



Introduction

High-temperature superconductivity has remained one of the most enigmatic phenomena in modern physics. Understanding the mechanisms behind superconductivity is crucial, as it could pave the way for revolutionary technological advancements everywhere from energy transmission to medical diagnostics. Recently, ladder structures in cuprates (copper oxide-based materials), characterized by two-dimensional CuO₂ planes interconnected by oxygen atoms, have gained considerable attention due to their unique electronic properties, making them ideal candidates for researching high-T_c superconductivity [1, 2, 3].

Hubbard model and 3D ladders

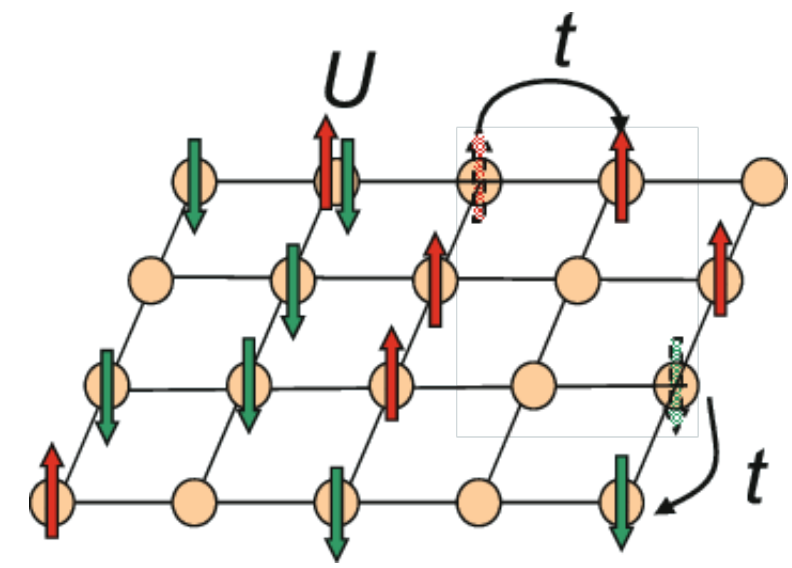


Figure 1. Electron hopping in the Hubbard model (Wikipedia: Hubbard Model).

The Hubbard model is a simple model used in physics, particularly in the study of magnetism and electron correlation effects in solids. The model captures the essential physics of electrons in a lattice, balancing the kinetic energy (which promotes electron delocalization) against the potential energy arising from electron-electron interactions.

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

We can host this general Hubbard model on 3D lattices as such $H = H_0 + t_\perp H_\perp$ with the inclusion of chemical potential and conserving particle number where [3]:

$$H_0 = \sum_{\langle i,j \rangle, \sigma} -t(c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - \mu \sum_{i,\sigma} n_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \quad (2)$$

$$H_\perp = - \sum_{\langle i,j \rangle \in \mathcal{R}, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.) \quad (3)$$

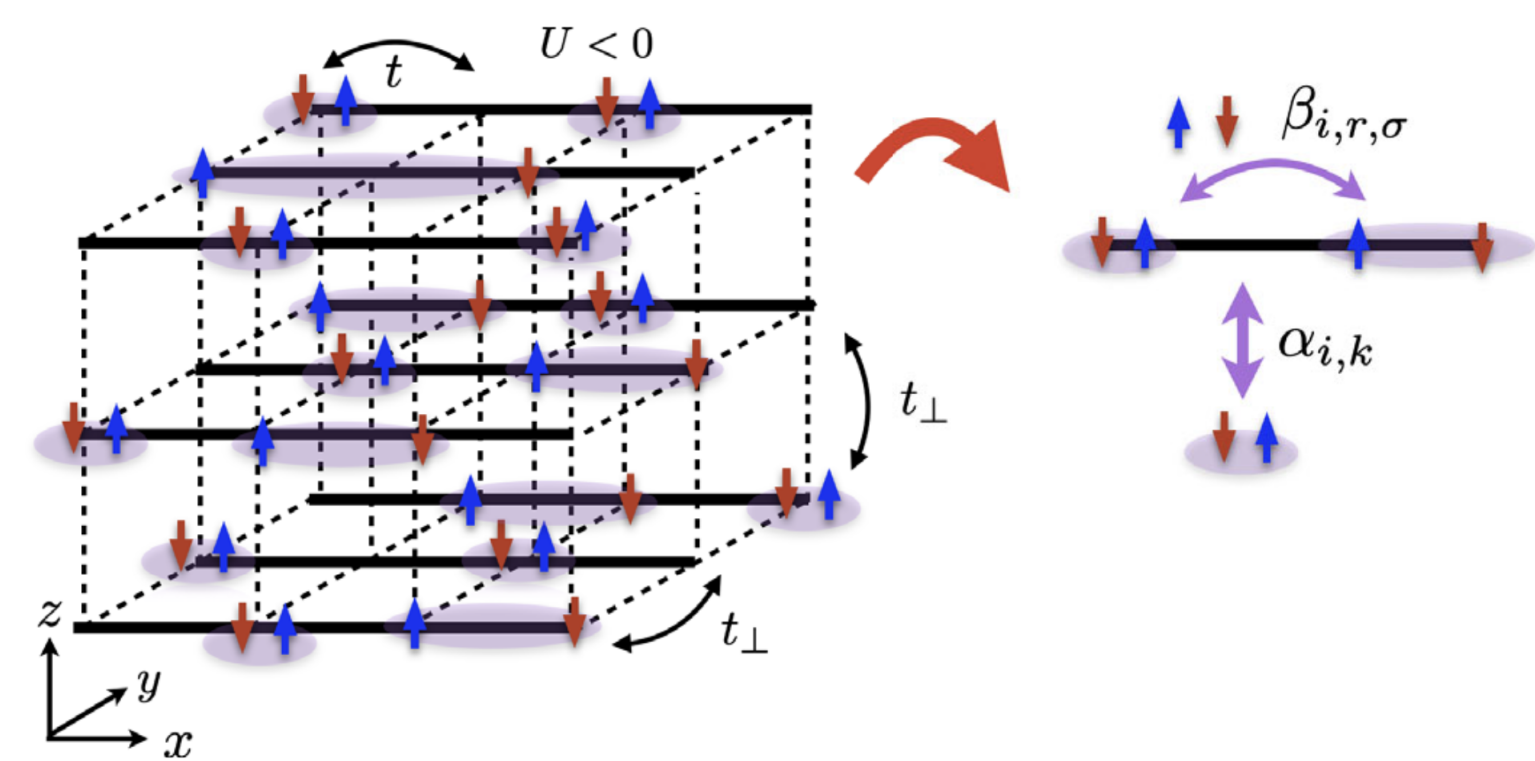


Figure 2. Diagram showing the 3-D ladder structure reducing to the quasi-1D chain [3].

Superconductivity in a 1D Hubbard Chain

Introducing the 1D chain, we seek to monitor our superconducting order parameter to make parallels/verify our effective Hamiltonians. Note that the 1D Hubbard model has a superconducting phase with attractive U (U<0) as it favors the formation of Cooper pairs.

We define the superconducting pair correlation function as:

$$\Delta(i, j) = \langle c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger c_{j,\downarrow} c_{j,\uparrow} \rangle$$

where:

- $\Delta(i, j)$ measures the correlation between a Cooper pair created at site i and annihilated at site j .
- This function allows us to monitor how correlations decay with distance.

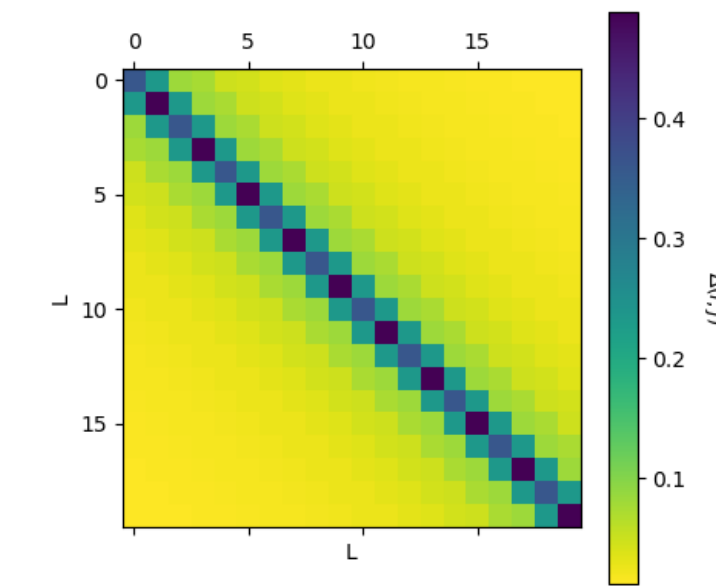


Figure 3. Displayed matrix of the superconducting pair correlation function via DMRG at half-filling.

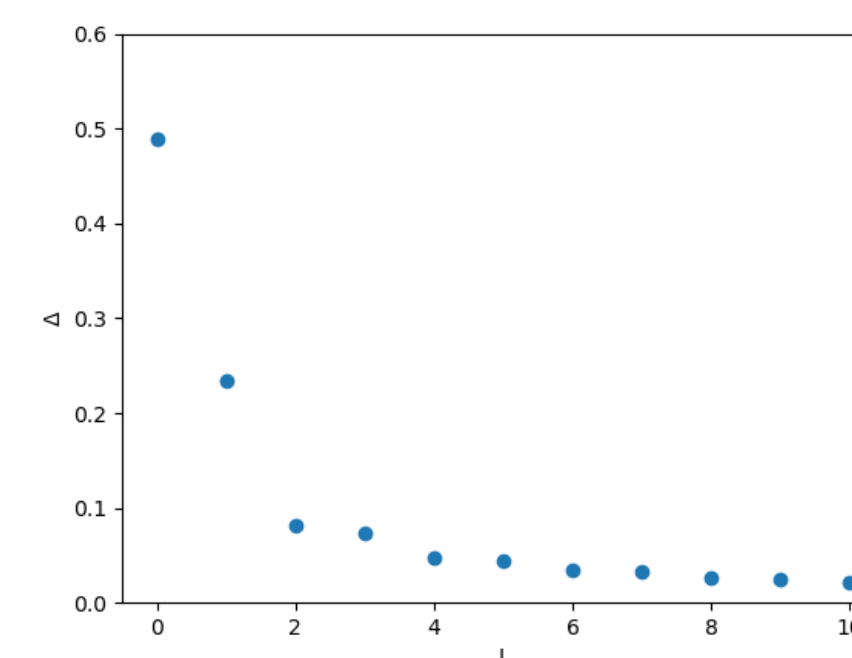


Figure 4. Plotted pair correlation function as a function of distance. We can see a power law correlation from the graph as expected (Tomonaga-Luttinger Liquid (TLL) behavior) [2].

Effective Mean Field Hamiltonian

We use the following ansatz to reduce our 3D Hamiltonian to a quasi-1D Hamiltonian and also assume that the expectation of operators that create/annihilate particles on different chains is 0:

$$\langle c_i c_j c_k c_l \rangle = \langle c_i c_j \rangle \langle c_k c_l \rangle + \langle c_i c_l \rangle \langle c_j c_k \rangle - \langle c_i c_k \rangle \langle c_j c_l \rangle \quad (4)$$

After reducing, we end up with [3]:

$$H_{\text{MF}} = H_0(R_i) - \sum_{i,k} \alpha_{i,k} (c_{i,\uparrow} c_{k,\downarrow} + c_{k,\downarrow}^\dagger c_{i,\uparrow}^\dagger) + \sum_{i,\sigma} \sum_{r=1}^{L-i} \beta_{i,r,\sigma} (c_{i+r,\sigma}^\dagger c_{i,\sigma} + c_{i,\sigma}^\dagger c_{i+r,\sigma}) \quad (5)$$

- Where we have the following coefficients describing tunneling in and out of parts of the 3D system [3]:
 - $\alpha_{i,k} = \frac{2ze^2}{\Delta E_p} \langle c_{i,\uparrow} c_{k,\downarrow} \rangle$
 - $\beta_{i,r,\sigma} = \frac{2ze^2}{\Delta E_p} \langle c_{i+r,\sigma}^\dagger c_{i,\sigma} \rangle$
- Each R_i denotes an individual chain.

MPS+MF Algorithm

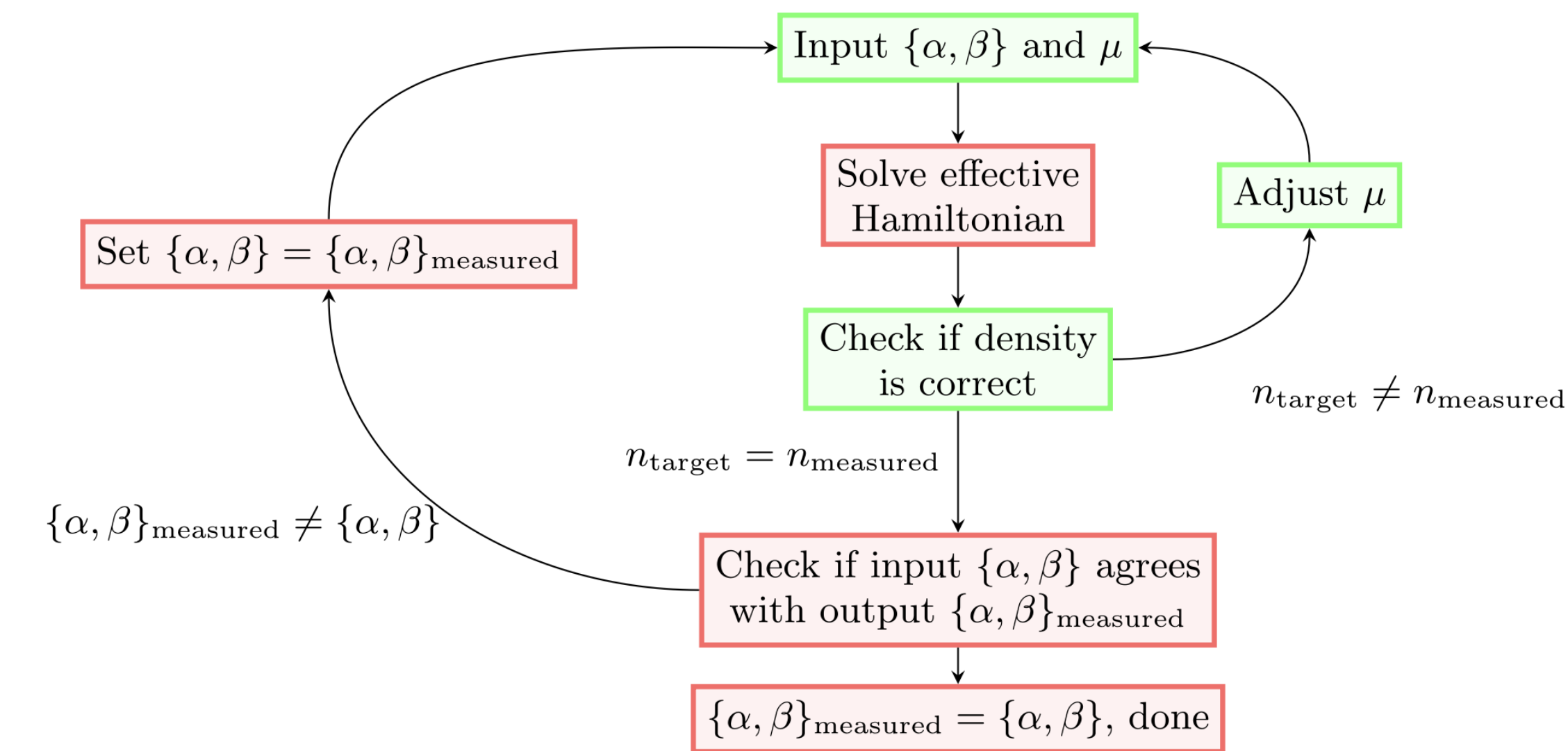


Figure 5. A schematic diagram of the MPS+MF convergence process [3]

- Note that we do not conserve particle number with our effective 1D Hamiltonian although this was the case in our explicit 3D Hamiltonian.
- We use a density matrix renormalization group algorithm (DMRG) via TenPy to iterate to convergence.
- Our scheme largely depends on initial guesses of coefficients and also scales with bond dimension as well as system size (due to DMRG).

Outlook

- Determine the MPS+MF method's validity for use in broader applications such as two-dimensional triangular lattices [4].
- Seek to make improvements to the MPS+MF method with convergence.

References

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