

1D Hubbard Model

BA-LDA

Student: Felipe D. Picoli*

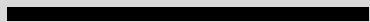
Supervisor: Luiz Nunes de Oliveira

Contents

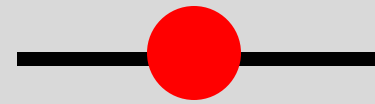
- **Hubbard Model**
- **Bethe Ansatz Solution**
- **DFT – Scheme and Results**
- **TD-DFT – Scheme and Results**

Hubbard Model

Creation and Annihilation Operators



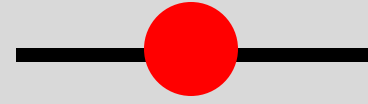
$$|0\rangle$$



$$|1\rangle = c^\dagger |0\rangle$$



$$|0\rangle = c |1\rangle$$



$$0 = c^\dagger c^\dagger |0\rangle$$



$$0 = c |0\rangle$$



$$c^\dagger c |1\rangle = (1) \times |1\rangle$$

$$n \equiv c^\dagger c$$

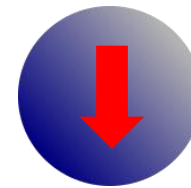
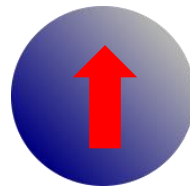
Let's consider ONLY ONE atom **only one orbital** for simplicity:



EMPTY

$$E = 0$$

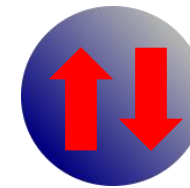
$$|sitio\rangle = |0\rangle$$



SINGLE OCCUPANCE

$$E = v_0$$

$$|sitio\rangle = c_{0,\sigma}^\dagger |0\rangle$$



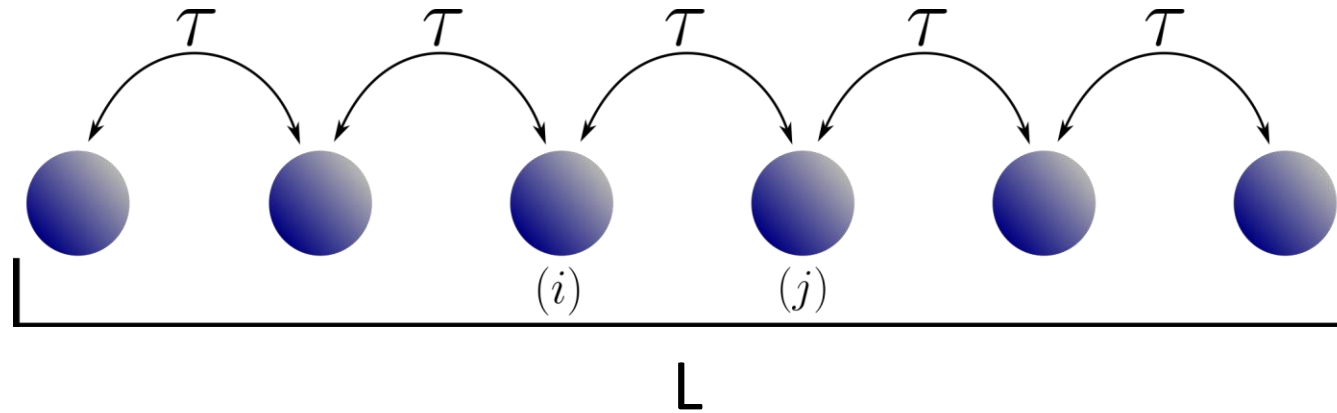
DUBLE OCCUPANCE

$$E = 2v_0 + \mathcal{U}$$

$$|sitio\rangle = c_{0,\uparrow}^\dagger c_{0,\downarrow}^\dagger |0\rangle$$

Hubbard Model

Now, we can set up a 1D chain with L those atoms. We may also allow the electrons to hop between them with a probability τ .



The system's Hamiltonian is

$$\mathcal{H} = \boxed{-\tau \sum_{i,\sigma} \left(c_{i,\sigma}^\dagger c_{i+1,\sigma} + h.c. \right)} + \boxed{\sum_{i,\sigma} v_{i,\sigma} n_{i,\sigma}} + \boxed{\mathcal{U} \sum_i n_{i,\uparrow} n_{i,\downarrow}}$$

Kinetic Energy **Atomic Orbital Energy** **Coulomb Repulsion**

Bethe Ansatz Solution*

The Bethe ansatz solution starts assuming a general form for the system's eigenstate

$$|\Psi\rangle = \sum_{1 < x_1 < \dots < x_n < N} \sum_{p \in S_N} A_p e^{i \sum_{j=1}^n k_{p_j} x_j} |x_1, \dots, x_n\rangle$$

From this, we can obtain the ground-state energy in the half-filling case

$$E_0 = -4L \int_0^\infty \frac{J_0(x) J_1(x)}{x(1 + e^{xU/2})} dx$$

While the energy per site is a function of the occupation number (density),

$$e^{BA}(n, U) = -\frac{2\beta(U)}{\pi} \sin\left(\frac{n\pi}{\beta(U)}\right) \quad n \leq 1$$

$$e^{BA}(n, U) = -\frac{2\beta(U)}{\pi} \sin\left(\frac{(2-n)\pi}{\beta(U)}\right) + U(n-1) \quad 1 < n \leq 2$$

Such that $\beta(U)$ can be obtained from, considering $n=1$,

$$-\frac{2\beta(U)}{\pi} \sin\left(\frac{\pi}{\beta(U)}\right) = -4 \int_0^\infty \frac{J_0(x) J_1(x)}{x(1 + e^{xU/2})} dx$$

*E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

DFT – Scheme*

The Kohn-Sham Hamiltonian is

$$\mathcal{H}_{KS} = -\tau \sum_j (c_{j,\sigma}^\dagger c_{j+1,\sigma} + h.c.) + \sum_{j,\sigma} v_{j,\sigma}^{KS} n_{j,\sigma} - \mu \sum_{j,\sigma} n_{j,\sigma}$$

Such the external potentials are

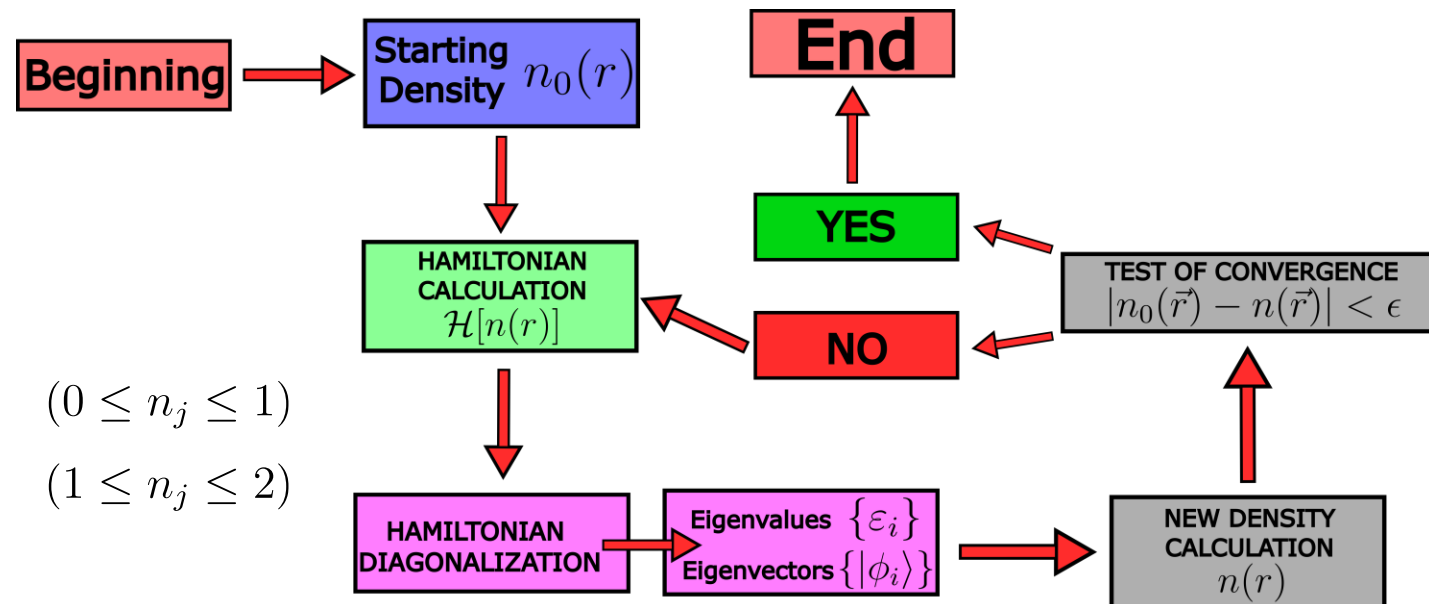
$$v_{j,\sigma}^{KS} = v_{j,\sigma} + v_j^H[n_j] + v_j^{xc}[n_j]$$

$$v_j^H[n_j] = \frac{U}{2} n_j$$

$$v_j^{xc}[n_j] = 2 \sin \frac{\pi n_j}{2} - \frac{U}{2} n_j - 2 \begin{cases} \cos \left(\frac{\pi n_j}{\beta(U)} \right), & (0 \leq n_j \leq 1) \\ -\cos \left(\frac{\pi(2-n_j)}{\beta(U)} \right) + U, & (1 \leq n_j \leq 2) \end{cases}$$

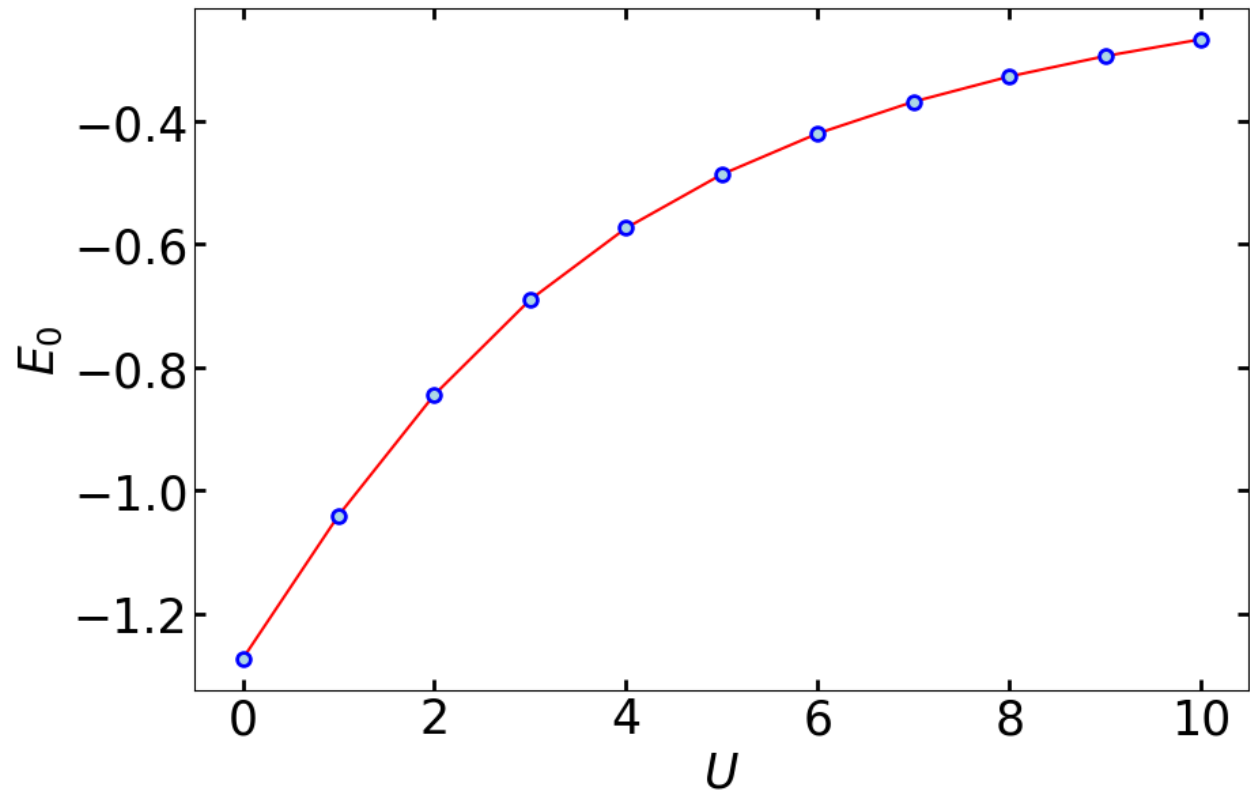
The total energy is

$$E[n] = -\frac{2\beta(U)}{\pi} \sum_j \begin{cases} \sin \left(\frac{\pi n_j}{\beta(U)} \right), & (0 \leq n_j \leq 1) \\ -\sin \left(\frac{\pi(2-n_j)}{\beta(U)} \right) + U(n_j - 1), & (1 \leq n_j \leq 2) \end{cases}$$

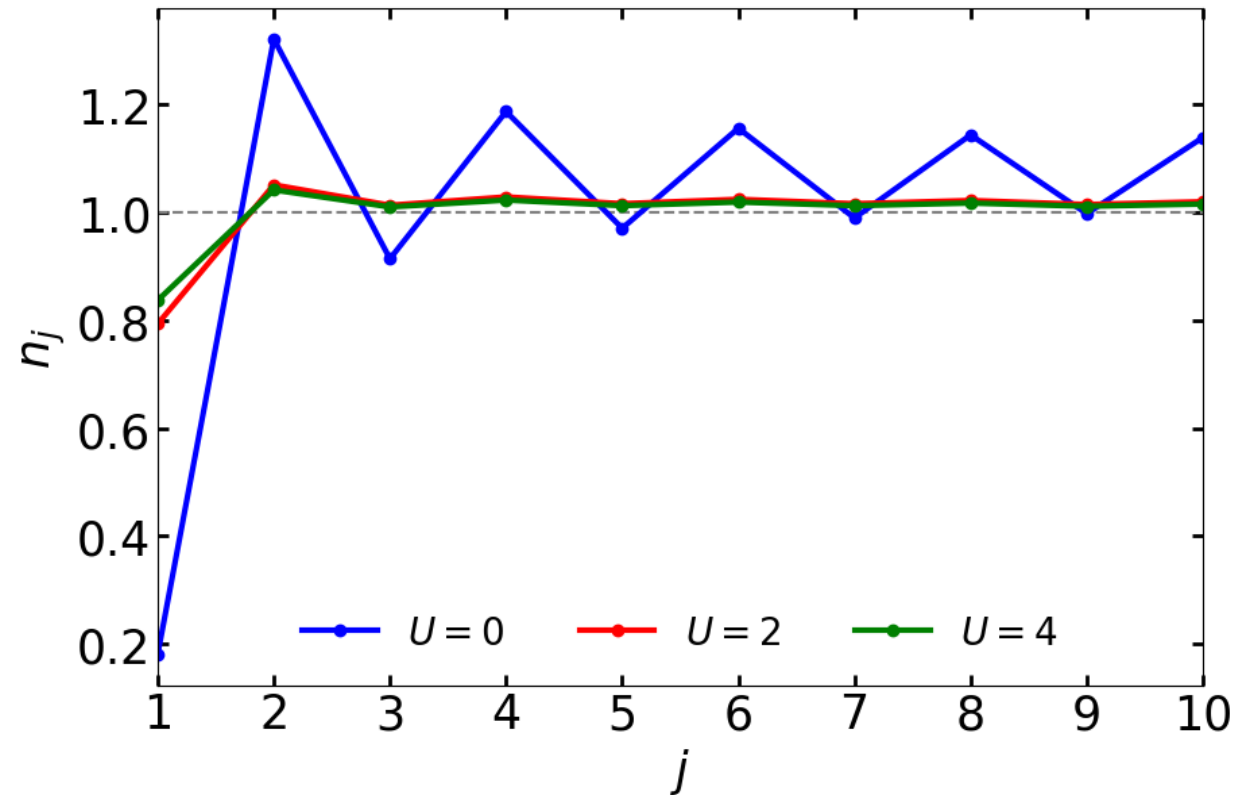


*N. A. Lima, M. F. Silva, L. N. Oliveira, and K. Capelle, Phys. Rev. Lett. **90**, 146402 (2003).

DFT – Results



Ground state energy as a function of the Hubbard interaction in the homogenous case.



Occupation number for a chain of 10 sites considering different many-body interaction values. A positive potential is applied at the first site.

TD-DFT – Scheme*

We have to solve the Schrödinger equation

$$-i\frac{\partial|\Psi(t)\rangle}{\partial t} = \mathcal{H}|\Psi(t)\rangle$$

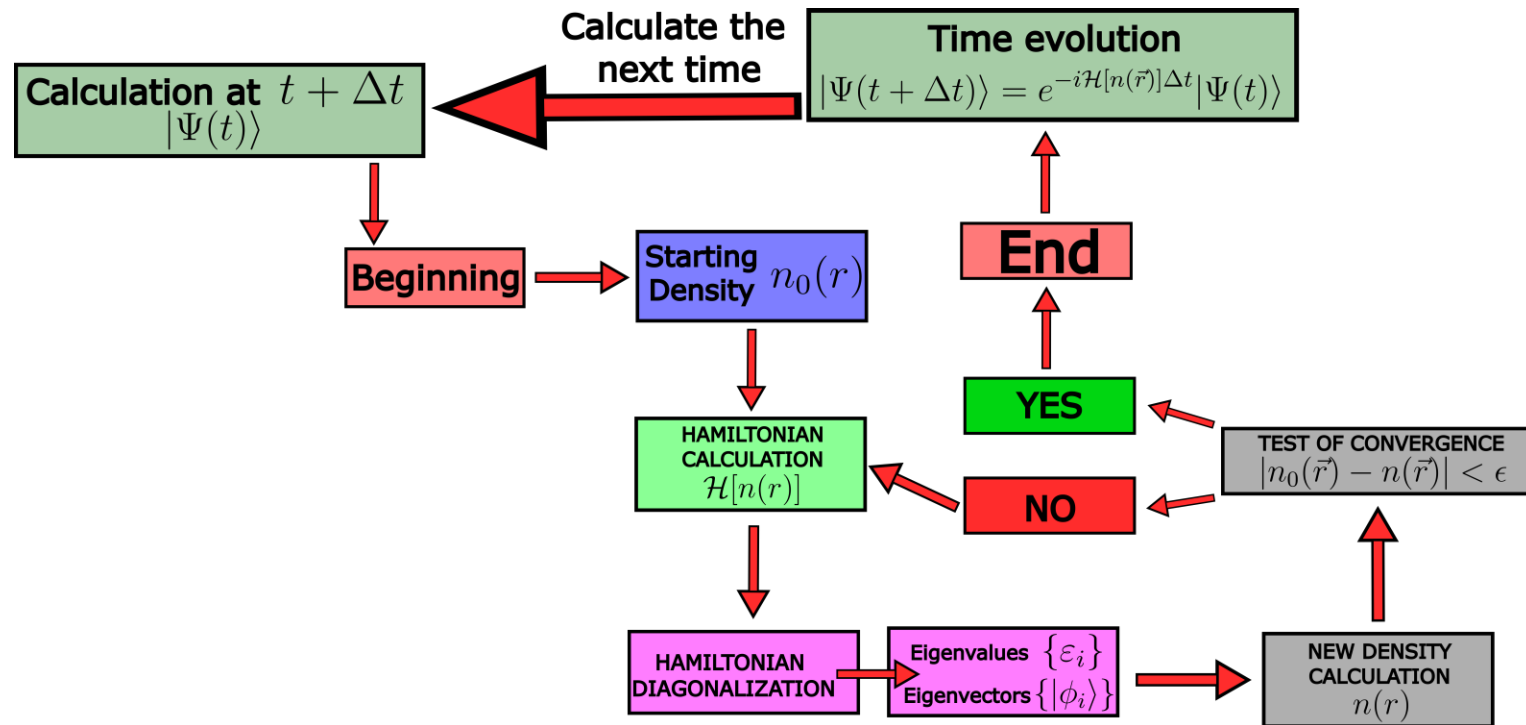
Whose Hamiltonian is calculated by the KS scheme.

Our initial state is the initial ground state.

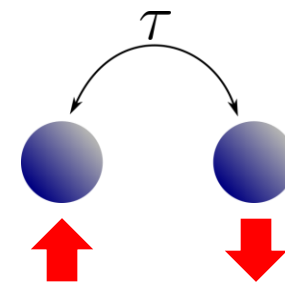
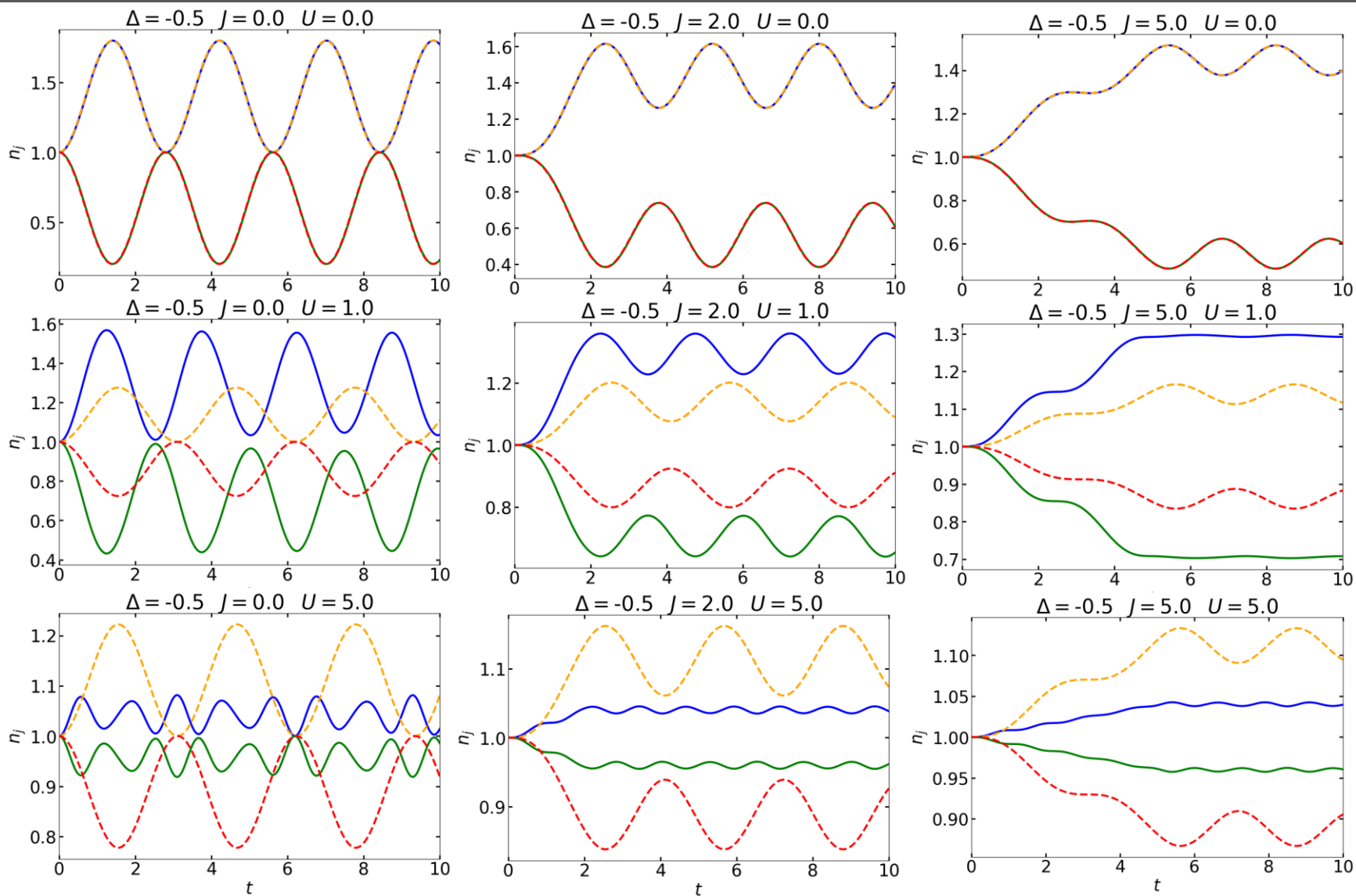
We have changed the external potential following the ramp up protocol,

$$v(t) = \frac{\Delta t}{J}$$

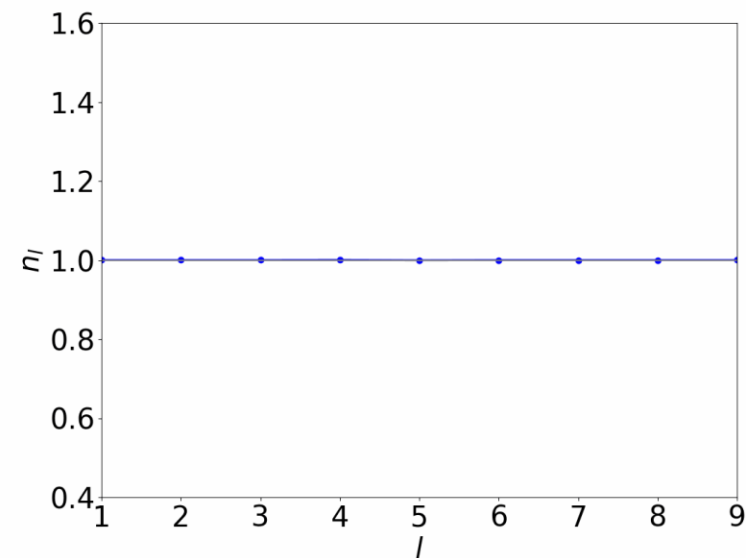
Where we apply positive (negative) potential in odd (even) sites.



TD-DFT – Results: Hubbard dimer



Dashed line: Exact Diagonalization
Continuum line: TD-DFT Calculation



References:

- Ullrich, Carsten A. "Time-dependent density-functional theory: concepts and applications." (2011);
- N. A. Lima, M. F. Silva, L. N. Oliveira, and K. Capelle, Phys. Rev. Lett. **90**, 146402(2003);
- Elliott H. Lieb and F. Y. Wu, Phys. Rev. Lett. **21**, 192 (1968);
- Nardi, Lucas Marcelo Cavalari. *O modelo de Hubbard unidimensional via DFT: o potencial de troca e correlação e o funcional híbrido*. Diss. Universidade de São Paulo, 2016;
- Herrera, M., Serra, R.M. & D'Amico, I. *Sci Rep* **7**, 4655 (2017).

THANKS!!

Code:

<https://github.com/FelipePicoli/Hubbard-Model---DFT-and-TD-DFT>