec{\mathbf{p}}_i}{2m} + \frac{m\omega^2}{2} \vec{\mathbf{r}}_i \right) + \sum_{i}^{N} \sum_{j>i}^{N} \frac{e^2}{4\pi\epsilon_0 \Delta \mathbf{r}_{ij}}$$

System

- **3-dimensional harmonic oscillator:**

$$\mathbf{H} = \sum_{i}^{N} \left(\frac{\vec{\mathbf{p}}_i}{2} + \frac{\omega^2}{2} \vec{\mathbf{r}}_i \right) + \sum_{i}^{N} \sum_{j>i}^{N} \frac{1}{\Delta \mathbf{r}_{ij}}$$

System

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$$\mathbf{H} = \sum_{i}^{N} \left(\frac{\vec{\mathbf{p}}_i}{2} + \frac{\omega^2}{2} \vec{\mathbf{r}}_i \right) + \sum_{i}^{N} \sum_{j>i}^{N} \frac{1}{\Delta \mathbf{r}_{ij}}$$

- $N = 2$ and $N = 8$
- $\omega \in \{ 0.01 , 0.10 , 0.25 , 0.50 , 0.75 , 1.00 \}$
- $3^3 = 27$ one-body basis states

System

harmonic oscillator energy eigenbasis (HO basis)

- **3-dimensional harmonic oscillator:**

$$\mathbf{H} = \sum_i^N \left(\frac{\vec{\mathbf{p}}_i}{2} + \frac{\omega^2}{2}\vec{\mathbf{r}}_i \right) + \sum_i^N \sum_{j>i}^N \frac{1}{\Delta \mathbf{r}_{ij}}$$

- N = 2 and N = 8
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Methods

- **Slater state:**

$$|\Phi\rangle = \ltimes \; |\phi_1 \ldots \phi_N\rangle \,/\sqrt{N!}$$

Methods

- **Slater state:**

$$|\Phi_{\vec{i}}\rangle = \ltimes \; |\phi_{i_1} \ldots \phi_{i_N}\rangle \,/\sqrt{N!}$$

Methods

- **Slater state:**

$$|\Phi_{\vec{i}}\rangle = \bigotimes |\phi_{i_1} \ldots \phi_{i_N}\rangle \, / \sqrt{N!}$$

- **Configuration Interaction (CI):**

  / Multi-Configurational Time-Dependent Hartree-Fock (MCTDHF):

$$|\Psi\rangle = \sum_{\vec{i}} C_{\vec{i}} |\Phi_{\vec{i}}\rangle = \sum_{\vec{i}} C_{\vec{i}} \bigotimes |\phi_{i_1} \ldots \phi_{i_N}\rangle \, / \sqrt{N!}$$

Methods

- **Slater state:**

$$|\Phi_{\vec{\imath}}\rangle = \rtimes \; |\phi_{i_1} \dots \phi_{i_N}\rangle \,/ \sqrt{N!}$$

Hartree-Fock basis (HF basis)

- **Configuration Interaction (CI):**

/ Multi-Configurational Time-Dependent Hartree-Fock (MCTDHF):

$$|\Psi\rangle = \sum_{\vec{\imath}} C_{\vec{\imath}} |\Phi_{\vec{\imath}}\rangle = \sum_{\vec{\imath}} C_{\vec{\imath}} \rtimes \; |\phi_{i_1} \dots \phi_{i_N}\rangle \,/ \sqrt{N!}$$

Methods

- **Coupled-Cluster (CC):**

$$|\Psi\rangle = \exp(\mathbf{X})\,|\Phi_0\rangle$$

$$= \sum_n \frac{\mathbf{X}^n}{n!}\,|\Phi_0\rangle = \sum_n \frac{(\mathbf{X}_1 + \mathbf{X}_2 + \ldots)^n}{n!}\,|\Phi_0\rangle$$

Methods

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- **Density Functional Theory (DFT):**

$$\mathbf{n} = \sum_i |\phi_i\rangle\langle\phi_i|$$

Methods

- Coupled-Cluster (CC):

$$|\Psi\rangle = \exp(\mathbf{X})\,|\Phi_0\rangle$$
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- Density Functional Theory (DFT):

$$\mathbf{n} = \sum_i |\phi_i\rangle\langle\phi_i|$$

Kohn-Sham basis (KS basis)

Results

HO basis:

Frequency	2e$^-$			8e$^-$		
	CI(SD)	CC	MCTDHF	CI(SD)	CC	MCTDHF
0.01	0.0797	0.0797	0.0797		-	1.27909
0.10	0.5007	0.5007	0.5008		6.1390	6.04836
0.25	1.0915	1.0915	1.0917		11.9122	11.6825
0.50	2.0026	2.0026	2.0030		20.0764	19.5312
0.75	2.8761	2.8761	2.8766		27.6379	26.6105
1.00	3.7297	3.7297	3.7303		34.5705	33.2865

Results

HF basis:

	2e⁻			8e⁻		
Frequency	CI(SD)	CC	MCTDHF	CI(SD)	CC	MCTDHF
0.01	0.0797	0.0797	0.0797		1.3330	1.27905
0.10	0.5007	0.5007	0.5008		6.1664	6.04836
0.25	1.0915	1.0915	1.0917		11.6190	11.6825
0.50	2.0026	2.0026	2.0030		19.4528	19.5312
0.75	2.8761	2.8761	2.8766		26.5295	26.6105
1.00	3.7297	3.7297	3.7303		33.2043	33.2865

Results

KS basis:

	2e⁻			8e⁻		
Frequency	CI(SD)	CC	MCTDHF	CI(SD)	CC	MCTDHF
0.01	0.0833	0.0833	0.0836		1.1997	1.2004
0.10	0.5227	0.5227	0.5228		6.0383	6.1024
0.25	1.1351	1.1351	1.1354		11.7963	11.8761
0.50	2.0779	2.0779	2.0784		19.8942	19.9838
0.75	2.9810	2.9810	2.9816		27.2202	27.3144
1.00	3.8631	3.8631	3.8638		34.1332	34.8992

Outlook

- Dynamics
- Correlations

Input or Questions?