# Phases of the half-filled extended Fermi-Hubbard model

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**Abstract:** This work has consisted on finding Mott insulating phases for a Hubbard model at half-filling. The numerical simulations have been performed with Time-Evolving Block Decimation, a tensor network method. Two interaction terms have been considered: on-site repulsion $U$ and next-neighbour repulsion $V$. The introduction of the first has allowed to observe a spin density wave phase that lost kinetic energy with on-site repulsion strength, and the latter has shown a distortion of the SDW antiferromagnetic ordering with a phase transition at $V = U/2$, in which the fermion ordering changes to charge density wave. The results show that simulations of the Hubbard model can be carried out in an optimal and satisfactory way using tensor network formalism.
**Keywords:** Hubbard model, tensor networks, imaginary time evolution, Coulomb repulsion, Mott insulator.
**SDGs:** This work is related to sustainable-development goals 4 and 12 (see page 6).

## I. INTRODUCTION

The study of the properties of electrons in a lattice is one of the most important problems of condensed matter physics. As essential as it is, it poses a practically impossible task to solve, since one should account for all particle-wise interactions in the crystal, both atomic and electronic, to obtain an exact solution. The most standard hypothesis to make when attempting to solve this problem is a mean field approximation that neglects direct particle interactions and models their collective effect as a mean potential field with which all particles interact. This gives rise to band theory, which assumes any electron interacts with a mean periodic potential and extrapolates a material's conductive properties based on the filling of its energy bands or quantum states: partially-filled bands give rise to metallic behaviour, completely full bands are insulating. There are materials, however, that present a conductivity orders of magnitude lower than is predicted by band theory: such is the case of oxides like MnO, CoO and NiO, as de Boer and Verwey first pointed out [1]. However, it was Nevill Mott and Rudolf Peierls who proposed that this could be an effect of strong electron-electron repulsion [2].

Motivated by this, one may take a different approach: instead of defining a general potential with which all electrons interact, the problem can be attacked from a quantum many-body standpoint, where particle-wise interactions are considered explicitly. From this perspective, the most essential actions a particle can perform are to move to another site and interact with another particle: this implies that every particle will obey a Hamiltonian with a kinetic term and a potential term. With no interaction, particles will move freely across the lattice, and become delocalised. The point at which electron-wise repulsion reduces the conductivity of a material is known as a Mott insulator phase, where Coulomb repulsion between electrons becomes significant enough that the particle wavefunctions localise to reduce their overlap. Formally, a Mott insulator is any insulating phase that is not predicted by band theory, and thus arises purely from particle interaction.

Throughout this project, a numerical solution for a 1D Hubbard model has been implemented to observe the consequences of applying explicit Coulomb repulsion to a lattice with fermions at half-filling. To solve this problem in an optimal way, tensor network formalism has been employed, which enables to operate with large quantities of entangled data in an efficient way by narrowing entanglement. Time-Evolving Block Decimation has been the method of choice to converge the system into the ground state. With it we have been able to observe two types of phases of Mott insulating nature; a spin density wave and a charge density wave.

## II. THEORETICAL BACKGROUND

### A. The Hubbard model

The Hubbard model describes the behaviour of particles in a lattice using the following Hamiltonian:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + U \sum_i n_\uparrow n_\downarrow, \qquad (1)$$

where $t$ is the tunnelling amplitude and $U$ is the on-site interaction strength: the second term adds an energetic cost of $U$ for every doubly-occupied site. For repulsive systems, $U > 0$. Although the model can be employed for bosons as well (Bose-Hubbard model), this work will focus on its fermion version (Fermi-Hubbard), as we strive to simulate the behaviour of electrons in a lattice, which is clearly fermionic. We will consider only non-degenerate ($s$) orbitals, which can only allocate up to two electrons. This implies a Fock basis of $\langle 0, \uparrow, \downarrow, \uparrow\downarrow \rangle$: a site can either be unoccupied, occupied by a spin up or

spin down electron, or occupied by both. Being a quantum model, our wavefunctions will return a set of amplitudes at any site giving the probability of observing each Fock state in it. In the non-interacting case ($U = 0$), particles tunnel arbitrarily throughout the whole lattice and become delocalised. Technically, particles become fully localised only in the limit $U \to \infty$, but throughout this work we will refer to particles as "localised" when found in an identifiable ordering that reduces kinetic energy, which for us is any ground-state for $U > 0$. As the on-site repulsion is increased, in half-filling conditions (same amount of $\uparrow$ and $\downarrow$ particles, half per site) particles will tend to occupy a single cell to avoid wavefunction overlap, which will become increasingly costly in energy: however, it will not be fully eliminated, as a compromise between repulsion and kinetic tendencies must be found. Following that concept, Coulomb repulsion, modelled by $U$, is less significant than Pauli exclusion: particles will favour a neighbour with which their wavefunctions can even slightly overlap, instead of being fundamentally excluded. An alternate explanation is considering that the probability for a particle to jump to one of its nearest sites is not null for finite $U$, giving rise to an effective spin coupling. This effect is known as superexchange [3], and results in antiferromagnetic ordering for large on-site repulsion: $|\uparrow,\downarrow,\uparrow,\downarrow ...\rangle$. The resulting alternating spin arrangement is also known as a spin density wave, as the site spin is spatially modulated in a wave-like manner (two-site period).

Following the Coulomb repulsion consideration introduced with $U$, one may extend the effect adding a nearest-neighbour interaction term, obtaining the extended Hubbard model:

$$\mathcal{H}_{\text{extended}} = \mathcal{H}_{\text{Hubbard}} + V \sum_{\langle i,j \rangle} n_i n_j, \tag{2}$$

where $n_i$ is the total number of particles at site $i$. This term adds an energetic cost of $V$ for two adjacent particles. Again, only repulsive interactions will be considered, corresponding to $V \geq 0$. Upon increasing $V$ to a value comparable to that of $U$, there arrives a point at which the combined repulsion of the adjacent sites beats the on-site one, and the particles order themselves in spin pairs, leaving an empty site between them. In second quantisation notation, $|2, 0, 2, 0, ...\rangle$. Since both up and down electrons have the same charge, this phase is known as a charge density wave, as the site charge is spatially modulated in a two-site periodic manner [4]. This phase implies particle localisation as well, making it another example of a Mott insulating phase at half-filling.

On another note, all systems with explicit correlation between particles exhibit an additional complication when one intends to solve them numerically: computational cost. To perform correct simulations and keep computation efficient and relevant we must choose an adequate method.

### B. Tensor network formalism

The Hubbard model for $s$ orbitals describes a system with a local Hilbert space of dimension $d = 4$: as such, the Hilbert space of a 1D Hubbard lattice of N sites has a dimension of $4^N$. Being a superposition of all possible states, a random wavefunction $\Psi$ from this system will have the same dimension as the Hilbert space. Since it grows exponentially with system size, the Hilbert space quickly becomes infeasible to fully explore via traditional methods like exact diagonalisation. Tensor networks offer an alternative to this explicit representation with the factorisation of $\Psi$ into lower-rank tensors with explicit entanglement connections [5]:

$$|\Psi\rangle = \sum_{\{s_i\}} A^{s_1}_{\alpha_1} A^{s_2}_{\alpha_1\alpha_2} A^{s_3}_{\alpha_2\alpha_3} ... A^{s_N}_{\alpha_{N-1}\alpha_N} |s_1 s_2 ... s_N\rangle. \tag{3}$$

This is what is known as a matrix product state, and it is one of the most standard tensor network structures. With it, the information of every site is stored in its own tensor, each with its own set of Fock basis amplitudes regarding the probability of that site being in each state (stored in what is known as the physical index $s_i$), as well as pairwise-shared indices (known as virtual or internal bonds $\alpha_i$) that connect adjacent sites. Internal bonds contain information about the entanglement between both sides of the partition said bond represents: for a given bond dimension $\chi$, an internal bond can represent an entanglement entropy of up to $\log \chi$. This is where another great advantage of tensor network notation comes into play: it can be shown that ground states of one-dimensional gapped systems with local interactions follow an area law for the entanglement entropy [6] [7]. This property implies that the ground states of such systems exhibit limited entanglement, and this quantity scales as one dimension less than the system's. In the case of a 1D system, this means that the entanglement entropy of the ground state saturates at a certain value constant with system size, and therefore the bond dimension that can store this given value allows for a precise representation of the state. Imposing an upper threshold for the bond dimension regardless of size is a huge advantage, as it allows to set a limit to the number of operations necessary to simulate the system correctly, that is notably smaller than when working with a complete representation.

The concept of maximum bond dimension becomes particularly understandable when the system is evolved. Suppose one wishes to perform an operation that involves two adjacent sites (for example, as we will see in the following section, time-evolving them): the tensors belonging to these two sites will be first contracted together via their internal bond $\alpha_i$, leaving a two-site tensor of indices $\chi \times d \times d \times \chi$, where $\chi$ are internal indices and $d$ are physical indices. A two-site operator can be applied onto this tensor by contracting the operator via the shared physical indices. After performing this operation,

the following step is to split back the total tensor into sites to recover the MPS form. The most standard procedure to do so is Singular Value Decomposition (SVD), which factorises an arbitrary $m \times n$ matrix into a $n \times n$ rotation matrix $V$, a $m \times n$ rescaling array of eigenvalues $S$, and a $m \times m$ rotation $U$, such that $A = USV^*$. SVD is performed on matrices, two-index tensors, which can easily be derived from arbitrary tensors by index combinations and rearrangements that will be undone after the partition: in this case, the tensor is reshaped following $\chi \times d \times d \times \chi \to \chi d \times \chi d$. Clearly, eigenvectors corresponding to the largest-magnitude eigenvalues will be the ones with the greatest contribution to the total quantum state. We can construct a good enough approximation of the site tensors keeping only the greatest-magnitude $\chi$ eigenvalues: this is known as truncation. Software implementations of SVD commonly return the result matrices in such a way that $S$ is an array of eigenvalues in descending order, making truncation easy to implement.

In the context of splitting across a tensor derived from two sites, the array of eigenvalues will contain information about the entanglement of the system at both sides of the split, as it finds itself in the midst of the new internal bond. By limiting the amount of eigenvalues, one is limiting the maximum entanglement entropy that can be expressed between two system partitions; however, we know by the area law that this is an affordable limitation, as the entanglement entropy naturally saturates at a given value. Even if the bond dimension imposed is not precisely the one that satisfies the area law, the lowest eigenvalues are the ones with lesser contributions to the complete state.

### C. Time-Evolving Block Decimation

This section describes the method with which the ground state wavefunctions have been computed for an initial random state and a given Hamiltonian. An arbitrary wavefunction $\Psi(x,t)$ can be expressed as a linear combination of Hamiltonian eigenstates:

$$\Psi(x,t) = \sum c_n \psi_n(x) e^{-iE_n t/\hbar} \tag{4}$$

Where $c_n$ are the amplitudes of each eigenstate in this particular $\Psi(x,t)$, and $E_n$ are the energies of the respective eigenstates $\psi_n(x)$. The ground state is the Hamiltonian eigenstate of lowest energy, and a particularly interesting state to understand the properties of a system, especially at low temperatures. In terms of Fourier series, as is defined the wavefunction above, the ground state will be the eigenstate that oscillates at the lowest frequency, being the component with the smallest exponent (in magnitude) in the time evolution operator $e^{-iE_0 t/\hbar}$. A change of variables can be done such that $\tau = it$, where $\tau$ is the imaginary time. Having removed the imaginary unit from the exponent, the time evolution operators become decaying exponentials:

$$\lim_{\tau\to\infty} \Psi(x,\tau) = \lim_{\tau\to\infty} \sum c_n \psi_n(x) e^{-E_n \tau/\hbar}. \tag{5}$$

Upon advancing in imaginary time $\tau$, all exponential terms will decay at a certain rate, with the lowest rate being that of the ground state term. If instead of doing a full projection to $\tau \to \infty$ one applies imaginary time steps $\delta\tau$ and normalises the wavefunction after each step, the state will evolve to an increasing spectral domination of the ground state, and this can be iterated until all higher-energy states have a negligible contribution: with due normalisation, the lowest-energy coefficient $c_0$ becomes trivial and $\Psi(x, \tau \to \infty) \approx \psi_0(x)$.

To implement this projection numerically a time evolution operator must be constructed by exponentiating the Hamiltonian $\mathcal{H}$: this is not trivial when terms do not commute, as is the case of hopping and interaction terms in the Hubbard model. The Hamiltonian can, however, be expressed as a sum of commuting terms:

$$e^{-\mathcal{H}\tau} = e^{-(\mathcal{H}_o + \mathcal{H}_e)\tau} = \lim_{n\to\infty} \left( e^{-\mathcal{H}_o \tau/n} e^{-\mathcal{H}_e \tau/n} \right)^n \tag{6}$$

Such operator is thus split into two subsets, the elements of which all commute; notice that $\delta\tau = \tau/n$. This process is known as Suzuki-Trotter decomposition or Trotterization. The common procedure is splitting the Hamiltonian into odd terms ($\mathcal{H}_o = \sum h_i h_{i+1}$ for odd $i$, acting on site pairs starting with an odd index like 1-2, 3-4...) and even terms ($\mathcal{H}_e$). Now, the application of one of these two partitions $\mathcal{H}_i$ onto $\Psi$ is equivalent to applying their terms $h_i h_{i+1}$ individually (just two-site interaction tensors, known as gates), as they commute. Thus, it is only necessary to employ these gates, of dimension $d^4$, to evolve the system into the projected ground state, effectively breaking down the action of a full exponentiated matrix into a sequence of gate applications, each consisting of $\chi^2 d^4$ operations. The splitting (decimation) of the full time evolution operator into local gates is what is known as Time-Evolving Block Decimation. Recall now the MPS representation introduced earlier: if a N-site wavefunction were described by a vector of $d^N$ coefficients, its imaginary time step operator $e^{-\delta\tau\mathcal{H}}$ would be described by a matrix of dimension $d^N \times d^N$, and every imaginary time step (in which said operator is applied onto the wavefunction) would consist of $d^{2N}$ operations (in other words, have a complexity of $d^{2N}$). By splitting the Hamiltonian into gates, one must apply $N$ ($N-1$ for open boundary conditions) gates onto the sites, resulting in a time step of complexity $N\chi^2 d^4$ (not accounting for SVD, that has a complexity of $\chi^3 d^3$). Keep in mind that truncation is implemented after every gate application: when the full tensor is split to recover MPS form using SVD, the eigenvalue array is limited to its $\chi$ greatest elements.

Overall, this is an extraordinary improvement in computing cost: TEBD time steps scale linearly with system size, not exponentially. This allows for much more versatile simulation sweeps and lighter memory loads.

## III. RESULTS

In this section the measurements of the ground-state wavefunctions obtained by TEBD are discussed. Tensor operations have been programmed with Julia and using the ITensors and ITensorMPS libraries, which allow for explicit quantum number conservation in finite MPS, necessary to impose half-filling. A TEBD algorithm for such MPS objects has been implemented with direct gate contractions and normalisation, and different observables have been defined to study the ground-state properties. Initial wavefunctions were generated with random coefficients at half-filling. The code is available at [11].

### A. Convergence

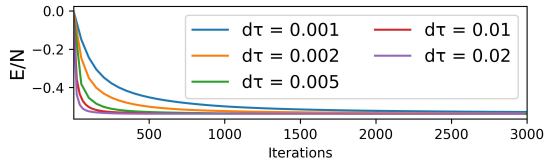


Figure 1: Energy per site as a function of TEBD iterations, for $N = 10$ and $U = 4$. The full energy of the system decays in a practically exponential manner, as is expected from imaginary time evolution. The decay rate is proportional to the time step, $d\tau$.

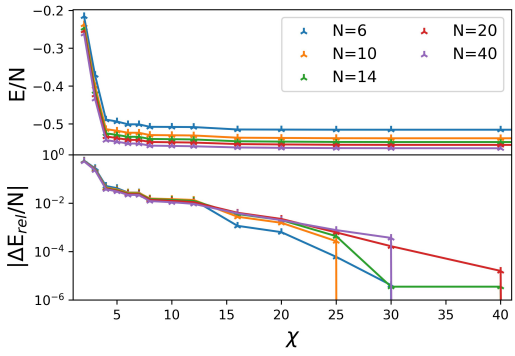


Figure 2: Converged energy per site and relative energy per site error (considering the maximum simulated bond dimension as the standard value, $\chi = 60$ except for N=40) as a function of bond dimension for different system sizes ($U = 4$, $V = 0$).

A bond dimension of 20 has been deemed sufficient to simulate the following ground states from here on, as a bond dimension of 60 yields a result with a relative difference of $\sim 0,5\%$. It's easy to see that increasing bond dimension incorporates increasingly low-energy terms, to a point where their addition becomes trivial. Since the simulations performed in this work are of open-boundary conditions and run in a conventional laptop, boundary effects are unavoidable due to insufficient scaling capabilities, as the $N = 40$ systems were already time-costly to simulate: however, a limited number of sites still allows for a heuristic interpretation of the effects of direct particle interaction, which is the aim of this project. All simulations have been run with $d\tau = 0.01$ and an energy convergence precision of $10^{-6}$.

### B. On-site interaction

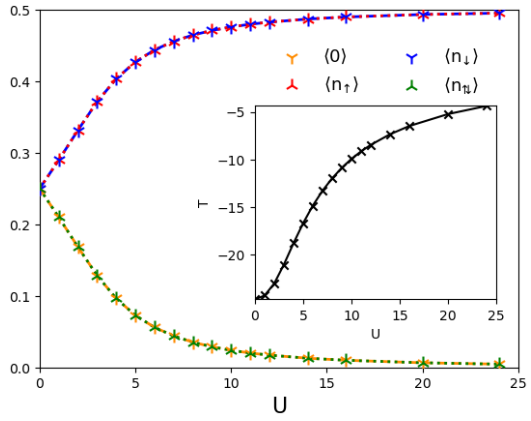


Figure 3: Average expectation value of the Fock basis states and kinetic energy $T$ as a function of the on-site potential $U$ for a lattice of $N = 20$.

This plot successfully recovers the diagram shown in the third figure of [8], being the expected result of the on-site potential repulsion and the display of Mott insulating behaviour. One can see that for $U = 0$ all states are equiprobable, no electron organisation is favoured. However, upon introducing $U > 0$, doubly-occupied and empty sites are slightly disfavoured, and this fact becomes more notorious for larger values of $U$. This localisation comes with a decrease in the kinetic energy: notice that since the hopping term of the Hamiltonian is negative, a decrease in absolute value of the measured kinetic energy translates to a lower tunnelling probability between sites. For near-zero values of $n_{\uparrow\downarrow}$, recalling that we have imposed half-filling, the electrons are practically localised, one in each site, in alternating values of spin. This alternating ordering can be seen using the spin-spin correlation function, which gives information of how similar two expected values of spin are.

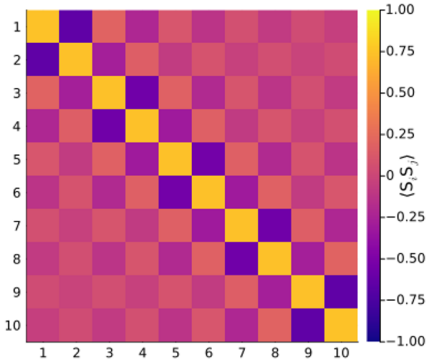


Figure 4: Spin correlation matrix for $U = 10$ and a lattice of size $L = 10$.

A chequerboard pattern is manifest, indicating negative spin correlation among nearest neighbours, corresponding to an antiferromagnetic ordering. It can be shown that the correlation magnitude of two sites decays exponentially with the distance [9]. The block-diagonal high correlations are a consequence of the open boundary conditions and can be seen to vanish away from the boundaries as lattice size is increased.

### C. Extended model

A common choice for the order parameter of the SDW-CDW phase transition is the staggered charge density[10]:

$$\Delta_{CDW} = \frac{1}{N}\sum_i (-1)^i \langle n_{i,\uparrow\downarrow}\rangle \tag{7}$$

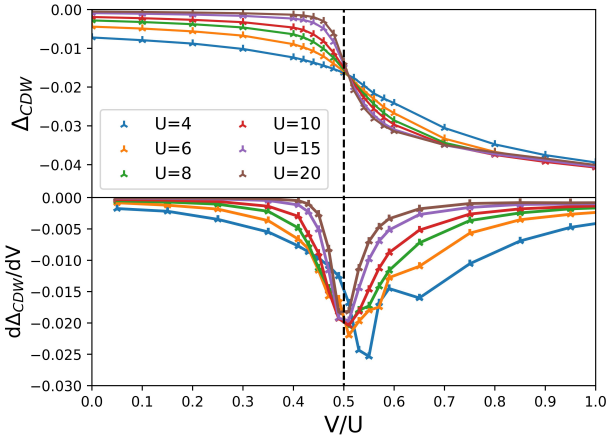


Figure 5: Evolution of the staggered charge density $\Delta_{CDW}$ as a function of $V/U$ for $L = 10$.

As is easy to see, this value will increase in the case of double occupancy in alternating sites, and will approach zero if electrons are regularly distributed throughout the lattice (such that the expected number of electrons in one site is similar to that of its nearest neighbours). This is a comfortable choice for an order parameter because it is local: that is, it is a sum of local expectation values, making it a relatively easy quantity to compute.

Rescaling of N.N. repulsion $V$ sweeps to the ratio $V/U$ helps see the point where the phase transition takes place. The precise value can be more easily seen in the numerical derivative plot, in which the rescaled peaks are all centred at $V = U/2$, indicating a change in curve slope. Since the staggered charge density displays very low values for low $V$ (no spatial charge modulation) and increases in magnitude with $V/U$, the plot shows a phase transition from spin density wave (initial state with just on-site repulsion) to charge density wave.

## IV. CONCLUSIONS

Using an MPS model and Time-Evolving Block Decimation, we have observed two Mott insulating phases in a half-filled one-dimensional Hubbard lattice. Electron localisation and spin-spin anti-correlations in the presence of an on-site repulsion potential have been observed, characterising the spin density wave phase. After that, a next-neighbour repulsion term has been incorporated, which introduced spatial charge modulation and a phase transition to a charge density wave at $V = U/2$. Overall, this project has helped to see how an explicit consideration of electron-electron repulsion in a lattice gives rise to insulating phases at half-filling.

### Acknowledgments

I would like to thank the Quantic group at BSC for their guidance and attentiveness, as well as my tutors Artur and Bruno for their support. Also, a heartfelt thank you to my family and friends for supporting me through this journey.

[1] J. de Boer and E. Verwey. Semi-conductors with partially and with completely filled 3d-lattice bands. *Proceedings of the Physical Society*, 49(4S):59, August 1937.
[2] N. F. Mott and R. Peierls. Discussion of the paper by de Boer and Verwey. *Proceedings of the Physical Society*, 49(4S):72, August 1937.
[3] S. Trotzky et al. Time-resolved observation and control of superexchange interactions with ultracold atoms in optical lattices. *Science*, 319(5861):295–299, January 2008.
[4] S Ejima and S Nishimoto. Phase Diagram of the One-Dimensional Half-Filled Extended Hubbard Model. *Phys. Rev. Lett.*, 99(21):216403, November 2007.
[5] R. Orús. A practical introduction to tensor networks: Matrix product states and projected entangled pair states. *Annals of Physics*, 349:117–158, 2014.
[6] M B Hastings. An area law for one-dimensional quantum systems. *Journal of Statistical Mechanics: Theory and Experiment*, 2007(08):P08024, August 2007.
[7] U. Schollwöck. The density-matrix renormalization group in the age of matrix product states. *Annals of Physics*, 326(1):96–192, 2011.
[8] Wing Chi Yu. Density matrix spectra and order parameters in the 1D extended Hubbard model. *The European Physical Journal B*, 89(10):212, October 2016.
[9] M. B. Hastings. Lieb-schultz-mattis in higher dimensions. *Physical Review B*, 69(10), March 2004.
[10] C. Borgs et al. The staggered charge-order phase of the extended Hubbard model in the atomic limit. *Journal of Physics A*, 29(4):733, February 1996.
[11] https://github.com/mlimonv12/codi_TFG

# Fases del model de Hubbard estès a mig omplir

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**Resum:** Aquest treball ha consistit en trobar fases aïllants pel model de Hubbard a mig omplir. Les simulacions s'han dut a terme amb TEBD, un mètode de xarxes tensorials. S'han considerat dos termes d'interacció: repulsió *in situ* $U$ i repulsió a primers veïns $V$. La introducció del primer ha permès observar una fase d'ona de densitat d'espín que perdia energia cinètica amb la repulsió *in situ*, i la segona ha mostrat una distorsió de l'ordenament antiferromagnètic anterior amb una transició de fase a $V = U/2$, on l'ordenament dels electrons canviava a ona de densitat de càrrega. Els resultats mostren que es poden dur a terme simuacions del model de Hubbard de manera òptima i satisfactòria fent servir el formalisme de xarxes tensorials.
**Paraules clau:** Model de Hubbard, xarxes tensorials, evolució en temps imaginari, repulsió de Coulomb, aïllant de Mott.
**ODSs:** Aquest TFG està relacionat amb els Objectius de Desenvolupament Sostenible (SDGs)

**Objectius de Desenvolupament Sostenible (ODSs o SDGs)**

| | | | |
|---|---|---|---|
| 1. Fi de la es desigualtats | | 10. Reducció de les desigualtats | |
| 2. Fam zero | | 11. Ciutats i comunitats sostenibles | |
| 3. Salut i benestar | | 12. Consum i producció responsables | X |
| 4. Educació de qualitat | X | 13. Acció climàtica | |
| 5. Igualtat de gènere | | 14. Vida submarina | |
| 6. Aigua neta i sanejament | | 15. Vida terrestre | |
| 7. Energia neta i sostenible | | 16. Pau, justícia i institucions sòlides | |
| 8. Treball digne i creixement econòmic | | 17. Aliança pels objectius | |
| 9. Indústria, innovació, infraestructures | | | |

El contingut d'aquest TFG, part d'un grau universitari de Física, es relaciona amb els Objectius de Desenvolupament Sostenible 4 i 12. La relació amb l'ODS 4 és clara, sent educació de qualitat, ja que contribueix a l'educació a nivell universitari, explorant de forma intuitiva la simulació del model de Hubbard emprant el formalisme de xarxes tensorials. Tanmateix, el treball també es relaciona amb l'ODS 12, posant èmfasi en la necessitat d'optimitzar els càlculs d'un problema de molts cossos per obtenir bons resultats, i la possibilitat de fer-ho fins poder dur a terme simulacions massives a un ordinador personal.