1D Hubbard Model

BA-LDA

(Bethe Ansatz Local Density Approximation)

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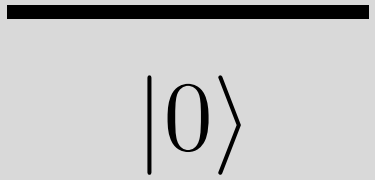
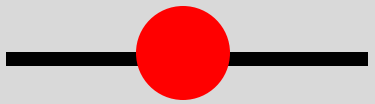
Hubbard Model

Criation and Aniquilation Operators

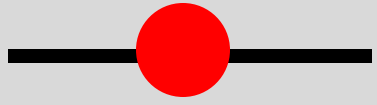


$$|0\rangle$$



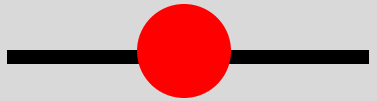
$$|1\rangle = c^\dagger|0\rangle$$

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



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

$$0 = c|0\rangle$$



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

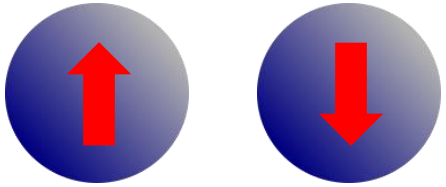
$$n \equiv c^\dagger c$$

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

EMPTY

$$E = 0$$

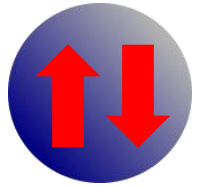
$$|sitio\rangle = |0\rangle$$



SIMGLE OCCUPANCE

$$E = v_0$$

$$|sitio\rangle = c^\dagger_{0,\sigma}|0\rangle$$



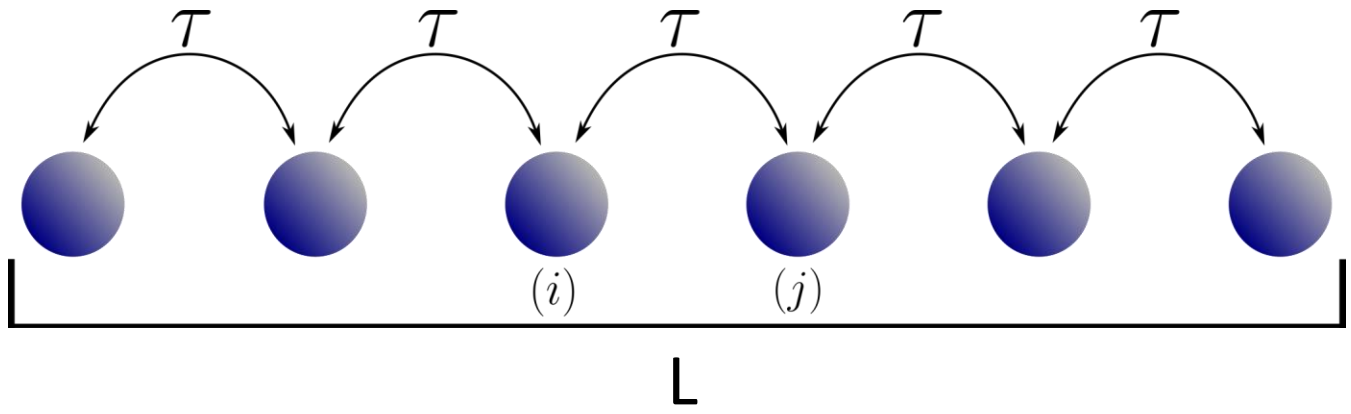
DUBLE OCCUPANCE

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

$$|sitio\rangle = c^\dagger_{0,\uparrow}c^\dagger_{0,\downarrow}|0\rangle$$

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

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

Kinetic Energy

Atomic Orbital Energy

Coulomb Repulsion

Bethe Ansatz Solution*

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

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

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),

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

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

Such that β(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

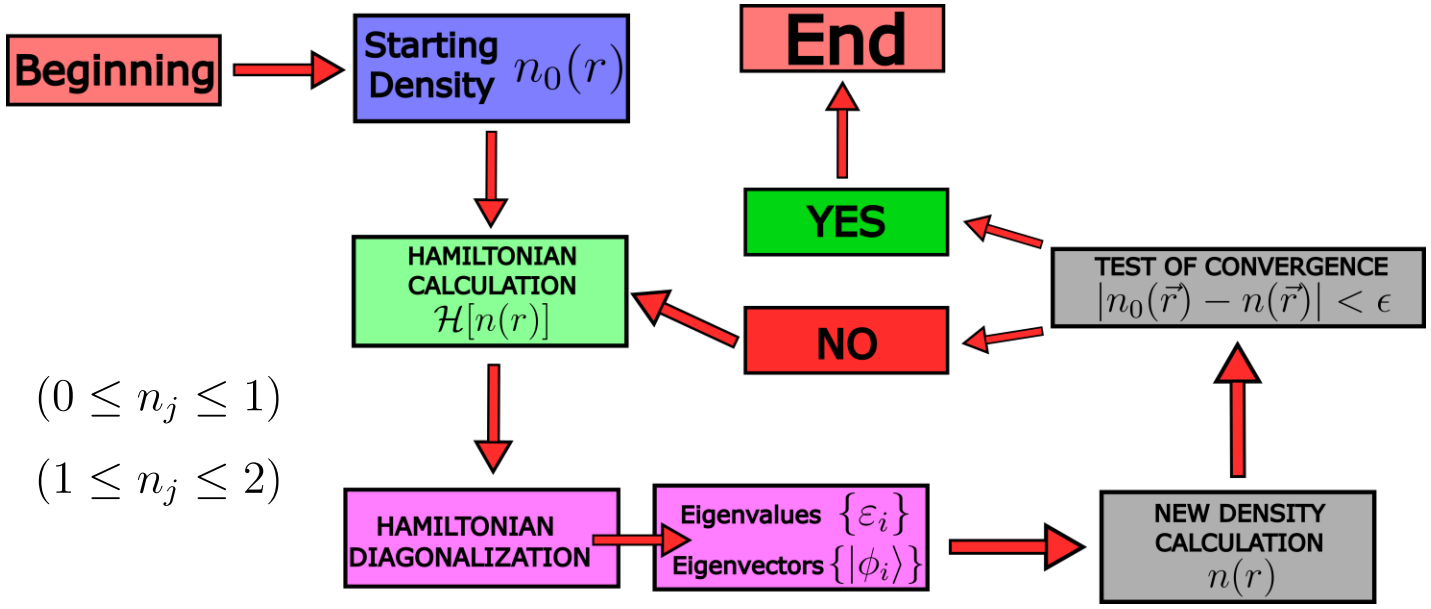
$$\mathcal{H}_{KS} = -\tau \sum_j (c^\dagger_{j,\sigma} c_{j+1,\sigma} + h.c.) + \sum_{j,\sigma} v^{KS}_{j,\sigma} n_{j,\sigma} - \mu \sum_{j,\sigma} n_{j,\sigma}$$

Such the external potentials are

$$v^{KS}_{j,\sigma} = v_{j,\sigma} + v^H_j[n_j] + v^{xc}_j[n_j]$$

$$v^H_j[n_j] = \frac{U}{2} n_j$$

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

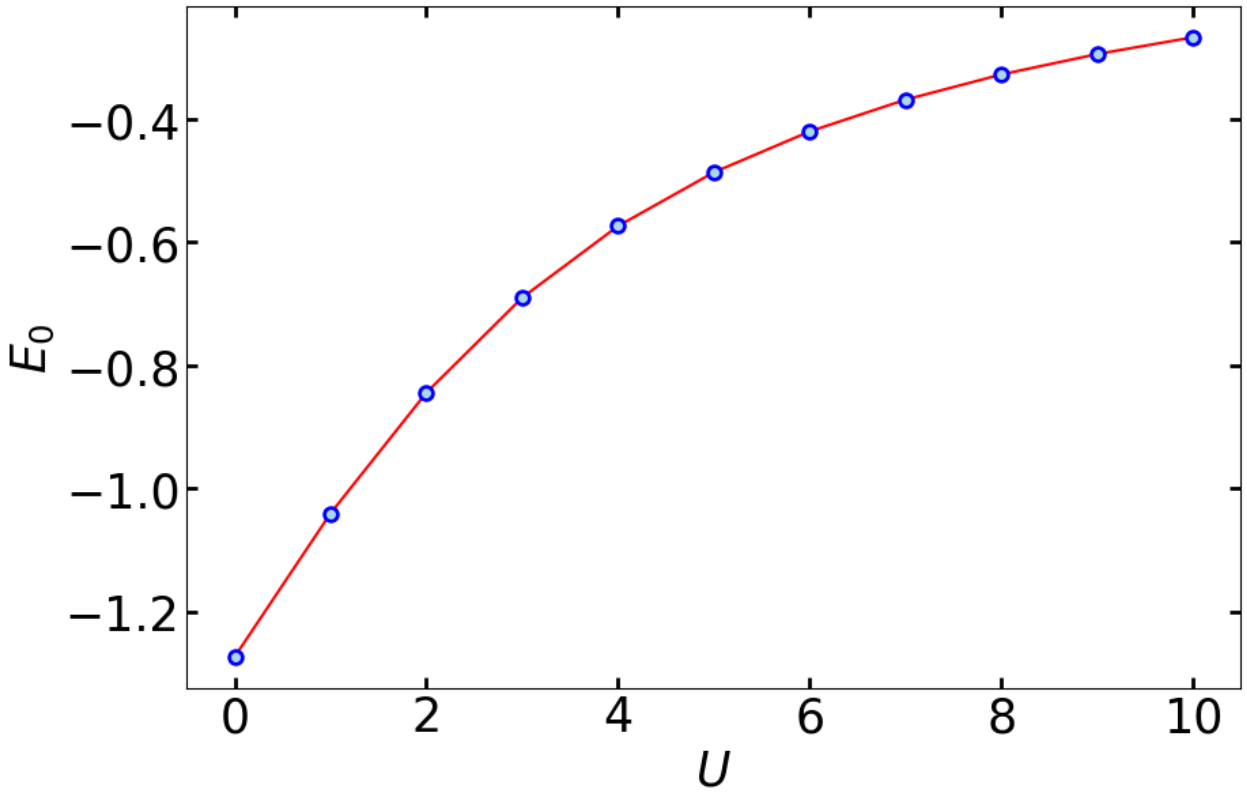


The total energy is

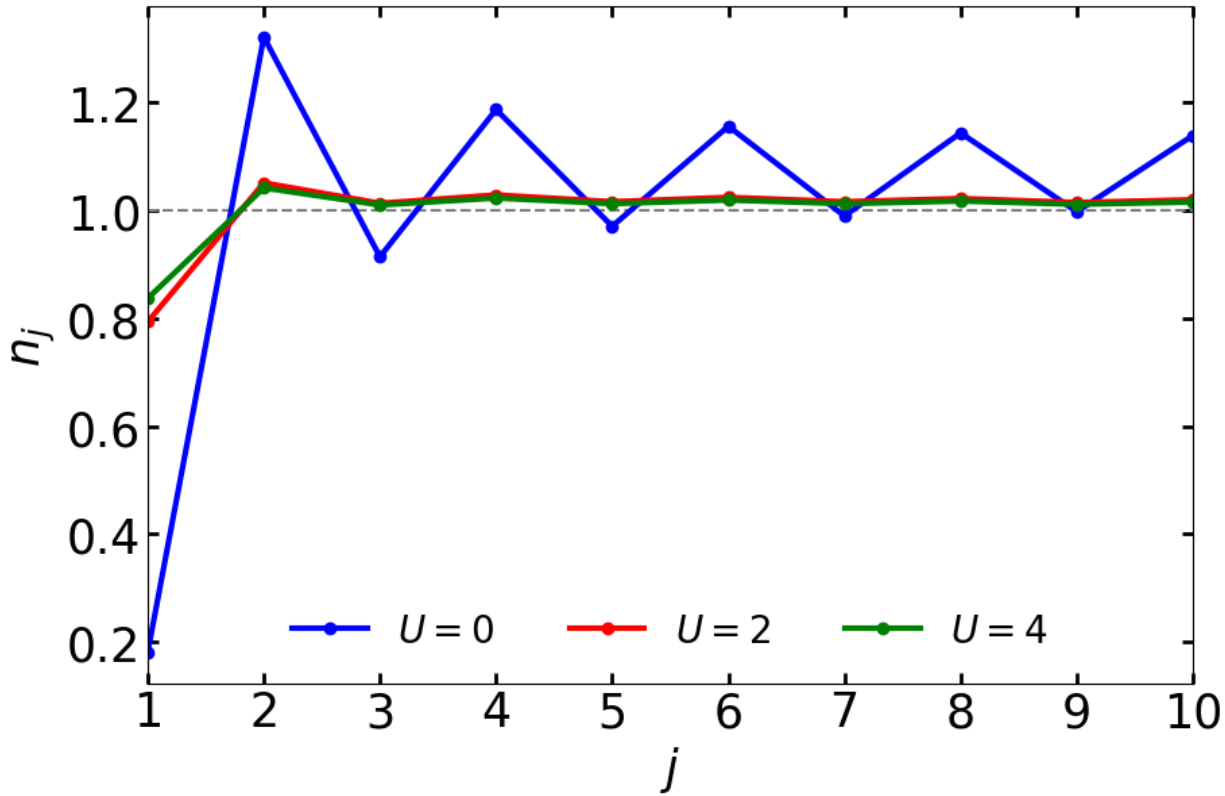
$$E[n] = -\frac{2\beta(U)}{\pi} \sum_j \begin{cases} \sin\left(\frac{\pi n_j}{\beta(U)}\right), & (0 \le n_j \le 1) \\ -\sin\left(\frac{\pi(2-n_j)}{\beta(U)}\right) + U(n_j - 1), & (1 \le n_j \le 2) \end{cases}$$

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

DFT – Results



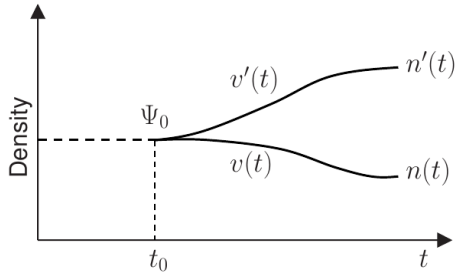
Ground state energy as a function of the Hubbard interaction in the homogenous case.

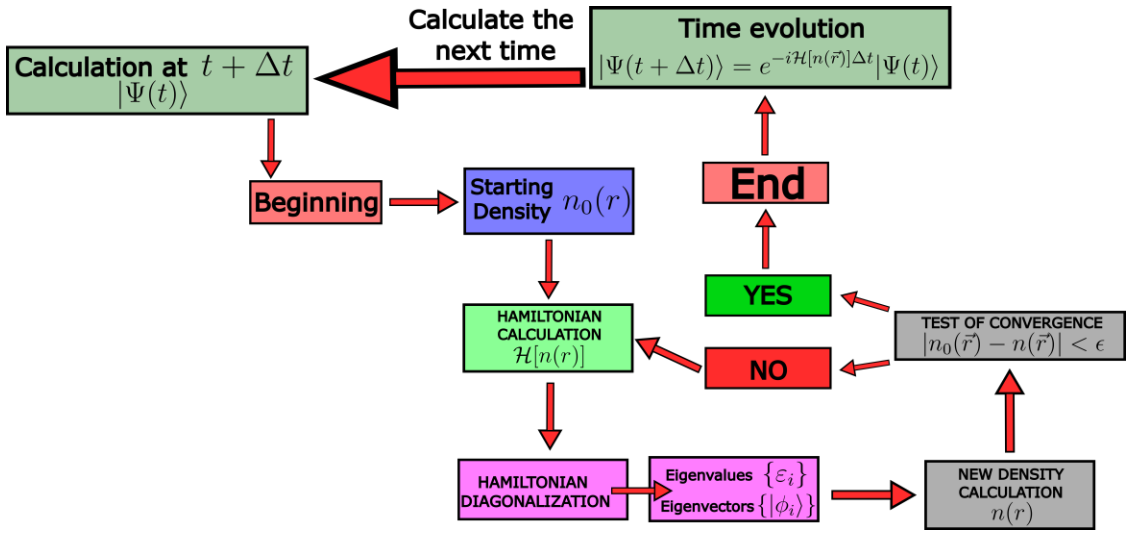


Occupation number for a chain of 10 sites considering different many-body interaction values. A positive potential is applied at the first site.

TD-DFT – Scheme*

Runge–Gross theorem. Two densities $n(\mathbf{r},t)$ and $n'(\mathbf{r},t)$, evolving from a common initial many-body state Ψ_0 under the influence of two different potentials $v(\mathbf{r},t)$ and $v'(\mathbf{r},t) \neq v(\mathbf{r},t)+c(t)$ (both assumed to be Taylor-expandable around t_0), will start to become different infinitesimally later than t_0. Therefore, there is a one-to-one correspondence between densities and potentials, for any fixed initial many-body state.





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.

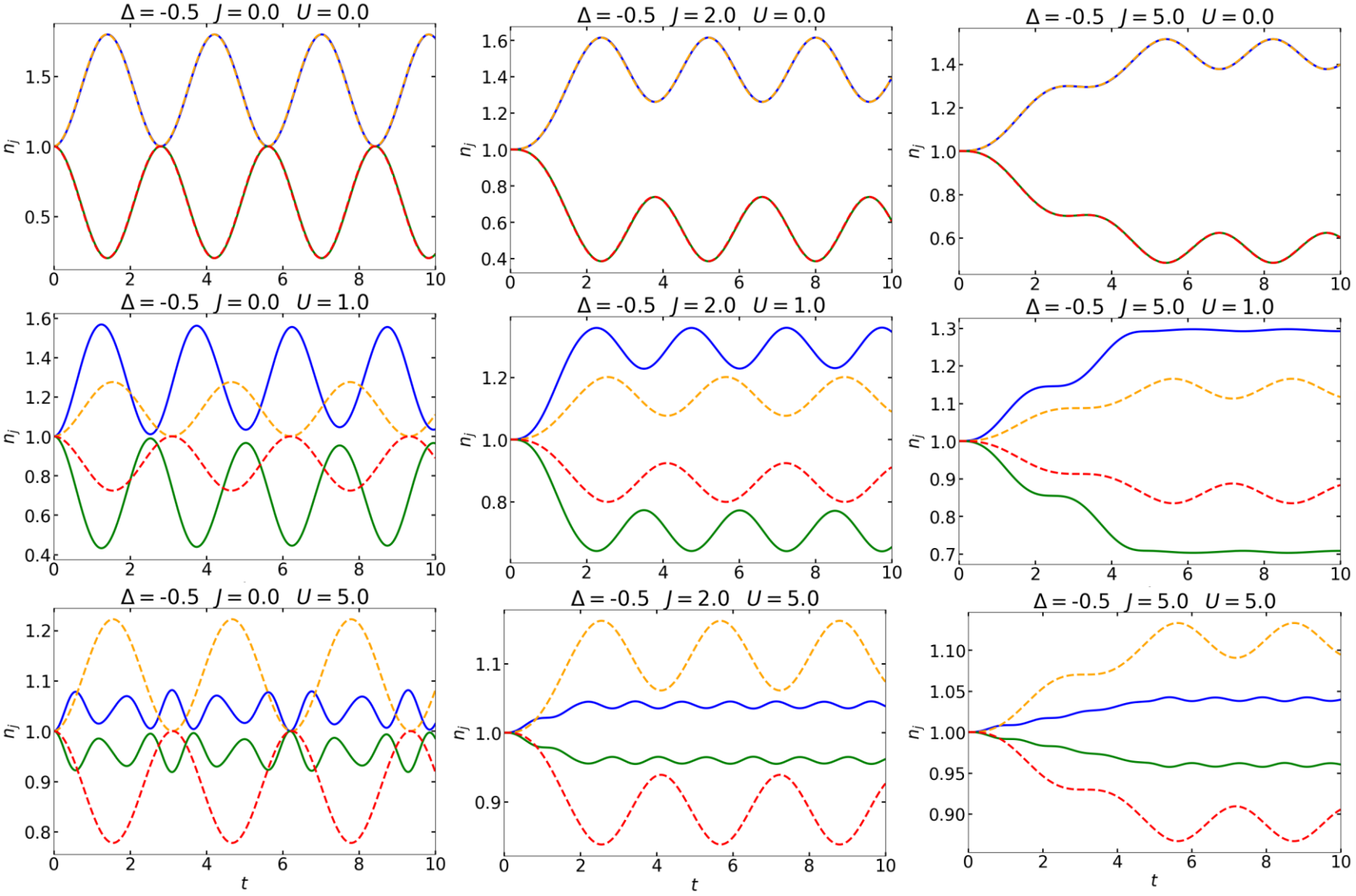
We have changed the external potential following the ramp up protocol**,

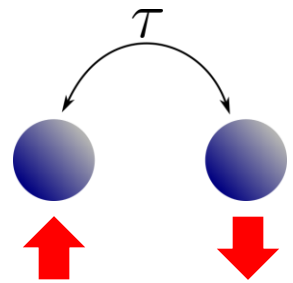
$$v(t) = \frac{\Delta t}{J}$$

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

*Ullrich, Carsten A. "Time-dependent density-functional theory: concepts and applications." (2011);**Herrera, M., Serra, R.M. & D'Amico, I. *Sci Rep* **7**, 4655 (2017).

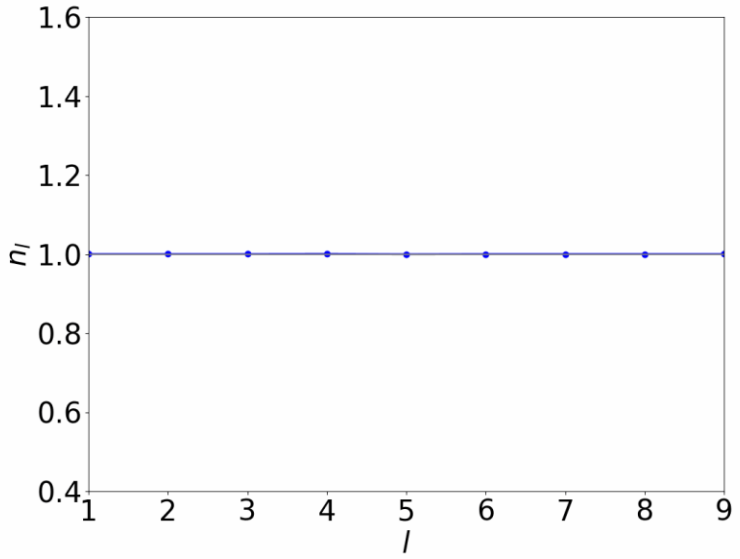
TD-DFT – Results: Hubbard dimer





Dashed line: Exact Diagonalization

Continuum line: TD-DFT Calculation



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- 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);
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- 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