ASP Online Seminars

Exact Kohn-Sham Density Functional Theory on a Lattice

Kossi Amouzouvi

September, 2021.

Outline

1. **Bibliography**

2. PhD Thesis
   - One dimensional lattice
   - 1D Hubbard Hamiltonian
   - Lattice - DFT
   - Exact method

3. Maths Initiative: Togo Maths Camp

Bio

1. 2011: Maitrise en Science Es Math‘ematiques, University of Lom‘e
2. 2014: PGD @ AIMS Ghana (Graduated from University of Cape Coast)
3. 2014: ASP Meeting, Senegal
4. 2018: Ph.D in Computational and Applied Physics (University of Witwatersrand)
5. 2018-2020: Teaching Assistant at AIMS
6. 2021: Lecturer at KNUST

ASP 2014

Outline

PhD Thesis: Motivation

- Density Functional Theory (DFT) is an elegant reformulation of quantum mechanics in which the density distribution is the variable that formally contains all the information about a system.
- For small lattice sizes described by the Hubbard model, the exact solutions can be found numerically and for a uniform infinite chain an analytic solution is available.
- The exact solutions can be used as a reference to approximate implementations of DFT.

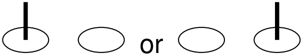
Two-site lattice with $n_e = 0, 1, 2, 4$

- Two sites lattice with zero electron

Two-site lattice with $n_e = 0, 1, 2, 4$

- Two sites lattice with zero electron

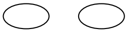
- Two sites lattice with one electron



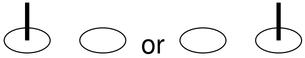
where | is either a spin up $\uparrow$ or a spin down $\downarrow$ electron.

Two-site lattice with $n_e = 0, 1, 2, 4$

- Two sites lattice with zero electron

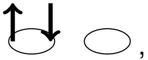


- Two sites lattice with one electron



where | is either a spin up ↑ or a spin down ↓ electron.

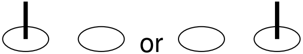
- Two sites lattice with two electrons



Two-site lattice with $n_e = 0, 1, 2, 4$

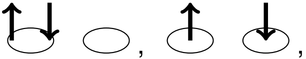
- Two sites lattice with zero electron

- Two sites lattice with one electron



where | is either a spin up ↑ or a spin down ↓ electron.

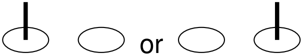
- Two sites lattice with two electrons



Two-site lattice with $n_e = 0, 1, 2, 4$

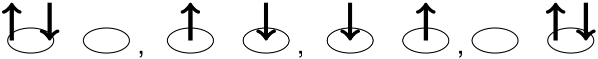
- Two sites lattice with zero electron

- Two sites lattice with one electron



where | is either a spin up $\uparrow$ or a spin down $\downarrow$ electron.

- Two sites lattice with two electrons

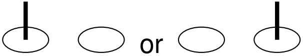


and two others.

Two-site lattice with $n_e = 0, 1, 2, 4$

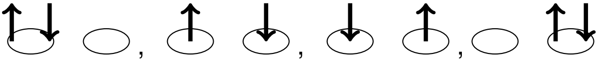
- Two sites lattice with zero electron

- Two sites lattice with one electron



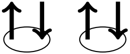
where | is either a spin up ↑ or a spin down ↓ electron.

- Two sites lattice with two electrons



and two others.

- Two sites lattice with four electrons



One Dimensional Hubbard Hamiltonian (1D HH)

The Hamiltonian, $\hat{H}$, of a quantum system gives information about the total energy of the system. In our case,

One Dimensional Hubbard Hamiltonian (1D HH)

The Hamiltonian, $\hat{H}$, of a quantum system gives information about the total energy of the system. In our case,

$\hat{H}$ is the single chain Hubbard Hamiltonian [a] used to describe discrete quantum systems (Lattice):

- t the nearest-neighbor hopping amplitude,
- u_0 the on-site interaction,
- v_i the on-site spin-independent external potential

[a] J. Hubbard, *Proc. R. Soc. (London) A* **276**, 238–257 (1963).

$\hat{H} = \hat{T} + \hat{u} + \hat{v}$:

- $$\hat{T} = -t \sum_{<ij>,\sigma}^{n_e} \hat{C}^{\dagger}_{j\sigma} \hat{C}_{i\sigma}$$
- $$\hat{u} = u_0 \sum_{i}^{n_e} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$
- $$\hat{v} = \sum_{i,\sigma}^{n_e} v_i \hat{n}_{i\sigma}$$

where $\hat{n}_{i\sigma} = \hat{C}^{\dagger}_{i\sigma} \hat{C}_{i\sigma}$ is the on-site particle number operator, and $\hat{C}^{\dagger}_{i\sigma}$ and $\hat{C}_{i\sigma}$ are the creation and annihilation operators.

1D HH

☛ To see how the different operators account for the physics that undergo the electrons, let us consider a two sites lattice with two electrons.

The case $n_e = 2$ is relevant since it easily points out the physics behind the Hubbard model.

1D HH: Kinetic operator

Let us denote by $\hat{t}_{ji\sigma}$ the operator $\hat{C}^{\dagger}_{j\sigma}\hat{C}_{i\sigma}$. The kinetic operator for a two sites lattice takes the expression

$$\begin{aligned}\hat{T} &= -t \sum_{<ij>,\sigma}^{2} \hat{C}^{\dagger}_{j\sigma}\hat{C}_{i\sigma} \\ &= -t \sum_{<ij>,\sigma}^{2} \hat{t}_{ji\sigma} \\ &= -t\left(\hat{t}_{21\uparrow} + \hat{t}_{12\uparrow} + \hat{t}_{21\downarrow} + \hat{t}_{12\downarrow}\right). \end{aligned} \tag{1}$$

From the following configurations, let us see how the kinetic operator conveys the idea of moving an electron from one site to the nearest neighbour sites. This characterized the motion of a valence electron from one atom to another.

1D HH: Kinetic operator

ϕ_i	$\hat{t}_{21\uparrow}\phi_i$	$\hat{t}_{12\uparrow}\phi_i$
$\phi_1 = \hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{2\uparrow}\|\rangle$:= 	$\hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{2\uparrow}\|\rangle = \|\rangle$:=  This state is not allowed	$-\hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{1\uparrow}\|\rangle = \|\rangle$:=  This state is not allowed
$\phi_2 = \hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{1\downarrow}\|\rangle$:= 	$\hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{1\downarrow}\|\rangle = \phi_4$:= 	$\|\rangle$:=  Complete annihilation
$\phi_3 = \hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{2\downarrow}\|\rangle$:= 	$\hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{2\downarrow}\|\rangle = \phi_5$:= 	$\|\rangle$:=  Complete annihilation
$\phi_4 = \hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{1\downarrow}\|\rangle$:= 	$\|\rangle$:=  Complete annihilation	$\hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{1\downarrow}\|\rangle = \phi_2$:= 
$\phi_5 = \hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{2\downarrow}\|\rangle$:= 	$\|\rangle$:=  Complete annihilation	$\hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{2\downarrow}\|\rangle = \phi_3$:= 
$\phi_6 = \hat{c}^\dagger_{1\downarrow}\hat{c}^\dagger_{2\downarrow}\|\rangle$:= 	$\|\rangle$:=  Complete annihilation	$\|\rangle$:=  Complete annihilation

Table: Images $\hat{t}_{ij\sigma}\phi_i$ of the basis elements ϕ_i by $\hat{t}_{21\uparrow}$ and $\hat{t}_{12\uparrow}$.

1D HH: Kinetic operator

tiny

ϕ_i	$\hat{t}_{21\downarrow}\phi_i$	$\hat{t}_{12\downarrow}\phi_i$
$\phi_1 = \hat{C}^\dagger_{1\uparrow}\hat{C}^\dagger_{2\uparrow}\lvert\rangle$:= ↑ ↑	$\lvert\rangle$:= ○ ○ Complete annihilation	$\lvert\rangle$:= ○ ○ Complete annihilation
$\phi_2 = \hat{C}^\dagger_{1\uparrow}\hat{C}^\dagger_{1\downarrow}\lvert\rangle$:= ↑↓ ○	$\hat{C}^\dagger_{1\uparrow}\hat{C}^\dagger_{2\downarrow}\lvert\rangle = \phi_3$:= ↑ ↓	$\lvert\rangle$:= ○ ○ Complete annihilation
$\phi_3 = \hat{C}^\dagger_{1\uparrow}\hat{C}^\dagger_{2\downarrow}\lvert\rangle$:= ↑ ↓	$\lvert\rangle$:= ○ ○ Complete annihilation	$\hat{C}^\dagger_{1\uparrow}\hat{C}^\dagger_{1\downarrow}\lvert\rangle = \phi_2$:= ↑↓ ○
$\phi_4 = \hat{C}^\dagger_{2\uparrow}\hat{C}^\dagger_{1\downarrow}\lvert\rangle$:= ↓ ↑	$\hat{C}^\dagger_{2\uparrow}\hat{C}^\dagger_{2\downarrow}\lvert\rangle = \phi_5$:= ○ ↓↑	$\lvert\rangle$:= ○ ○ Complete annihilation
$\phi_5 = \hat{C}^\dagger_{2\uparrow}\hat{C}^\dagger_{2\downarrow}\lvert\rangle$:= ○ ↑↓	$\lvert\rangle$:= ○ ○ Complete annihilation	$\hat{C}^\dagger_{2\uparrow}\hat{C}^\dagger_{1\downarrow}\lvert\rangle = \phi_4$:= ↓ ↑
$\phi_6 = \hat{C}^\dagger_{1\downarrow}\hat{C}^\dagger_{2\downarrow}\lvert\rangle$:= ↓ ↓	$\hat{C}^\dagger_{2\uparrow}\hat{C}^\dagger_{2\downarrow}\lvert\rangle = \lvert\rangle$:= ○ ↓↓ This state is not allowed	$-\hat{C}^\dagger_{1\downarrow}\hat{C}^\dagger_{1\downarrow}\lvert\rangle = \lvert\rangle$:= ↓↓ ○ This state is not allowed

Table: Images $\hat{t}_{ij\sigma}\phi_i$ of the basis elements ϕ_i by $\hat{t}_{12\downarrow}$ and $\hat{t}_{21\downarrow}$.

1D HH: Kinetic operator

In summary,

$$
\begin{aligned}
&\hat{T}\phi_1 = 0 && \hat{T}\phi_2 = -t\phi_4 - t\phi_3, && \hat{T}\phi_3 = -t\phi_5 - t\phi_2,\\
&\hat{T}\phi_4 = -t\phi_2 - t\phi_5, && \hat{T}\phi_5 = -t\phi_3 - t\phi_4, && \hat{T}\phi_6 = 0.
\end{aligned} \tag{2}
$$

1D HH: Kinetic operator

In summary,

$$
\begin{aligned}
&\hat{T}\phi_1 = 0 && \hat{T}\phi_2 = -t\phi_4 - t\phi_3, && \hat{T}\phi_3 = -t\phi_5 - t\phi_2, \\
&\hat{T}\phi_4 = -t\phi_2 - t\phi_5, && \hat{T}\phi_5 = -t\phi_3 - t\phi_4, && \hat{T}\phi_6 = 0.
\end{aligned}
\tag{2}
$$

	$\hat{T}\phi_1$	$\hat{T}\phi_2$	$\hat{T}\phi_3$	$\hat{T}\phi_4$	$\hat{T}\phi_5$	$\hat{T}\phi_6$
ϕ_1	0	0	0	0	0	0
ϕ_2	0	0	$-t$	$-t$	0	0
ϕ_3	0	$-t$	0	0	$-t$	0
ϕ_4	0	$-t$	0	0	$-t$	0
ϕ_5	0	0	$-t$	$-t$	0	0
ϕ_6	0	0	0	0	0	0

$$
\begin{aligned}
\phi_1 &= \hat{C}^{\dagger}_{1\uparrow}\hat{C}^{\dagger}_{2\uparrow}|\rangle \\
\phi_2 &= \hat{C}^{\dagger}_{1\uparrow}\hat{C}^{\dagger}_{1\downarrow}|\rangle \\
\phi_3 &= \hat{C}^{\dagger}_{1\uparrow}\hat{C}^{\dagger}_{2\downarrow}|\rangle \\
\phi_4 &= \hat{C}^{\dagger}_{2\uparrow}\hat{C}^{\dagger}_{1\downarrow}|\rangle \\
\phi_5 &= \hat{C}^{\dagger}_{2\uparrow}\hat{C}^{\dagger}_{2\downarrow}|\rangle \\
\phi_6 &= \hat{C}^{\dagger}_{1\downarrow}\hat{C}^{\dagger}_{2\downarrow}|\rangle
\end{aligned}
$$

Table: Matrix representation of the kinetic operator.

1D HH: Onsite interaction operator

The onsite interaction operator for two sites and two electrons is read

$$\hat{u} = u_0 \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} + u_0 \hat{n}_{2\uparrow} \hat{n}_{2\downarrow}. \tag{3}$$

1D HH: Onsite interaction operator

The onsite interaction operator for two sites and two electrons is read

$$\hat{u} = u_0 \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} + u_0 \hat{n}_{2\uparrow} \hat{n}_{2\downarrow} . \tag{3}$$

	$\hat{u}\phi_1$	$\hat{u}\phi_2$	$\hat{u}\phi_3$	$\hat{u}\phi_4$	$\hat{u}\phi_5$	$\hat{u}\phi_6$
ϕ_1	0	0	0	0	0	0
ϕ_2	0	u_0	0	0	0	0
ϕ_3	0	0	0	0	0	0
ϕ_4	0	0	0	0	0	0
ϕ_5	0	0	0	0	u_0	0
ϕ_6	0	0	0	0	0	0

Table: Matrix representation of the interaction operation.

$$\phi_1 = \hat{C}^\dagger_{1\uparrow} \hat{C}^\dagger_{2\uparrow} |\rangle$$
$$\phi_2 = \hat{C}^\dagger_{1\uparrow} \hat{C}^\dagger_{1\downarrow} |\rangle$$
$$\phi_3 = \hat{C}^\dagger_{1\uparrow} \hat{C}^\dagger_{2\downarrow} |\rangle$$
$$\phi_4 = \hat{C}^\dagger_{2\uparrow} \hat{C}^\dagger_{1\downarrow} |\rangle$$
$$\phi_5 = \hat{C}^\dagger_{2\uparrow} \hat{C}^\dagger_{2\downarrow} |\rangle$$
$$\phi_6 = \hat{C}^\dagger_{1\downarrow} \hat{C}^\dagger_{2\downarrow} |\rangle$$

1D HH: External potential operator

Electrons of the lattice experience the external potential described by

$$\hat{v} = v_1(\hat{n}_{1\uparrow} + \hat{n}_{1\downarrow}) + v_2(\hat{n}_{2\uparrow} + \hat{n}_{2\downarrow}). \quad (4)$$

	$\hat{u}\phi_1$	$\hat{u}\phi_2$	$\hat{u}\phi_3$	$\hat{u}\phi_4$	$\hat{u}\phi_5$	$\hat{u}\phi_6$
ϕ_1	$v_1 + v_2$	0	0	0	0	0
ϕ_2	0	$2v_1$	0	o	0	0
ϕ_3	0	0	$v_1 + v_2$	0	0	0
ϕ_4	0	0	0	$v_1 + v_2$	0	0
ϕ_5	0	0	0	0	$2v_2$	0
ϕ_6	0	0	0	0	0	$v_1 + v_2$

$\phi_1 = \hat{C}^\dagger_{1\uparrow}\hat{C}^\dagger_{2\uparrow}|\rangle$
$\phi_2 = \hat{C}^\dagger_{1\uparrow}\hat{C}^\dagger_{1\downarrow}|\rangle$
$\phi_3 = \hat{C}^\dagger_{1\uparrow}\hat{C}^\dagger_{2\downarrow}|\rangle$
$\phi_4 = \hat{C}^\dagger_{2\uparrow}\hat{C}^\dagger_{1\downarrow}|\rangle$
$\phi_5 = \hat{C}^\dagger_{2\uparrow}\hat{C}^\dagger_{2\downarrow}|\rangle$
$\phi_6 = \hat{C}^\dagger_{1\downarrow}\hat{C}^\dagger_{2\downarrow}|\rangle$

Table: Matrix representation of the external potential operator.

1D HH: Exact diagonalization

The action of the HH on the one dimension two-electron lattice basis elements generates the Hubbard Hamiltonian matrix.

$$H = \begin{pmatrix} v_1 + v_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & u_0 + 2v_1 & -t & -t & 0 & 0 \\ 0 & -t & v_1 + v_2 & 0 & -t & 0 \\ 0 & -t & 0 & v_1 + v_2 & -t & 0 \\ 0 & 0 & -t & -t & u_0 + 2v_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & v_1 + v_2 \end{pmatrix}.$$

1D HH: Exact diagonalization

The action of the HH on the one dimension two-electron lattice basis elements generates the Hubbard Hamiltonian matrix.

$$H = \begin{pmatrix} v_1+v_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & u_0+2v_1 & -t & -t & 0 & 0 \\ 0 & -t & v_1+v_2 & 0 & -t & 0 \\ 0 & -t & 0 & v_1+v_2 & -t & 0 \\ 0 & 0 & -t & -t & u_0+2v_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & v_1+v_2 \end{pmatrix}.$$

Example

For $t=1$,

$u_0=-2$ *and*

$v_{i\sigma}=1$, *the Hamiltonian reads*

$$H = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & -1 & 2 & 0 & -1 & 0 \\ 0 & -1 & 0 & 2 & -1 & 0 \\ 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}$$

1D HH: Exact diagonalization

The action of the HH on the one dimension two-electron lattice basis elements generates the Hubbard Hamiltonian matrix.

$$H = \begin{pmatrix} v_1+v_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & u_0+2v_1 & -t & -t & 0 & 0 \\ 0 & -t & v_1+v_2 & 0 & -t & 0 \\ 0 & -t & 0 & v_1+v_2 & -t & 0 \\ 0 & 0 & -t & -t & u_0+2v_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & v_1+v_2 \end{pmatrix}.$$

Example

For $t=1$,

$u_0=-2$ *and*

$v_{i\sigma}=1$, *the Hamiltonian reads*

$$H = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & -1 & 2 & 0 & -1 & 0 \\ 0 & -1 & 0 & 2 & -1 & 0 \\ 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}$$

The Shrödinger equation or eigenvalue problem: $\hat{H}\psi_i = E_i\psi_i$.
This can be solved by performing an Exact Diagonalization (ED):
$\psi_0 = 0.602\phi_2 + 0.372\phi_3 + 0.372\phi_4 + 0.602\phi_5$ is the ground state wave function.

1D HH: Exact diagonalization

Except for small number of site or lattice sizes, the eigenvalue problems is really difficult to be solved by ED.

Therefore numerical approximations draw upon methods like the Lanczos algorithm or the Bethe ansatz [1] are used instead.

[1] E. H. Lieb, and F. Y. Wu, *Phys. Rev. Lett.*, **20**, 1445–1448 (1968).

Lattice - DFT

- Density Functional Theory (DFT), a theoretical reformulation of Quantum Mechanics which makes the density the controlling variable, is often used in condensed matter physics, material science and chemistry to study ground state properties of many body system (finite 1D lattice sytem or shortly lattice).
- It is almost impossible to solve straightforward the Schrödinger equation and find the ground state wave function.
- Functionals of the density are (or DFT is) used instead.

Lattice-DFT: What is done.

Interacting system: $\hat{H} = \hat{T} + \hat{u} + \hat{v}$

$\updownarrow$

Ψ, ρ^0, E_0

Lattice-DFT: What is done.

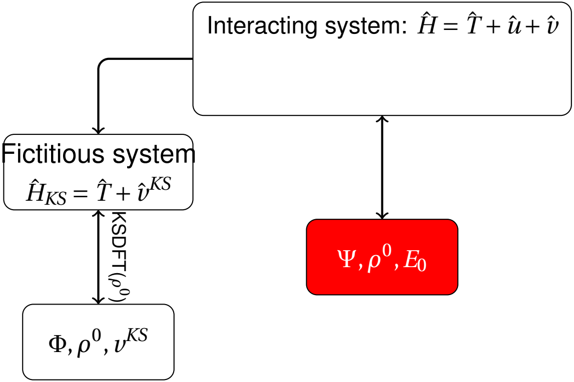
Interacting system: $\hat{H} = \hat{T} + \hat{u} + \hat{v}$

Fictitious system

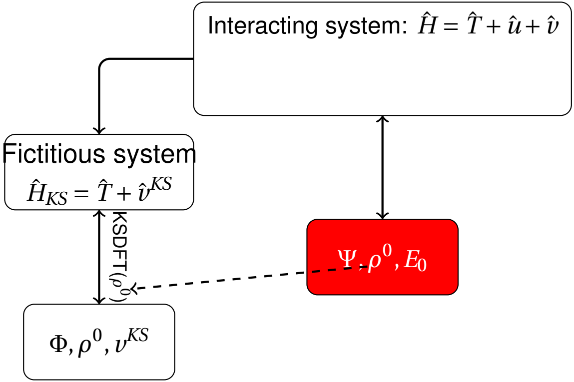
$\hat{H}_{KS} = \hat{T} + \hat{v}^{KS}$

Ψ, ρ^0, E_0

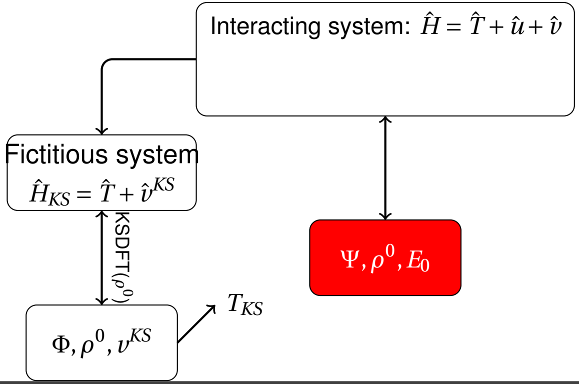
Lattice-DFT: What is done.



Lattice-DFT: What is done.



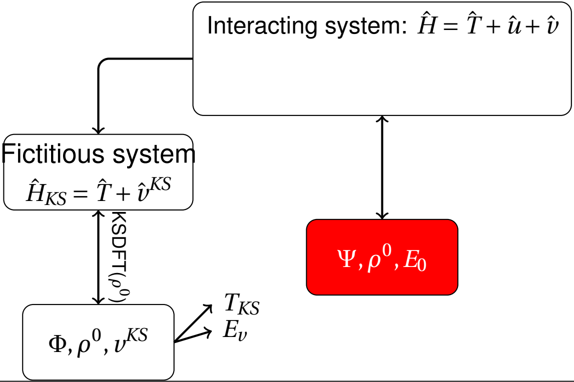
Lattice-DFT: What is done.



Energies from KSDFT

$$T_{KS} = \langle \Phi \mid \hat{T} \mid \Phi \rangle$$

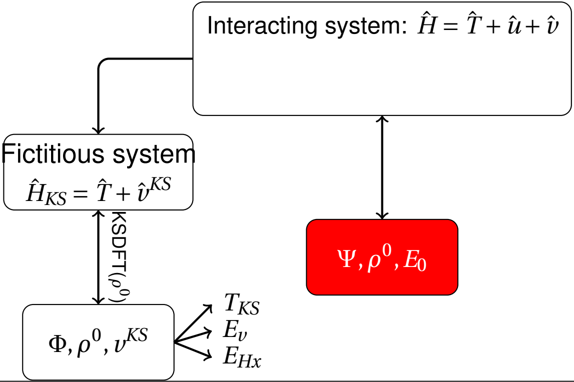
Lattice-DFT: What is done.



Energies from KSDFT

$$E_v = \langle \Phi \mid \hat{v} \mid \Phi \rangle$$

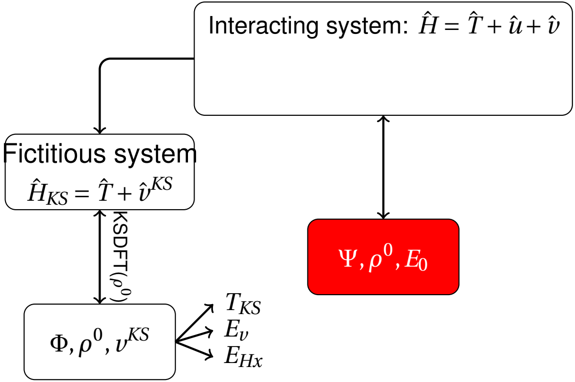
Lattice-DFT: What is done.



Energies from KSDFT

$$E_{Hx} = \langle \Phi \mid \hat{u} \mid \Phi \rangle$$

Lattice-DFT: What is done.



Energies from KSDFT

$$E_c \stackrel{?}{=} E_0 - (T_{KS} + E_{Hx} + E_v)$$

What we are doing: Hartree plus Exchange approximation.

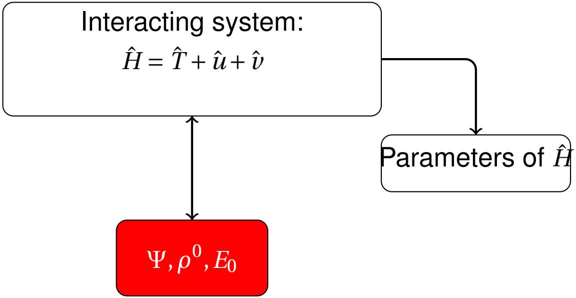
Interacting system:

$$\hat{H} = \hat{T} + \hat{u} + \hat{v}$$

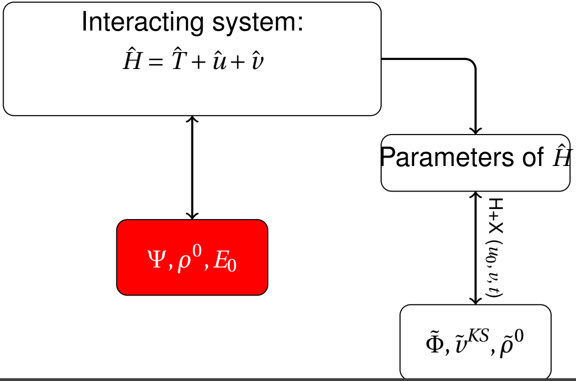
$$\updownarrow$$

$$\Psi, \rho^0, E_0$$

What we are doing: Hartree plus Exchange approximation.



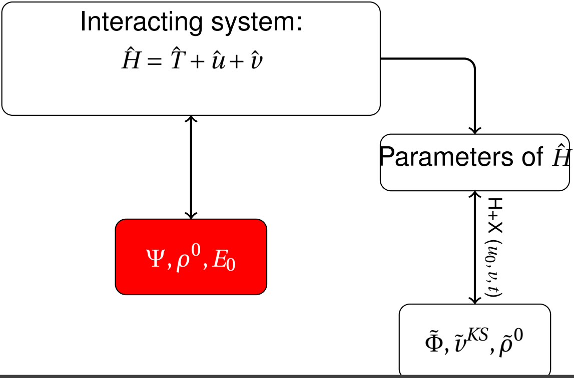
What we are doing: Hartree plus Exchange approximation.



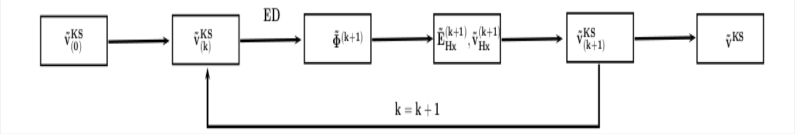
Approximate KS potential

$$v^{KS} = v_c + (v_H + v_x) + v \text{ and } \tilde{v}^{KS} = v_{Hx} + v$$

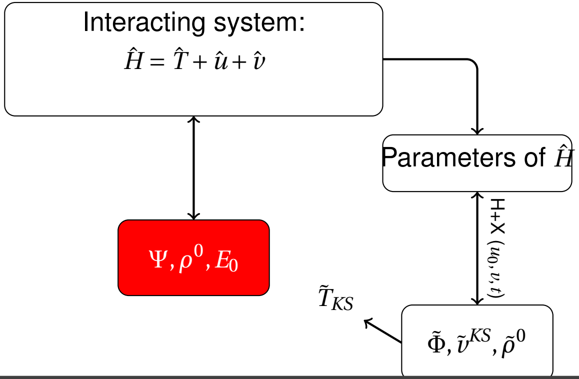
What we are doing: Hartree plus Exchange approximation.



Approximate KS potential



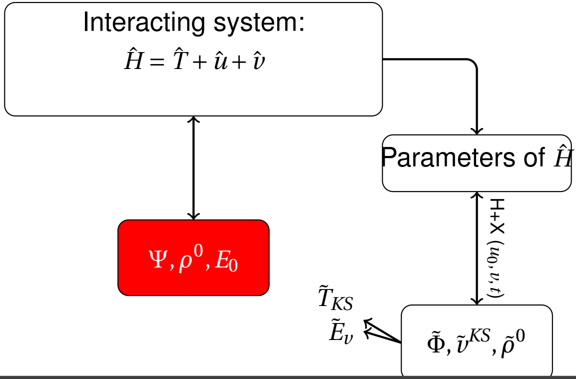
What we are doing: Hartree plus Exchange approximation.



Energies from H+X approximation

$$\tilde{T}_{KS} = \langle \tilde{\Phi} \mid \hat{T} \mid \tilde{\Phi} \rangle$$

What we are doing: Hartree plus Exchange approximation.



Energies from H+X approximation

$$\tilde{E}_v = \langle \tilde{\Phi} \mid \hat{v} \mid \tilde{\Phi} \rangle$$

What we are doing: Hartree plus Exchange approximation.

Interacting system:

$$\hat{H} = \hat{T} + \hat{u} + \hat{v}$$

Parameters of $\hat{H}$

$$\Psi, \rho^0, E_0$$

H+X (u_0, v, t)

$\tilde{T}_{KS}$

$\tilde{E}_v$

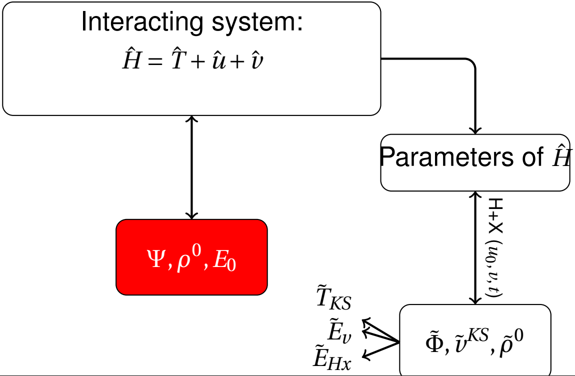
$\tilde{E}_{Hx}$

$$\tilde{\Phi}, \tilde{v}^{KS}, \tilde{\rho}^0$$

Energies from H+X approximation

$$\tilde{E}_{Hx} = \langle \tilde{\Phi} \mid \hat{u} \mid \tilde{\Phi} \rangle$$

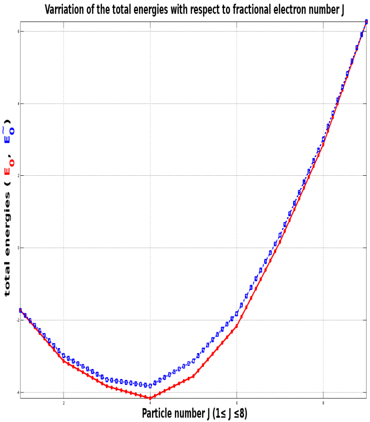
What we are doing: Hartree plus Exchange approximation.

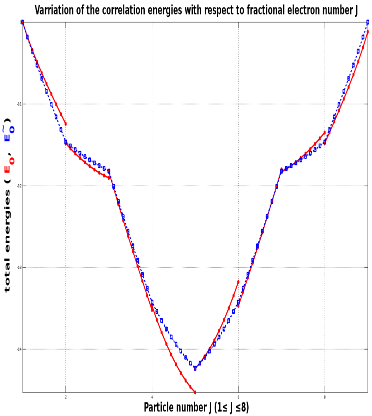


Energies from H+X approximation

$$\tilde{E}_c \overset{?}{=} \tilde{E}_0 - (\tilde{T}_{KS} + \tilde{E}_{Hx} + \tilde{E}_v)$$

Results: Correlation energy from H+X approximation

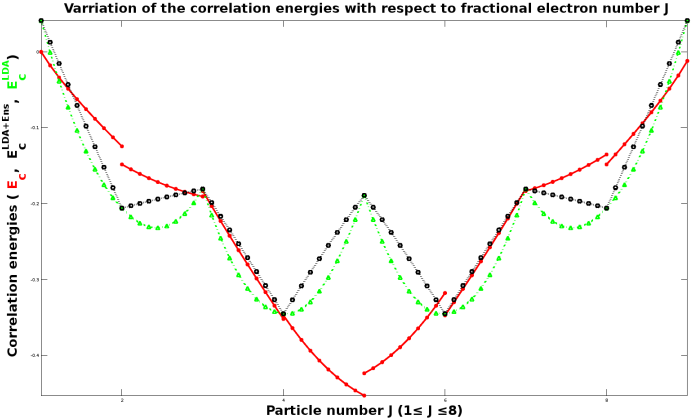




where

$$\tilde{E}_0 = \tilde{T}_{KS} + \tilde{E}_{Hx} + \tilde{E}_v \text{ and } \tilde{E}_c = E_0 - \tilde{E}_0$$

Results: Correlation energy from LDA

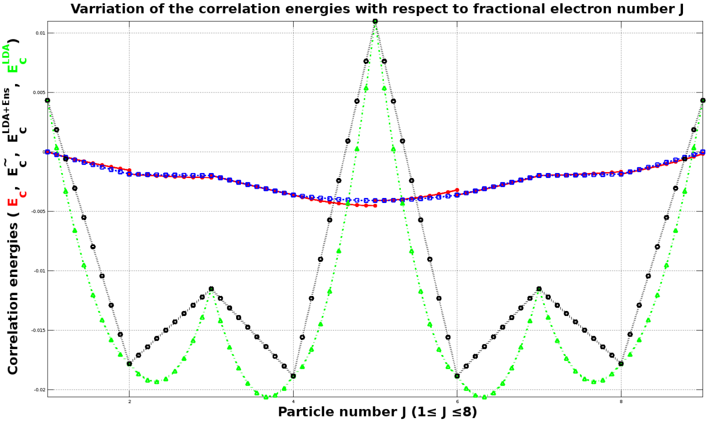


$$LDA \Longrightarrow E_{Hxc}^{LDA} \Longrightarrow E_c^{LDA}[\rho(J)] = E_{Hxc}^{LDA}[\rho(J)] - E_{Hx}^{LDA}[\rho(J)]$$

or

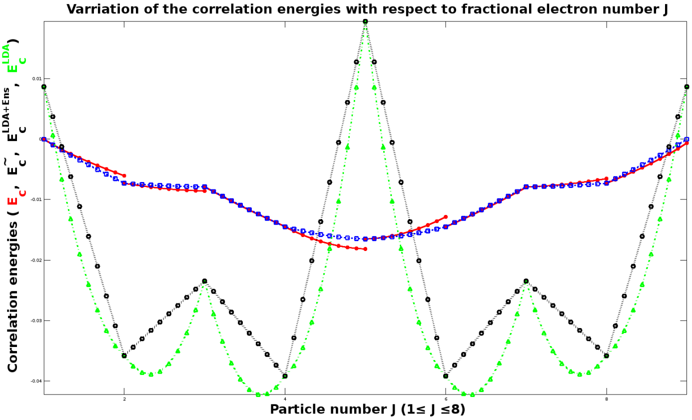
$$E_c^{LDA+Ens}[\rho(J)] = (1-\alpha)E_c^{LDA+Ens}[\rho[N_e, v^{KS}(J)]] + \alpha E_c^{LDA+Ens}[\rho[N_e+1, v^{KS}(J)]]$$

Results: All the correlation energies together



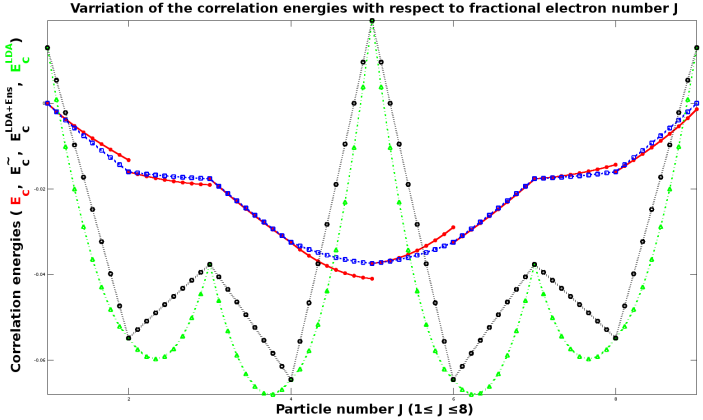
$v_i = 0, 1 \leq i \leq 10$ $\qquad u_0 = 0.2$ $\qquad t = 1$

Results: All the correlation energies together



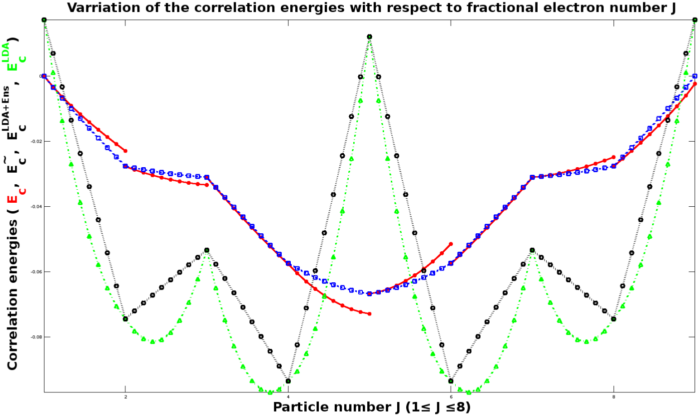
$v_i = 0, 1 \leq i \leq 10$ $\quad u_0 = 0.4$ $\quad t = 1$

Results: All the correlation energies together



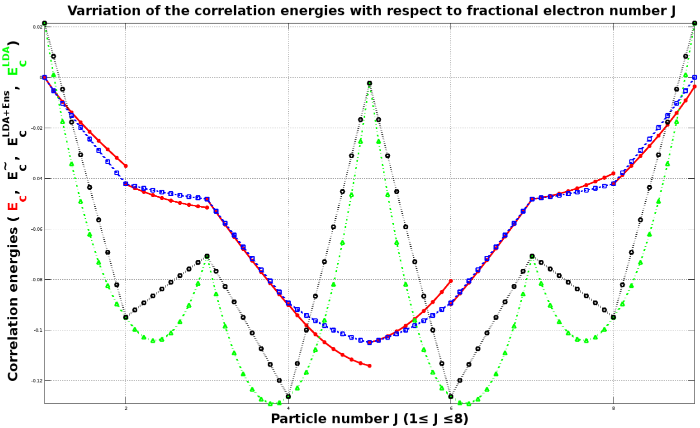
$v_i = 0, 1 \leq i \leq 10$ $\qquad u_0 = 0.6$ $\qquad t = 1$

Results: All the correlation energies together



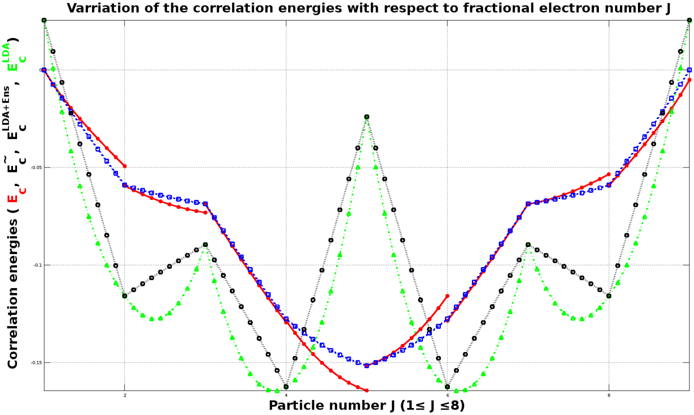
$v_i = 0, 1 \leq i \leq 10$ $\quad u_0 = 0.8$ $\quad t = 1$

Results: All the correlation energies together



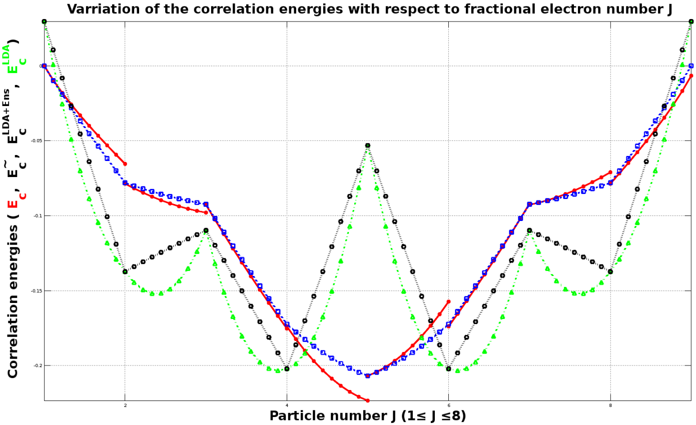
$v_i = 0, 1 \leq i \leq 10$ $\quad u_0 = 1.0$ $\quad t = 1$

Results: All the correlation energies together



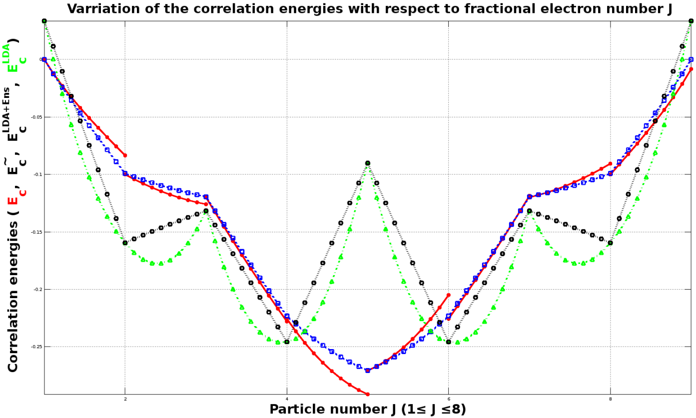
$v_i = 0, 1 \leq i \leq 10$ $\quad u_0 = 1.2$ $\quad t = 1$

Results: All the correlation energies together



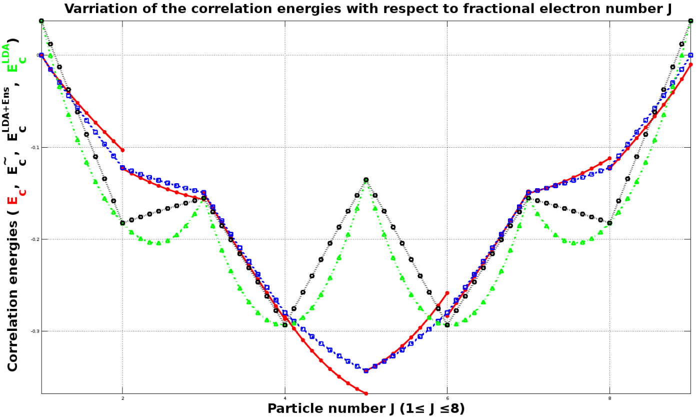
$v_i = 0, 1 \leq i \leq 10$ $\quad u_0 = 1.4$ $\quad t = 1$

Results: All the correlation energies together



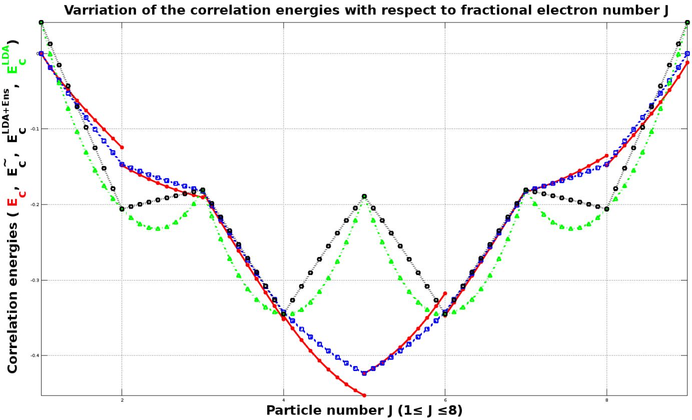
$v_i = 0, 1 \leq i \leq 10$ $\quad u_0 = 1.6$ $\quad t = 1$

Results: All the correlation energies together



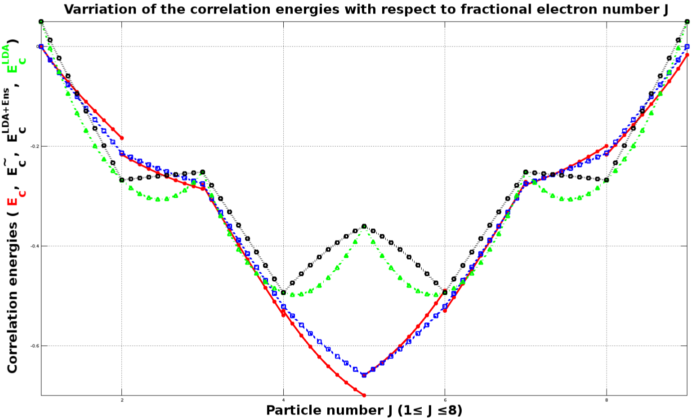
$v_i = 0, 1 \leq i \leq 10$ $\quad u_0 = 1.8$ $\quad t = 1$

Results: All the correlation energies together



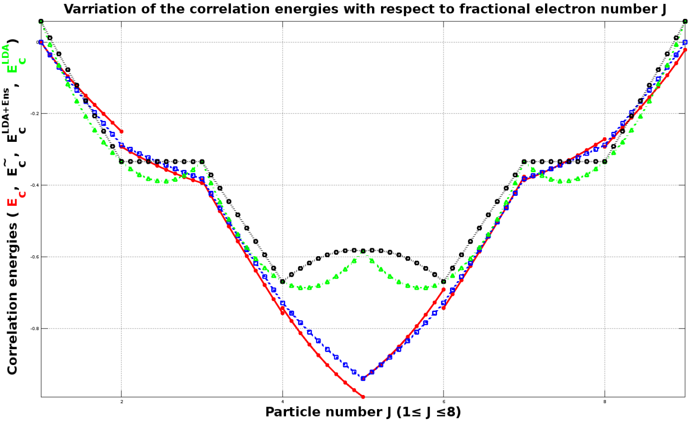
$v_i = 0, 1 \leq i \leq 10$ $\quad u_0 = 2.0$ $\quad t = 1$

Results: All the correlation energies together



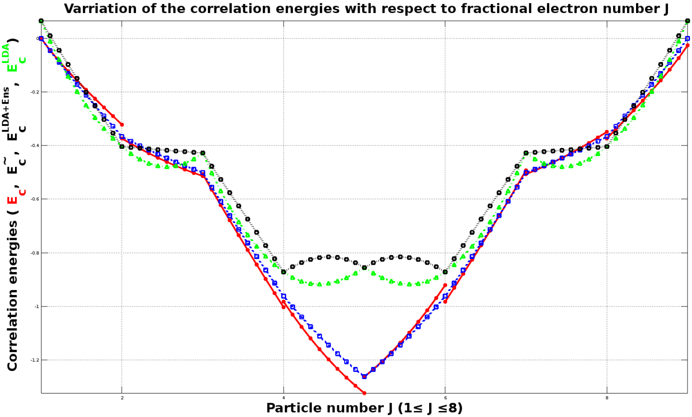
$v_i = 0, 1 \leq i \leq 10$ $\qquad u_0 = 2.5$ $\qquad t = 1$

Results: All the correlation energies together



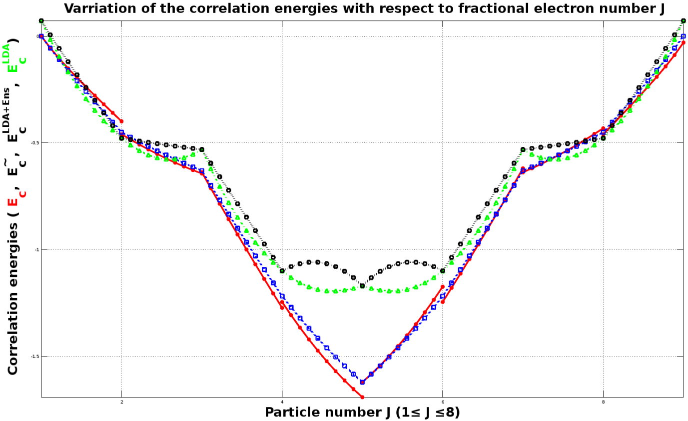
$v_i = 0, 1 \leq i \leq 10$ $\quad$ $u_0 = 3$ $\quad$ $t = 1$

Results: All the correlation energies together



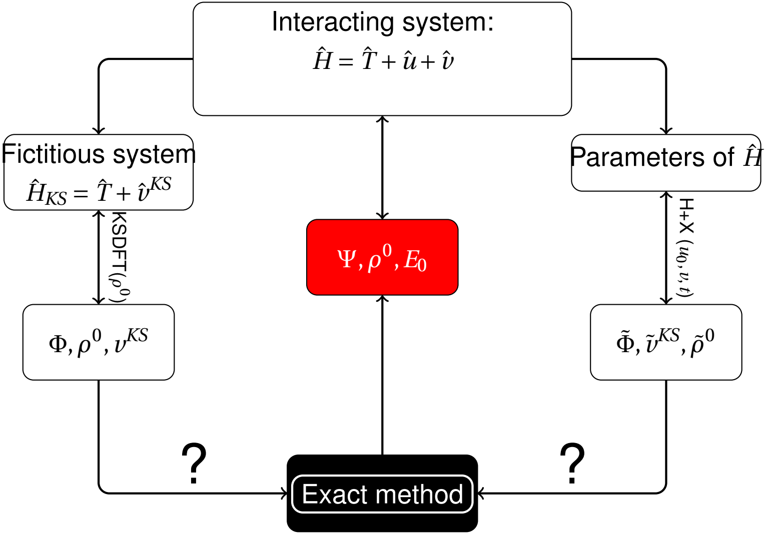
$v_i = 0, 1 \leq i \leq 10$ $u_0 = 3.5$ $t = 1$

Results: All the correlation energies together



$v_i = 0, 1 \leq i \leq 10$ $\quad u_0 = 4$ $\quad t = 1$

What we did: Main problem.



What we are doing: Exact method-Jastrow factor operator

- Our exact method is based on Jastrow factor $\hat{J}$ defined by

$$\hat{J} = e^{-\sum_{m=1}^{\#} \gamma_m \hat{P}_m}$$

so that

$$\Phi = \sum_{m=1}^{\#} \boxed{b_m} \phi_m \Longrightarrow \hat{J}\,\Phi = \sum_{m=1}^{\#} \boxed{b_m e^{-\gamma_m}} \phi_m$$

What we are doing: Exact method-Jastrow factor operator

- Our exact method is based on Jastrow factor $\hat{J}$ defined by

$$\hat{J} = e^{-\sum_{m=1}^{\#} \gamma_m \hat{P}_m}$$

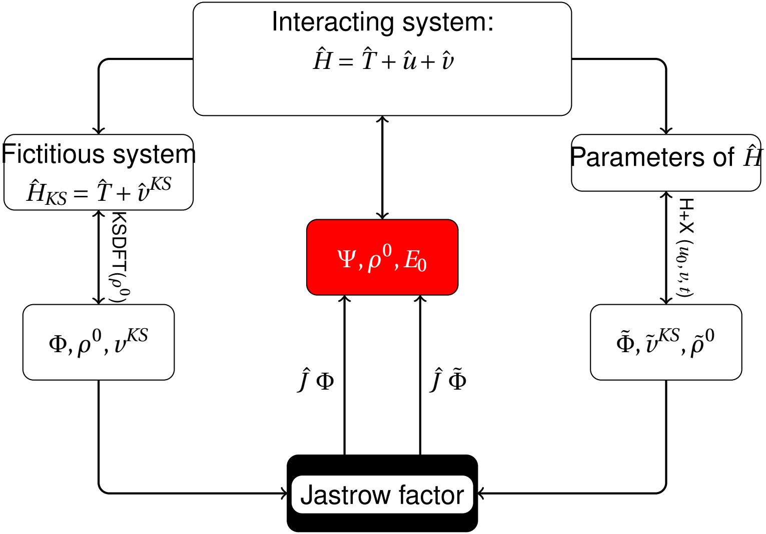
so that

$$\Phi = \sum_{m=1}^{\#} \boxed{b_m} \phi_m \Longrightarrow \hat{J}\,\Phi = \sum_{m=1}^{\#} \boxed{b_m e^{-\gamma_m}} \phi_m$$

- and

$$\hat{J}\,\Phi = \Psi$$

Completed diagram



Conclusion

- It is clear to us that the use of Jastrow factor, after performing a KSDFT, is a good way to investigate on possible way to map KSDFT results (Φ, E^{KS}) onto the noninteracting ones (Ψ, E_0).
- The H+X approximation appears to highly compete with the LDA approximation
- We seek for applying our methods to more complex Hubbard Hamiltonians from lattices to realistic systems.

Outline

What is a Math Camp

Math camps are two weeks camp consisted of an initial planning week for instructors or volunteers and a second week of activities for the students.

1. Initiated in 2011 by a group of educators (African Maths Initiative or AMI) based at the Maseno University in Kenya

What is a Math Camp

Math camps are two weeks camp consisted of an initial planning week for instructors or volunteers and a second week of activities for the students.

1. Initiated in 2011 by a group of educators (African Maths Initiative or AMI) based at the Maseno University in Kenya
2. Goal: Revolutionize how mathematics is taught in school and perceived by the students

What is a Math Camp

Math camps are two weeks camp consisted of an initial planning week for instructors or volunteers and a second week of activities for the students.

1. Initiated in 2011 by a group of educators (African Maths Initiative or AMI) based at the Maseno University in Kenya
2. Goal: Revolutionize how mathematics is taught in school and perceived by the students
3. Objectives: Come together in

What is a Math Camp

Math camps are two weeks camp consisted of an initial planning week for instructors or volunteers and a second week of activities for the students.

1. Initiated in 2011 by a group of educators (African Maths Initiative or AMI) based at the Maseno University in Kenya
2. Goal: Revolutionize how mathematics is taught in school and perceived by the students
3. Objectives: Come together in
    - shared learning and enjoyment, exploring rich ideas that go beyond what is traditionally taught in schools;

What is a Math Camp

Math camps are two weeks camp consisted of an initial planning week for instructors or volunteers and a second week of activities for the students.

1. Initiated in 2011 by a group of educators (African Maths Initiative or AMI) based at the Maseno University in Kenya
2. Goal: Revolutionize how mathematics is taught in school and perceived by the students
3. Objectives: Come together in
   - shared learning and enjoyment, exploring rich ideas that go beyond what is traditionally taught in schools;
   - solving puzzles and playing games;

What is a Math Camp

Math camps are two weeks camp consisted of an initial planning week for instructors or volunteers and a second week of activities for the students.

1. Initiated in 2011 by a group of educators (African Maths Initiative or AMI) based at the Maseno University in Kenya
2. Goal: Revolutionize how mathematics is taught in school and perceived by the students
3. Objectives: Come together in
   - shared learning and enjoyment, exploring rich ideas that go beyond what is traditionally taught in schools;
   - solving puzzles and playing games;
   - running workshops that allow students to discover the applications of maths in the real world;

What is a Math Camp

Math camps are two weeks camp consisted of an initial planning week for instructors or volunteers and a second week of activities for the students.

1. Initiated in 2011 by a group of educators (African Maths Initiative or AMI) based at the Maseno University in Kenya
2. Goal: Revolutionize how mathematics is taught in school and perceived by the students
3. Objectives: Come together in
    - shared learning and enjoyment, exploring rich ideas that go beyond what is traditionally taught in schools;
    - solving puzzles and playing games;
    - running workshops that allow students to discover the applications of maths in the real world;
    - doing extra-curriculum activities.

1. Supporting African Maths Initiatives (SAMI):

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
   - SAMI is committed to providing ongoing support to maths camp across Africa and UK.

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
    - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
    - SAMI helps to recruit and coordinate international volunteers.

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
    - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
    - SAMI helps to recruit and coordinate international volunteers.
    - SAMI develops exciting new themes and raise funds for student bursaries and core running costs.

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
   - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
   - SAMI helps to recruit and coordinate international volunteers.
   - SAMI develops exciting new themes and raise funds for student bursaries and core running costs.
2. Maths camp in Africa [2]

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
   - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
   - SAMI helps to recruit and coordinate international volunteers.
   - SAMI develops exciting new themes and raise funds for student bursaries and core running costs.
2. Maths camp in Africa [2]
   - Kenya

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
   - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
   - SAMI helps to recruit and coordinate international volunteers.
   - SAMI develops exciting new themes and raise funds for student bursaries and core running costs.
2. Maths camp in Africa [2]
   - Kenya
   - Ethiopia

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
   - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
   - SAMI helps to recruit and coordinate international volunteers.
   - SAMI develops exciting new themes and raise funds for student bursaries and core running costs.
2. Maths camp in Africa [2]
   - Kenya
   - Ethiopia
   - Ghana

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
    - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
    - SAMI helps to recruit and coordinate international volunteers.
    - SAMI develops exciting new themes and raise funds for student bursaries and core running costs.
2. Maths camp in Africa [2]
    - Kenya
    - Ethiopia
    - Ghana
    - Cameroon

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
   - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
   - SAMI helps to recruit and coordinate international volunteers.
   - SAMI develops exciting new themes and raise funds for student bursaries and core running costs.
2. Maths camp in Africa [2]
   - Kenya
   - Ethiopia
   - Ghana
   - Cameroon
   - Tanzania

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
    - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
    - SAMI helps to recruit and coordinate international volunteers.
    - SAMI develops exciting new themes and raise funds for student bursaries and core running costs.
2. Maths camp in Africa [2]
    - Kenya
    - Ethiopia
    - Ghana
    - Cameroon
    - Tanzania
    - Togo

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
   - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
   - SAMI helps to recruit and coordinate international volunteers.
   - SAMI develops exciting new themes and raise funds for student bursaries and core running costs.
2. Maths camp in Africa [2]
   - Kenya
   - Ethiopia
   - Ghana
   - Cameroon
   - Tanzania
   - Togo
   - Rwanda

[2] www.samicharity.co.uk/projects/maths-camps/

1. Supporting African Maths Initiatives (SAMI):
    - SAMI is committed to providing ongoing support to maths camp across Africa and UK.
    - SAMI helps to recruit and coordinate international volunteers.
    - SAMI develops exciting new themes and raise funds for student bursaries and core running costs.
2. Maths camp in Africa [2]
    - Kenya
    - Ethiopia
    - Ghana
    - Cameroon
    - Tanzania
    - Togo
    - Rwanda
    - UK.

[2] www.samicharity.co.uk/projects/maths-camps/

Togo Maths Camp 2019: Gallery











Togo Maths Camp 2019: Gallery

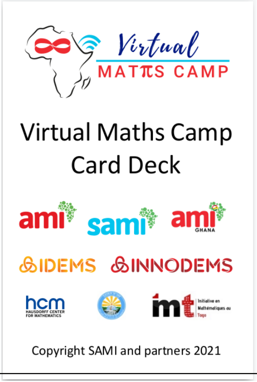
What Happened after COVID19 Outbreak

1. Virtual Math Camps [3]: SAMI and its partners joined efforts across Africa and internationally to create
    - a collection of resources across different countries
    - platforms and delivery mechanism with the potential to have long lasting impacts

[3] www.virtualmathscamp.com

What Happened after COVID19 Outbreak

1. Virtual Math Camps [3]: SAMI and its partners joined efforts across Africa and internationally to create
    - a collection of resources across different countries
    - platforms and delivery mechanism with the potential to have long lasting impacts



[3] www.virtualmathscamp.com

Togo Virtual Maths Camp 2020