

Investigating unconventional superconductivity in the 2D Hubbard-Kanamori model using Functional Renormalization Group (FRG)

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1 Abstract

The two-dimensional Hubbard model has attracted sustained scientific interest for decades, largely because of its ability to capture most of the underlying physics of the superconducting phase of the high-temperature cuprate superconductors [1]. Beyond its relevance to the cuprates, it also serves as a fundamental toy model in theoretical physics. This thesis conducts a detailed analysis of the 2D Hubbard model using the truncated-unity functional Renormalisation Group (TU²FRG) method, within the framework of spin-fluctuation-mediated superconductivity. The interplay between magnetism and superconductivity is explored by systematically varying model parameters such as the on-site Coulomb repulsion, chemical potential, Hund’s coupling, next-nearest-neighbor hopping, and the number of orbitals per site. This approach enables the identification of clear trends in the superconducting critical (T_c) temperature and order parameter, while also providing insights into the magnetic ordering and how well FRG works for a certain range of parameters.

2 Introduction

Since its discovery in 1911 [2], superconductivity has remained a topic of great scientific interest. This phenomenon, characterised by an abrupt drop in resistance at a so-called “Critical Temperature (T_c)” [3] is driven by an attractive interaction between electrons. This interaction leads to the formation of electron pairs, famously known as “Cooper pairs” [4]. For many years after the discovery of superconductivity, physicists were convinced that BCS-Eliashberg-electron-phonon theory [4] provided a complete explanation of the electron pairing mechanism in all superconducting materials. However, in 1979, the discovery of the first heavy-fermion superconductor [5] gave rise to a whole new class of materials: Unconventional Superconductors. These are condensates of cooper pairs formed by a different pairing mechanism than the electron-phonon coupling predicted by BCS theory [6]. For many materials, there is no consensus on what the mechanism otherwise is.

High-temperature superconductors are a special class of unconventional superconductors. They are defined by having a critical temperature greater than the boiling point of Nitrogen (77K). Ever since the discovery of the first high- T_c superconductor [7], the search for “(close to-) room temperature” superconductors has been extended to all kinds of unconventional superconductors. However, a comprehensive understanding of what drives the superconductivity is required in order to achieve this. There have been multiple attempts to model the pairing mechanism of some families of high- T_c superconductors, most of which have been greatly limited by the numerical challenges that working with complex lattice structures present.

Motivated by these challenges and by the need for simplified yet insightful models, this work turns to the two-dimensional Hubbard model—one of the most fundamental frameworks in condensed matter physics. Truncate Unity Functional Renormalisation Group (TU²FRG) [8] is employed to investigate the influence of the Coulomb repulsion (U) and chemical potential (μ) on the interplay between magnetism and superconductivity. This is done under the key assumption that superconductivity arises from spin-fluctuation mediation. In this work, regions of stable magnetic and superconducting order are identified, and trends in their respective ordering and

critical temperatures are presented. The study is further extended by examining how variations in the next-nearest-neighbor hopping amplitude and the inclusion of a second orbital per site impact all of the above.

3 Theoretical Background

3.1 Unconventional superconductivity

Most generally, the Hamiltonian for a superconducting state can be described as follows:

$$\hat{H} = \hat{H}^0 + \hat{H}^{cp} \quad (1)$$

where \hat{H}^{cp} describes the pairing interaction that leads to the formation of a Cooper pair and is given by:

$$\hat{H}^{cp} = \sum_{k,k'} \Gamma(k, k') c_{k,\uparrow}^\dagger c_{k',\downarrow}^\dagger c_{k',\uparrow} c_{-k,\downarrow} \quad (2)$$

In s-wave symmetric superconductors, the effective pairing interaction $\Gamma(k, k')$ is momentum-independent and thus remains constant. For many unconventional superconductors-including those with spin-fluctuation mediated pairing-the exact form of $\Gamma(k, k')$ has remained as an unanswered question for decades.

3.1.1 Spin-fluctuation mediated superconductivity

The prevailing assumption for the pairing mechanism in Iron-based or heavy-fermion compounds is that it is driven by spin fluctuations [9]. This section discusses how to model spin-fluctuation mediated superconductivity for the fluctuation-exchange approximation (FLEX) [10].

In such cases, the effective pairing interaction $\Gamma(k, k')$ is given by ¹:

$$\Gamma(k, k') = \frac{3}{2}U^2\chi^S(k - k') - \frac{1}{2}U^2\chi^C(k - k') + U \quad (3)$$

This equation is taken from [11]. Here, U is the on-site Coulomb repulsion and χ^S , χ^C are the interacting spin-susceptibilities in the Charge (C) and Spin(S) channel respectively. Their form is given below.

$$\chi^S(q) = \frac{\chi^0(q)}{1 - U\chi^0(q)} \quad (4)$$

$$\chi^C(q) = \frac{\chi^0(q)}{1 + U\chi^0(q)} \quad (5)$$

These interacting spin susceptibilities are expressed in terms of the non-interacting dynamic spin susceptibility (χ_{ps}^0) [9], stated below:

¹Note that this form of pairing interaction assumes that the ratio between the fluctuation frequency (w_f) and the Fermi energy is small.

$$\chi_{ps}^0(q, i\omega) = - \sum_k \int_0^\beta d\tau G_{ps}^0(k + q\tau) G_{sp}^0(k, -\tau) e^{i\omega\tau} \quad (6)$$

The calculations presented in this project are carried out in the spin-fluctuation framework. Whilst this theory has managed to successfully capture key features in the phase diagrams of unconventional superconductors, it also has its limitations. The most relevant example is that of the cuprate phase diagram: spin-fluctuation theory is able to capture the superconducting dome and the correct order parameter [12, 13] but fails to describe the characteristic pseudo-gap and Mott insulating phase [14].

3.2 Hubbard-Kanamori Model

3.2.1 Tight binding Models

The Tight Binding Model is a central element of condensed matter physics (7). In this model, electrons are bound in orbitals around the lattice ions. Due to the overlap between the quantum mechanical wave-functions that describe these orbitals, electrons are allowed to 'hop' to neighbouring sites. The probability that this hopping process will occur is given by a tunnelling amplitude, which can be calculated using a hopping integral.

This work is carried out in the tight-binding model framework, where the magnitude of the tunnelling amplitudes is at first treated as a free parameter. The starting point is a simple nearest-neighbour hopping tight binding model. The effect of introducing a next-nearest-neighbour hopping and an extra orbital per site is then investigated (*See Fig. 1*).

$$\hat{H}_{TB}(\mathbf{R}) = \sum_{ij\sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + h.c) \quad (7)$$

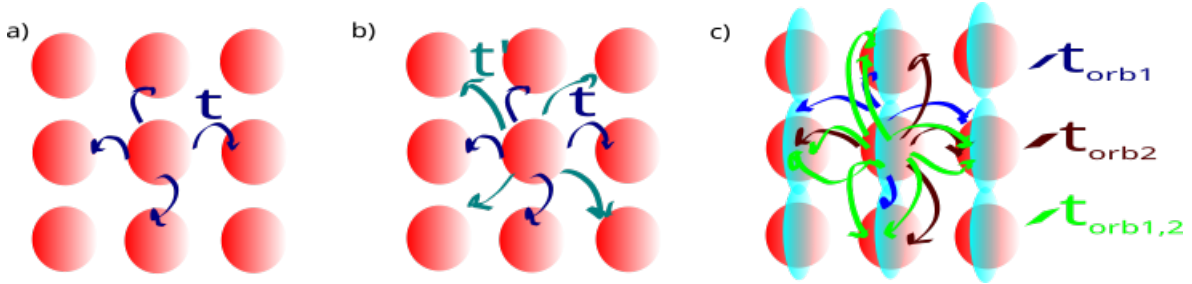


Figure 1: Two-Dimensional Tight-Binding Models: Three panels showing the tight binding models for the 1NN, 1NNN and 1NN2 models discussed in Section 5.1, 5.2 and 5.3 respectively. Panel a) shows the nearest-neighbour hopping case, where t depicts the hopping amplitude between the neighbouring sites. Panel b) shows the inclusion of the next-nearest neighbour hopping, the magnitude given by t' . Panel c) Shows the extension to the two-orbital case, depicting same orbital (t_{orb1} , t_{orb2}) and different orbital ($t_{orb1,2}$) nearest-neighbour hopping. Note that this is just a pictorial representation of the orbitals, and that it does not correspond to a particular choice of orbitals or their real space projection.

3.2.2 Hubbard Model

The tight binding model as defined above fails to account for any interactions between electrons. This motivates the extension of this model to the Hubbard model (8), which includes the (onsite) Coulomb repulsion between electrons. Despite its simple form, this model can describe very rich physical phenomena. In particular, it becomes very interesting to study when the Coulomb repulsion (U) and the nearest neighbour hopping (t) are of comparable order, since it highlights the competing phenomena that take place in correlated systems. The 2D Hubbard model is able to predict all sorts of correlated phases: it describes metals, insulators, superconductors and other exotic phases [15–18]. This model has been widely studied since it resembles the structure of the cuprate high-temperature superconductors [1].

$$\hat{H} = \sum_{ij\sigma} -t_{ij}(\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + h.c) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \quad (8)$$

3.2.3 Hubbard-Kanamori Model

In the case of materials with a multi-band and/or multi-orbital nature, the Hubbard model is not sufficient to capture all physical phenomena. This motivates the extension of the Hubbard model to the Hubbard-Kanamori model [19] by including a Hund's coupling term.

$$H_{int} = U \sum_{is} n_{i,s\uparrow} n_{i,s\downarrow} + \frac{V}{2} \sum_{i,s,t \neq s} n_{is} n_{it} - \frac{J}{2} \sum_{i,s,t \neq s} \vec{S}_{is} \cdot \vec{S}_{it} + \frac{J'}{2} \sum_{i,s,t \neq s} \sum_{\sigma} c_{is\sigma}^\dagger c_{is\bar{\sigma}}^\dagger c_{it\bar{\sigma}} c_{it\sigma} \quad (9)$$

Here, U and V represent the electronic interactions in the same and different orbitals respectively. For generality, the intraorbital exchange J and the 'pair hopping' term J' following from Hund's rule coupling have been separated. Note that this Hamiltonian is relevant for the later section of this project, where the model is extended to a two-orbital, two-dimensional Hubbard model.

3.3 Functional Renormalisation Group (FRG) theory

Solving the Hubbard-Kanamori Hamiltonian is rather challenging, which is why one resorts to numerical techniques such as FRG. FRG falls into the same category of many other weak-coupling techniques (such as Mean field-theory [20], perturbation theory [21], Density Functional theory [22] or Random Phase approximation [23]). In these theories, interactions between electrons are considered to be weak. This allows one to effectively model the electrons in the system as free particles and treat their interactions as a perturbation. In the non-interacting limit, the method is therefore exact. Beyond this limit, the method's precision is controlled by the ratio between the interaction strength and the bandwidth of the system.

In this section the theoretical framework for FRG calculations is outlined. The central element of FRG is a flow equation that describes the evolution of the effective action of the system with respect to a scalar/flow parameter Lambda (Λ) (*See section 3.3.1*). The flow equation can be solved exactly for a limited number of systems, so in most scenarios an approximation has to be made in order to reach a solution in a reasonable computational time. For the systems explored

in this project only two-particle interactions are considered and any higher order terms are neglected. This allows the separation of the effective action of the system into three terms. Each term represents one of the following three physical channels: Superconductivity, Spin-Density and Charge-Density Waves. The calculation is then performed to determine the first to diverge and hence "winning channel", this will correspond to the respective physical ground state that the model exhibits. This rather conceptual overview of FRG is represented in a flowchart below (See Fig.2).

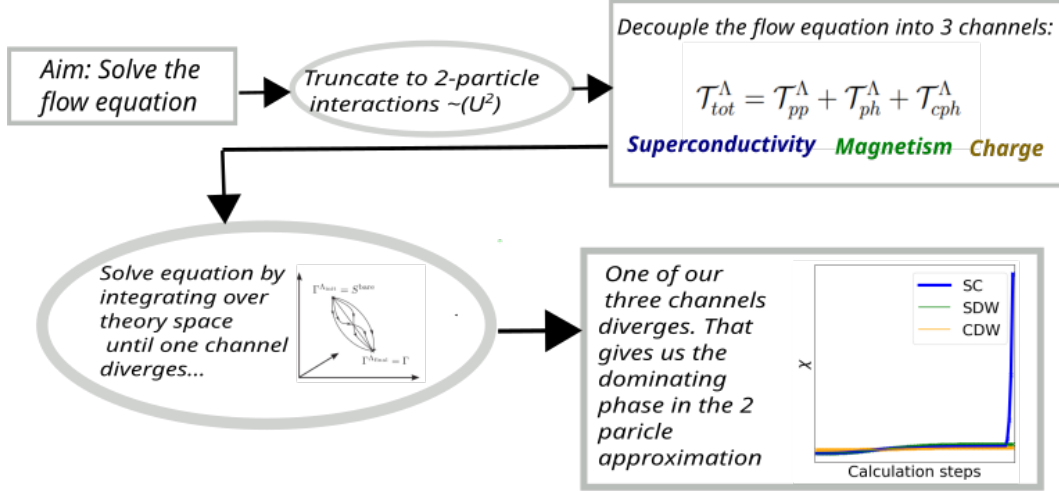


Figure 2: **FRG Flowchart:** Schematic illustration of the TU²FRG calculation process. The procedure begins by truncating the flow equation to two-particle interactions. This allows for the separation of the effective action into three distinct “physical” channels. Each channel is then computed independently, and the dominant phase is identified as the one in which the corresponding channel diverges.

3.3.1 Flow equation

In this section the derivation of the flow equation is outlined. If interested in the finer details of the derivation, the reader is referred to [24].

The central elements of statistical physics are the partition function, the canonical potential and its Legendre transformations. These are such powerful physical quantities that one can derive all physical observables from them. For quantum many-body problems, one works instead with partition functional, defined as follows in Eq.10:

$$\mathcal{Z}[\bar{\eta}, \eta] = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{\mathcal{S}[\bar{\psi}, \psi]} e^{(\bar{\eta}, \psi) + (\eta, \bar{\psi})} \quad (10)$$

In the case of fermionic systems, the action in the exponent of Eq.10 takes the form shown below.

$$\mathcal{S}[\psi, \bar{\psi}] = -(\bar{\psi}, G_0^{-1} \psi) + V[\psi, \bar{\psi}] \quad (11)$$

Here, $V[\psi, \bar{\psi}]$ is an arbitrary many-body interaction and G_0 represents the propagator of the non-interacting system. This equation contains the shorthand notation “(...)”, which represents the sum $\sum_x \bar{\psi}(x)(G_0^{-1}\psi)(x)$, $(G_0^{-1}\psi)(x) = \sum_{x'} G_0^{-1}(x, x')\psi(x')$. In this sum, the Grassman field index x encodes all the quantum numbers of the single-particle basis and imaginary time.

Note that in the limiting case where $V = 0$, the path integral in Eq.10 is exactly solvable. However, the situation becomes considerably more intricate when electronic correlations are taken into account. The main idea behind FRG is to introduce a cut-off in the non-interacting Green’s function ($G_0 \rightarrow G_0^\lambda = f(\lambda)G_0$). This cutoff is then interpolated between the solvable initial state and the full path integral solution by subsequently including electronic interactions. For a spin-independent system this would transform the bare propagator as shown in Equations (12) and (13).

$$G_0(k_0, \mathbf{k}) \rightarrow G_0^\lambda(k_0, \mathbf{k}) \quad (12)$$

$$\frac{1}{ik_0 - \xi_{\mathbf{k}}} \rightarrow \frac{\theta^{\mathbf{k}}}{ik_0 - \xi_{\mathbf{k}}} \quad (13)$$

where $\theta^\lambda(\mathbf{k})$ is defined, for example, as follows:

$$\theta^\lambda(\mathbf{k}) = \Theta(|\xi_{\mathbf{k}}| - \lambda) \quad (14)$$

With this particular choice of cutoff scheme, the calculation then excludes points close to the Fermi Surface (*See Fig.3*).

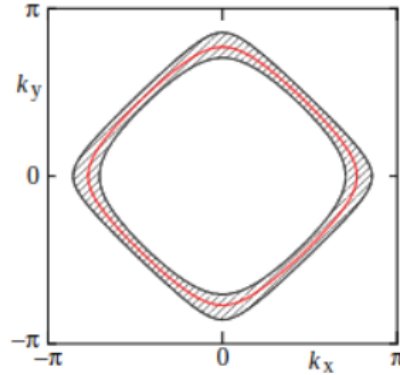


Figure 3: **Cut-off scheme example:** Momentum space region (shaded in grey) around the Fermi-surface (red) that is excluded by a momentum cut-off for a 2D square lattice. Taken from [24]

In the following steps the derivation will proceed in the framework of the so-called “effective action”² ($\mathcal{T}[\psi, \bar{\psi}]$). This is the Legendre transformation of the Greens function functional ($\mathcal{G}[\eta, \bar{\eta}]$), defined below in Equations (17) and (15, 16) respectively.

²If interested in why see Ref. [24]

$$\mathcal{G}[\eta, \bar{\eta}] = -\ln(\mathcal{Z}[\eta, \bar{\eta}]) \quad (15)$$

$$\mathcal{G}[\eta, \bar{\eta}] = -\ln \int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-\mathcal{S}[\psi, \bar{\psi}]} e^{(\bar{\eta}, \psi) + (\bar{\psi}, \eta)} \quad (16)$$

$$\mathcal{T}[\psi, \bar{\psi}] = (\bar{\eta}, \psi) + (\bar{\psi}, \eta) + \mathcal{G}[\eta, \bar{\eta}] \quad (17)$$

The next step is to introduce a scalar flow parameter (λ) into the generating functionals defined above. This is done in the same manner as outlined in the example shown in Equations 12 & 13. But, more generally, this has to be performed such that the generators recover their original structure at $\lambda = 0$. After a series of algebraic manipulations, which are omitted here but can be found in [24], one arrives at the exact functional flow equation for the effective action:

$$\frac{d}{d\Lambda} \mathcal{T}^\Lambda[\psi, \bar{\psi}] = (\bar{\psi}, \dot{Q}_0^\Lambda \psi) - \frac{1}{2} \text{tr}(\dot{Q}_0^\Lambda (\Gamma^{(2)\Lambda}[\psi, \bar{\psi}])^{-1}). \quad (18)$$

Where $\Gamma^{(2)\lambda}[\psi, \bar{\psi}]$ and \mathbf{Q}_0^Λ are given by equations (19) and (20) respectively.

$$\Gamma^{(2)\lambda}[\psi, \bar{\psi}] = \begin{bmatrix} \bar{\delta}\delta\Gamma[\psi, \bar{\psi}](x', x) & \bar{\delta}\bar{\delta}\Gamma[\psi, \bar{\psi}](x', x) \\ \delta\delta\Gamma[\psi, \bar{\psi}](x', x) & \delta\bar{\delta}\Gamma[\psi, \bar{\psi}](x', x) \end{bmatrix} \quad (19)$$

$$\mathbf{Q}_0^\Lambda = \begin{bmatrix} Q_0^\Lambda & 0 \\ 0 & -Q_0^{\Lambda t} \end{bmatrix} = \text{diag}(Q_0^\Lambda, -Q_0^{\Lambda t}), \quad (20)$$

This flow equation is the central element of FRG and the sections below outline how to solve it.

3.3.2 Truncation scheme (TU²FRG)

The flow equation derived above can be solved exactly only for a small class of systems; for most models, Functional Renormalisation Group (FRG) calculations are highly computationally expensive. In order to tackle this issue, the truncated unity approximation (TU²FRG) was introduced in 2017 [25] and later improved in 2020 [8]. The main idea behind this scheme is to find a new basis that, with a controlled loss of accuracy, can represent all required elements in a compressed way. It can be shown that such a basis can be constructed and is well-defined in the case where the calculation is constrained to terms in the order of U^2 (*two-particle interactions*) [26]. Partitions of unity³ are then introduced into a specific part of the flow equation. This reduces an otherwise computationally expensive nested integral to a matrix product.

Whilst the truncated scheme presents advantages in computational efficiency, particularly for lattice models with broken translational symmetry, it also has its limitations. TU²FRG relies on short-range interactions, thus struggling to capture strongly correlated phases. This is particularly relevant for the study of the 2D Hubbard model. TU²FRG will not be able to capture the characteristic Mott insulating phase of the Cuprate phase diagrams [27], which limits how well the results presented in this project can be directly compared with existing literature. More

³These can be essentially regarded as delta functions in momentum and real space. Their exact form can be found in [26].

importantly, the truncation scheme has a direct consequence on the accuracy of the predicted phase transition temperature (T_c). Whilst it is able to correctly capture the trends in T_c , the values predicted are much higher than what is reasonable to expect in real materials. Nevertheless, TU²FRG successfully captures the competition between magnetic and superconducting instabilities, a central focus of the results presented in this project.

3.3.3 Decoupling of flow equation

After constraining ourselves to the case of two-particle interactions in the framework of translationally invariant systems, one can decouple the two-particle coupling as a function of the flow parameter (λ) into three channels:

$$V(k_1, k_2, k_3, k_4) = V_{k_1, k_2, k_3, k_4}^{(0)} - \phi_{k_1+k_2, \frac{k_1-k_2}{2}, \frac{k_4-k_3}{2}}^P + \phi_{k_1-k_3, \frac{k_1+k_3}{2}, \frac{k_2+k_4}{2}}^C + \phi_{k_3-k_2, \frac{k_1+k_4}{2}, \frac{k_2+k_3}{2}}^D \quad (21)$$

Here, the three channels correspond to a particle-particle, crossed particle-hole and (three) direct particle-hole terms. These are strongly related to their respective effective actions (22-24). They represent all possible ways in which two particle can interact in the correlated system. The particle-particle (P), cross-particle-hole (C) and direct-particle-hole (D) channels correspond to the Superconducting, Charge and Magnetic phases respectively.

$$\dot{\phi}_{k_1+k_2, \frac{k_1-k_2}{2}, \frac{k_4-k_3}{2}}^P = -\mathcal{T}_{pp}(k_1, k_2, k_3) \quad (22)$$

$$\dot{\phi}_{k_1-k_3, \frac{k_1+k_3}{2}, \frac{k_2+k_4}{2}}^C = -\mathcal{T}_{cr-ph}(k_1, k_2, k_3) \quad (23)$$

$$\dot{\phi}_{k_3-k_2, \frac{k_1+k_4}{2}, \frac{k_2+k_3}{2}}^D = -\mathcal{T}_{d-ph}(k_1, k_2, k_3) \quad (24)$$

The decoupling outlined above enables the treatment of the effective action as a separable object:

$$\mathcal{T}[\psi, \bar{\psi}] = \mathcal{T}_{pp}[\psi, \bar{\psi}] + \mathcal{T}_{ph}[\psi, \bar{\psi}] + \mathcal{T}_{cph}[\psi, \bar{\psi}] \quad (25)$$

3.3.4 Instability calculation

This section provides an outline of the procedure following the decoupling the effective action and flow equation, for more details the reader is referred to [28]. In the TU²FRG method, the resulting decoupled flow equation is solved through nested integration, involving both a coarse momentum integration and a refined integration around each k point. This calculation yields the self-energy and the two particle vertex⁴. Although these quantities are not directly measurable, they serve as the foundation for further analysis. The first post-processing step involves identifying which of the three interaction channels diverges, revealing the leading susceptibility. Mean-field analysis [29] is then performed at the critical scale in order to determine the ordering symmetry and derive a

⁴For precise definitions of these quantities, see [24].

linearized gap equation for the superconducting channel⁵ (*See equation 26*) [28]. From this one can compute the superconducting gap and order parameter.

$$\Delta = aF(GG)|_{\Delta=0}\Delta \quad (26)$$

4 Computational Methods

After having discussed the required theoretical background, the implementation of the necessary concepts within the framework of this project is now addressed. The primary goal is to obtain a computational solution for the 2D Hubbard-(Kanamori) model, utilizing the divERGE package. This package implements the TU²FRG formalism discussed in Section 3.3.2. All calculations are conducted within the framework of spin-fluctuation mediated superconductivity (*see Section 3.1.1*), focusing solely on electronic interactions and neglecting other instabilities, such as lattice instabilities (e.g. charge density waves or phonon-mediated superconductivity). This section provides an overview of the divERGE package, together with the convergence tests required to ensure the accuracy of the results.

4.1 divERGE

divERGE is an open-source, high-performance, C/C++/Python library that includes a truncated unity FRG (TU²FRG) computational backend [30]. At the core of the truncated-unity calculation is a model that incorporates all the essential physical parameters. This model must accurately reflect the system’s kinematics, based on its real-space hopping parameters. It is equally important to define structural details such as the Bravais lattice vectors, the number of atoms per unit cell, and the number of orbitals per atom. Once the model is established, six input parameters must be specified for the calculation to proceed: the strengths of the Coulomb repulsion (U) and Hund’s coupling (J), the value of the chemical potential (μ), as well as the form factor cut-off, n_k and n_{k_f} values. (*The latter three terms are depicted in Fig.4 and discussed in more detail in Section 4.2*).

With the model constructed and all necessary parameters defined, the calculation can proceed. Under the approximations described in Section 3.3.2, the flow equations are integrated numerically from high energy scales ($\lambda = \infty$) down to low scales ($\lambda = 0$), by incrementally stepping from λ to $\lambda + d\lambda$. This integration continues until a phase transition is detected-signaled by the divergence of one of the interaction channels-or until a minimum value of λ is reached. In the latter case, the system is considered to remain in a Fermi-liquid state. All such computations were performed on the high-performance computing (HPC) cluster at the University of St Andrews.

4.2 Convergence of Calculation

In the truncated-unity approximation, several convergence tests must be performed to ensure that calculations are accurate. These tests include checking the form factor convergence and the

⁵The equation here is expressed in terms of the Greens functional G and vertex function F . Note that this form of linearised gap equation is valid for a small gap magnitude.

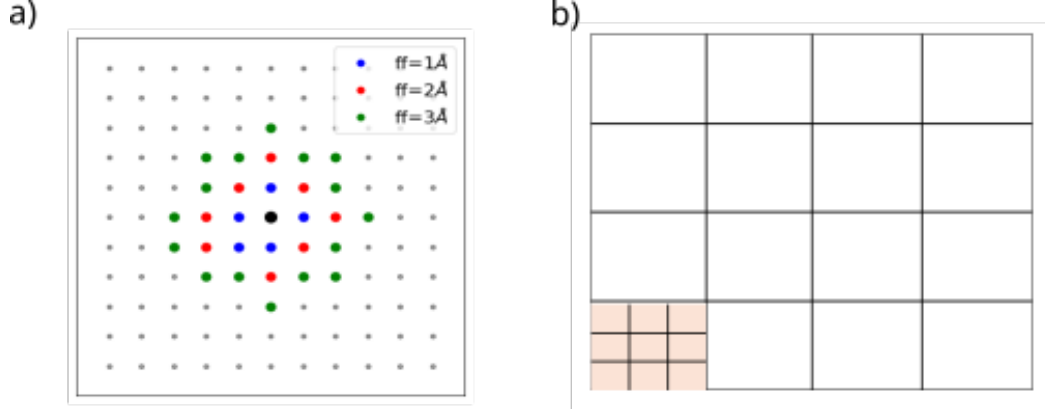


Figure 4: **Pictorial depictions of the form factor-cutoff, n_k and n_{k_f} :** *Panel a)* Form factor cut-off for a 2D square lattice. Increasing the form factor cut-off from 1-3Å increases the number of additional bonds that are included in a calculation for a given site. *Panel b)* A 3x4 $n_k \times n_{k_f}$ integration grid. n_k represents the number of k points used for the general momentum integral. In turn, n_{k_f} represents the number of k points for an additional momentum integral around each point. The outer loop is a 3x3 grid, which refined by a factor of 4 becomes a 12x12 grid.

number of k points.

4.2.1 Form factor convergence

The set of orthogonal basis functions (f_m) used to describe the truncated space (*See section 3.3.2*) in momentum representation is called the form factor basis [26]. In the case of the square lattice, the form factors take the form of delta functions in real space; they are arranged as circles with increasing radii around the origin. This effectively leads to a “bond-like” representation where the form-factor cut-off represents how many of the neighbouring bonds are accounted for in the calculation of each point in the phase diagram (*See Fig.4a*).

The divERGE package allows the user to modify the form-factor cutoff accordingly. Choosing appropriate values ultimately comes down to a trade-off between computational accuracy and expensiveness. For the results in this project, the form factor value was set at 4Å⁶ after the convergence of the calculations was tested accordingly for a range of points in the phase diagram (*an example of such tests is shown in Fig.5*). Moreover, this value is in agreement with values used in previous literature [26].

4.2.2 Convergence with number of k points

When integrating the flow equation, there are two parameters that can be further tuned to ensure convergence. These are the n_k and n_{k_f} values and they specify the number of k points used to carry out the nested integration of the decoupled flow equation. In particular, n_k refers to the number of k points used for the general momentum integral, and n_{k_f} to the number of k points

⁶This is equivalent to a number of form factor shells of 4 since the lattice spacing of the models here is set to 1Å.

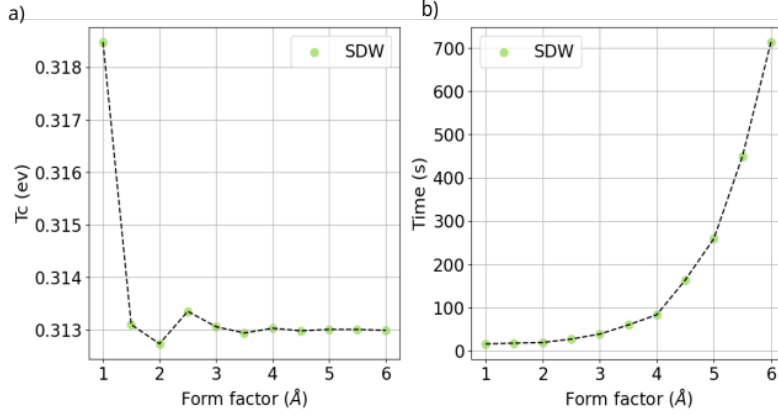


Figure 5: **Convergence testing:** Fig a) Transition temperature as a function of form factor for the nearest-neighbour 2D Hubbard model, $U = 5.00$, $\mu = 0.20\text{eV}$. Fig b) Time taken to complete the calculation as a function of form factor.

used for the additional sum around each k-point *See Fig.4b*. The calculations performed here were carried out with an integration grid of 20×5 ($n_k \times n_{k_f}$) points. The choice of parameters ensured that the calculations had converged appropriately and resulted in an average computational time of $\approx 180\text{s}$ per point for the simpler models⁷.

5 Results and discussion

The results of this thesis are discussed in three sections, each focusing on one of the models outlined in Fig. 1. These subsections explore the interaction between magnetism and superconductivity, highlighting trends in the superconducting order parameter and spin density wave nesting vectors. The effect of varying factors such as Coulomb repulsion, chemical potential, Hund's coupling, next-nearest-neighbor hopping, and the number of orbitals per site on the critical temperature of the superconducting regions is also examined.

5.1 Nearest-neighbour 2D Hubbard Model on a square lattice (1NN)

The 1NN model is defined as the 2D Hubbard model with a single orbital per site, allowing hopping between nearest-neighbour sites (*a diagrammatic representation can be found in Fig.1.a*). As discussed in Section 3.2.2, solving this model near half-filling presents significant challenges. This section investigates the solution to the 1NN Model Hamiltonian using two-particle interaction-truncated FRG. A phase diagram, plotted in terms of the on-site Coulomb repulsion U and chemical potential μ is presented and analyzed in detail. The calculations were performed using a 20×5 $n_k \times n_{k_f}$ grid and a form factor of 4\AA , with a nearest-neighbor hopping parameter of 1eV . These convergence parameters were selected based on the methods outlined in Section 4.2. The results cover Coulomb repulsion values ranging from 1 to 20 eV and chemical potential values spanning the full energy bandwidth of the model (from -4 eV to 4 eV). While previous FRG

⁷Note that the computational time increases as a function of Coulomb repulsion U .

studies on the 2D Hubbard model exist [31–33], they mostly focus on specific regions of the phase diagram. As a result, there has been limited investigation into the effects of varying the on-site Coulomb repulsion. The present work explores a much broader range of parameters than what has been previously studied.

There are several caveats to the results presented here. In real materials, the chemical potential is an easily tuneable parameter due to its strong connection to the electronic doping of the system. In turn, controlling the magnitude of the Coulomb repulsion between electrons is far from straightforward. Additionally, some of the interesting features discussed in this report fall outside the physical regime—specifically, the FRG calculation assumes a weak-coupling limit, meaning that any Coulomb repulsion values exceeding the bandwidth of the material (8 eV) are unphysical in this context. Therefore, the analysis conducted in this project should not be interpreted as a guide to enhance superconductivity in materials that closely resemble the models studied. Instead, the primary goal is to understand how variations in certain parameters (U , μ , t') influence the correlated phases observed in the model. It is also important to note, as discussed in Section 3.3.2, that any analysis of the superconducting transition temperature should be treated qualitatively. At no point does this work claim to have identified superconducting regions with transition temperatures of the order of thousands of Kelvin.

The complete phase diagram for the values discussed above is shown in Fig.6. As is expected for both the Hubbard model and the Cuprates [34–36], a pronounced competition between Magnetism and Superconductivity (SC) is observed. This interplay gives rise to a prominent magnetic dome, sandwiched between two narrower d-wave superconducting regions. This magnetic dome is anti-ferromagnetically (AFM) ordered and its width increases with increasing Coulomb repulsion. In other words, a stronger Coulomb repulsion favours the magnetic instability as the "winner" of this magnetism/SC competition for a larger range of doping values. Both AFM and d-wave SC arise from repulsive scattering between $(\pi, 0)$ and $(0, \pi)$ vectors. Therefore, their competition peaks closest to the Van-Hove singularity, where both instabilities are amplified and mutually reinforced [37,38]. Additionally, narrow magnetic stripes emerge at even-integer chemical potential values. At high values of U —those that exceed the material’s bandwidth—patches of a charge density wave (CDW) instability appear around regions of the superconducting dome.

The results presented here align with previous studies of the two-dimensional Hubbard model. Dynamical Mean Field Theory (DMFT) has previously captured the coexistence of antiferromagnetic (AFM) and superconducting (SC) order parameters within the same solution across a range of doping levels (analogous to variations in μ in this work) in the weak-coupling regime. A smooth transition between these two phases has also been reported [39]. However, the FRG treatment of the 2D 1NN Hubbard model has not been able to capture certain key features of the cuprate phase diagram—namely, the Mott insulating phase and the emergence of the pseudogap that have been found in other studies of the 2D Hubbard model [40,41].

5.1.1 Superconductivity in the 1NN Model

Recent findings have claimed that the 2D Hubbard model does not have a superconducting ground state [42]. Whilst the model in Ref. [42] is the same as the 1NN model explored in this section, the paper’s analysis is conducted in a slightly different framework than the one

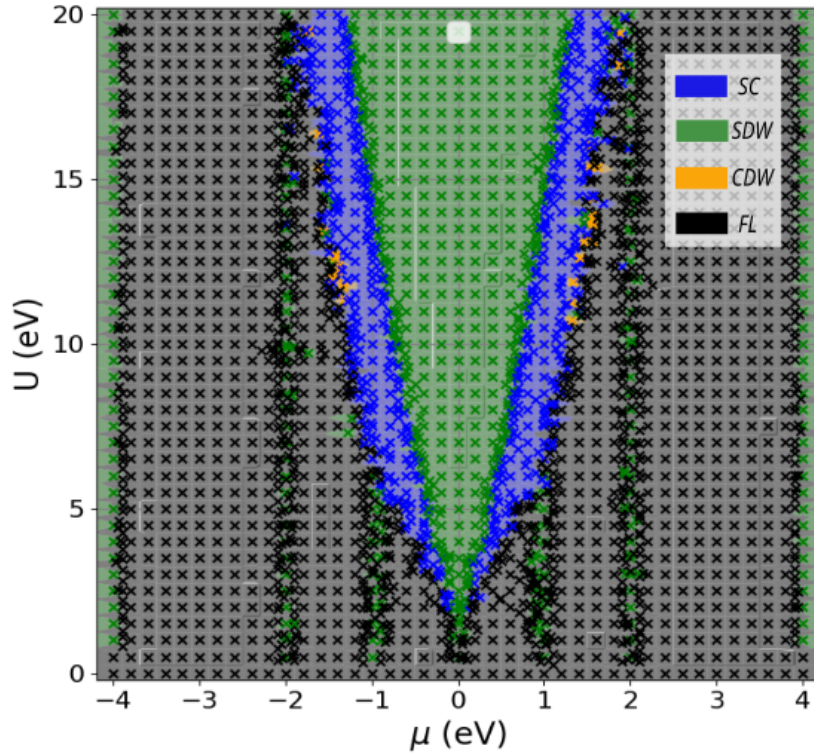


Figure 6: **Phase diagram for the 1NN model:** ($t = 1\text{eV}$, $n_k \times n_k = 20 \times 5$, $ff = 4\text{\AA}$) as a function of On-site Coulomb Repulsion U and chemical potential μ . Figure shows the four phases observed in the 1NN model: SC (Superconductivity), SDW (Spin-Density Wave), CDW (Charge Density Wave) and FL (Fermi-Liquid). Calculated points in the phase diagram are showed by the 'x' markers and a lighter-coloured background is used to depict interpolated regions between these points.

used in this project: using DMRG [43] at moderate-to-strong coupling and for values of U between 6-8eV (*which the paper claims to be the regime relevant to the cuprates*). The lack of superconductivity in their findings is attributed to a lack of competition between the magnetic and superconducting phases. Here, in the weak-coupling framework, both competition between magnetism and superconductivity and a stabilised superconducting region is found. The superconducting order parameter in this stable region is plotted on top of the Fermi-Surface for the first BZ (Fig.7a). The order parameter shows antisymmetry with respect to a 90 degree rotation and therefore one concludes that the bulk superconducting region is d-wave symmetric. This is in agreement with what is expected from the Cuprate superconductors [44].

After plotting the critical temperature (T_c) as a function of chemical potential (μ) for a constant Coulomb repulsion (U), one observes that the superconducting critical temperature is maximised closest to the magnetic instability (Fig.7b). This is in agreement with the idea that competition between instabilities enhance the phase transition temperature [45,46]. Moreover, the magnitude of the Coulomb repulsion and T_c are positively correlated, as is to be expected from the assumed of the pairing mechanism (*See Eq.3*). It is important to note that limiting the interactions accounted for in the FRG calculation to two-particle interactions acts as a bottle-neck for the accuracy of the T_c values calculated. Nevertheless, the trends in T_c remain trustworthy.

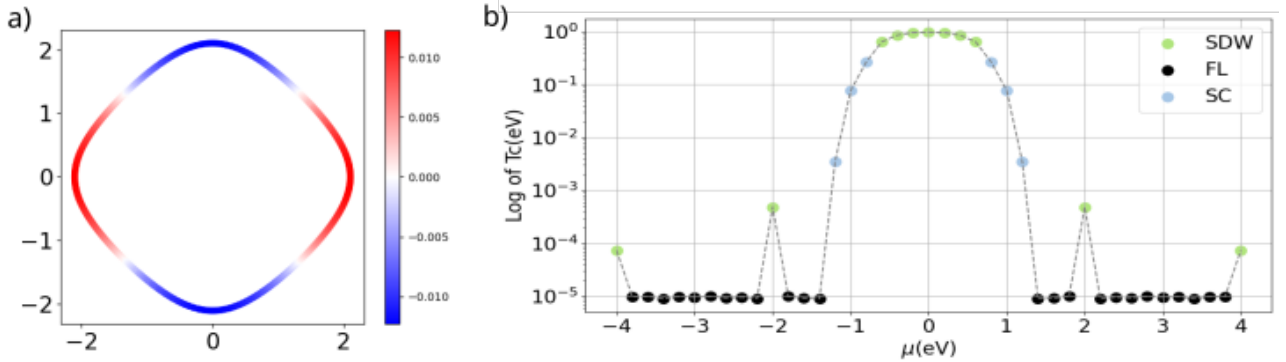


Figure 7: **Superconductivity in the 1NN model:** Fig a) Superconducting order parameter projected on Fermi Surface at $\mu = 1.00$ eV, for $U = 10.00$ eV. The order parameter is antisymmetric about a 90 degree rotation and hence it exhibits d-wave symmetry. Fig b) Transition temperature (T_c) plotted on a logarithmic scale as a function of chemical potential (μ) for $U = 10.00$ eV, showing a smooth transition between SC and SDW regions. T_c is enhanced closest to the magnetic instability. Although both plots are shown only specific for certain values of U and μ , the results they display hold for the entirety of the superconducting region of the phase diagram in Fig.6.

5.1.2 Magnetic stripes in the 1NN Model

Another distinctive feature of the Cuprates (*as well as of other unconventional superconductors* [47]) is the emergence of "stripes" in their phase diagram. These are patterns of alternating charge-density and spin density waves [48,49]. In the 1NN model discussed here, these patterns are not observed. However, magnetic regions of interest are found outside the main antiferromagnetic (AFM) dome. The 1NN phase diagram in Fig.6 reveals what will henceforth be referred

to as "magnetic stripes" occurring at even integer values of the chemical potential (μ). Most of them are ferromagnetically ordered and evolve to some commensurate nesting vector as the Coulomb repulsion is increased.

The physics becomes particularly interesting at a chemical potential of $\mu = 1.00\text{eV}$. In Cuprates, a doping of $\frac{1}{8}$ th is known as "the magical doping" [50], where stripes emerge and superconductivity is suppressed. In this model, the magical doping corresponds to a chemical potential of $\pm 1.00\text{eV}$ (which is $\frac{1}{8}$ th of the bandwidth). At low Coulomb repulsion values, a ferromagnetically ordered spin density wave (SDW) is observed. This SDW is suppressed by a superconducting phase, only to be revived at around $U \approx 15.00\text{eV}$, where it becomes antiferromagnetically ordered. The superconducting transition temperature T_c increases along the stripe (*See Fig.8*). While this behaviour is not the same as the conventional stripes seen in cuprates, it is fair to conclude that there is still something "magical" about the $\frac{1}{8}$ filling fraction in the 1NN model presented here.

It is worth noting that before conducting this analysis, the possibility of the stripes being a computational artifact was ruled out. This was done by increasing the $n_k \times n_{k_f}$ resolution for a single point in the stripe and confirming that the result remained unchanged. The appearance of these stripes as true outcomes of the calculations is further validated in Section 5.2.2.

5.2 Effect of next-nearest neighbour hopping (1NNN model)

The 1NNN model is an extension of the 1NN model described in previous sections, incorporating the next-nearest neighbour hopping amplitude as an additional free parameter. This section presents three additional phase diagrams for the two-dimensional Hubbard model, with next-nearest neighbour hopping amplitudes of 0.25, 0.50 and 0.75 eV (*See Fig.9*). The nearest neighbour hopping amplitude remains fixed at 1eV for all models. Furthermore, the chemical potential of the models is adjusted to ensure a constant number of electrons at half-filling, to allow for a direct comparison between the models.

As the next-nearest neighbour hopping is increased, the position of the Van-Hove singularity shifts to lower energies (*See Fig.9a*). This increase in t' also alters the Fermi-surface, which in turn changes the nesting vectors of the models. As a result of both these effects, the SC-SDW-SC sandwich region shifts toward the negative chemical potential regime as t' increases. The superconducting regions remain (in the most-part) d-wave symmetric and the emergence of magnetic stripes remains observable. Additionally, general trends in the superconducting transition temperature (T_c) are also observed: it is maximised closest to the magnetic instability and it increases as a function of U .

Several studies have explored the effect of t' in the 2D Hubbard model, employing both FRG [51] and other alternative methods [52], with a particular focus on using t' as a means to enhance T_c . The results presented here take a slightly different approach, aiming to compare the features of the 1NN and 1NNN phase diagrams.

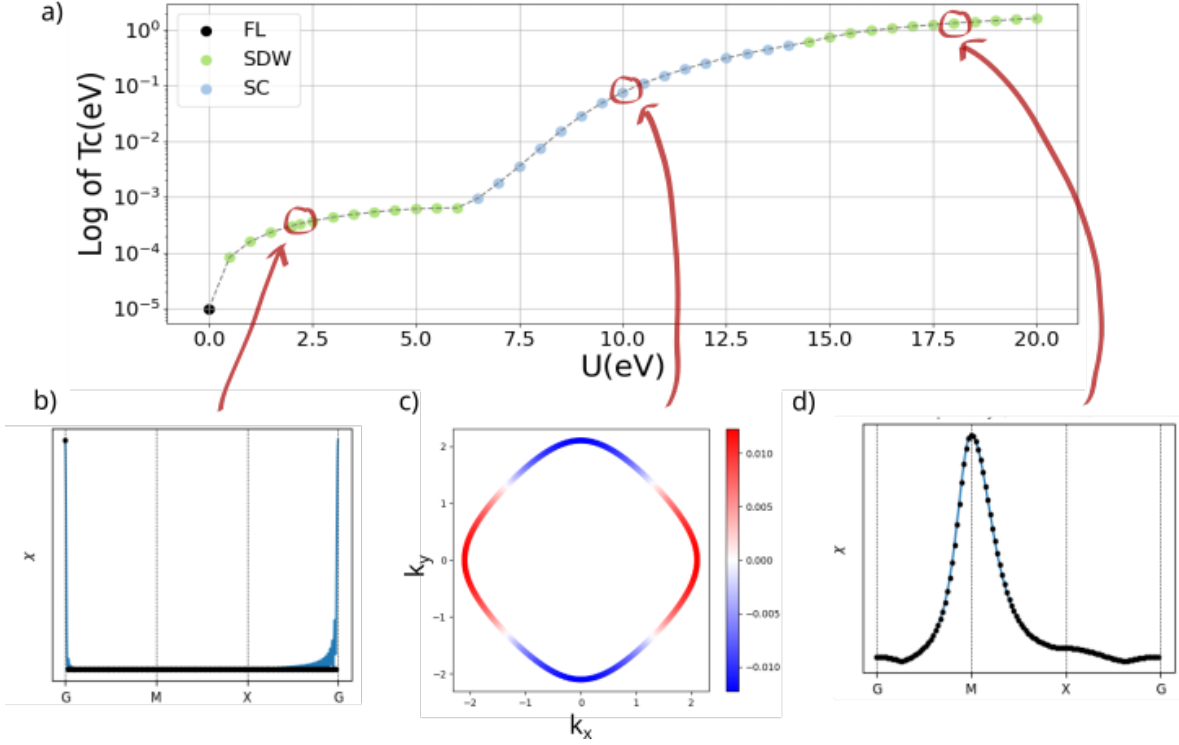


Figure 8: **Magnetic stripe in the 1NN model for doping at $\frac{1}{8}$ of the bandwidth:** Fig a) Transition temperature plotted in a Logarithmic scale as a function of Coulomb repulsion (U) along the Magnetic stripe at $\mu = 1\text{eV}$. Fig b) Magnetic susceptibility along high symmetry path for $U = 2.00\text{ eV}$. Fig c) Plot of the Superconducting order parameter projected on top of the Fermi-surface of the 1NN model for $U = 10.00\text{eV}$ and $\mu = 1.00\text{eV}$. Fig d) Magnetic susceptibility along high symmetry path for $U = 18.00\text{eV}$. The plots show the susceptibility as a function of q for both magnetic regions. The Ferromagnetic SDW is suppressed by a superconducting phase at $U \approx 6.00\text{eV}$. At larger values of U , the SDW phase is recovered but with an Anti-Ferromagnetic ordering instead.

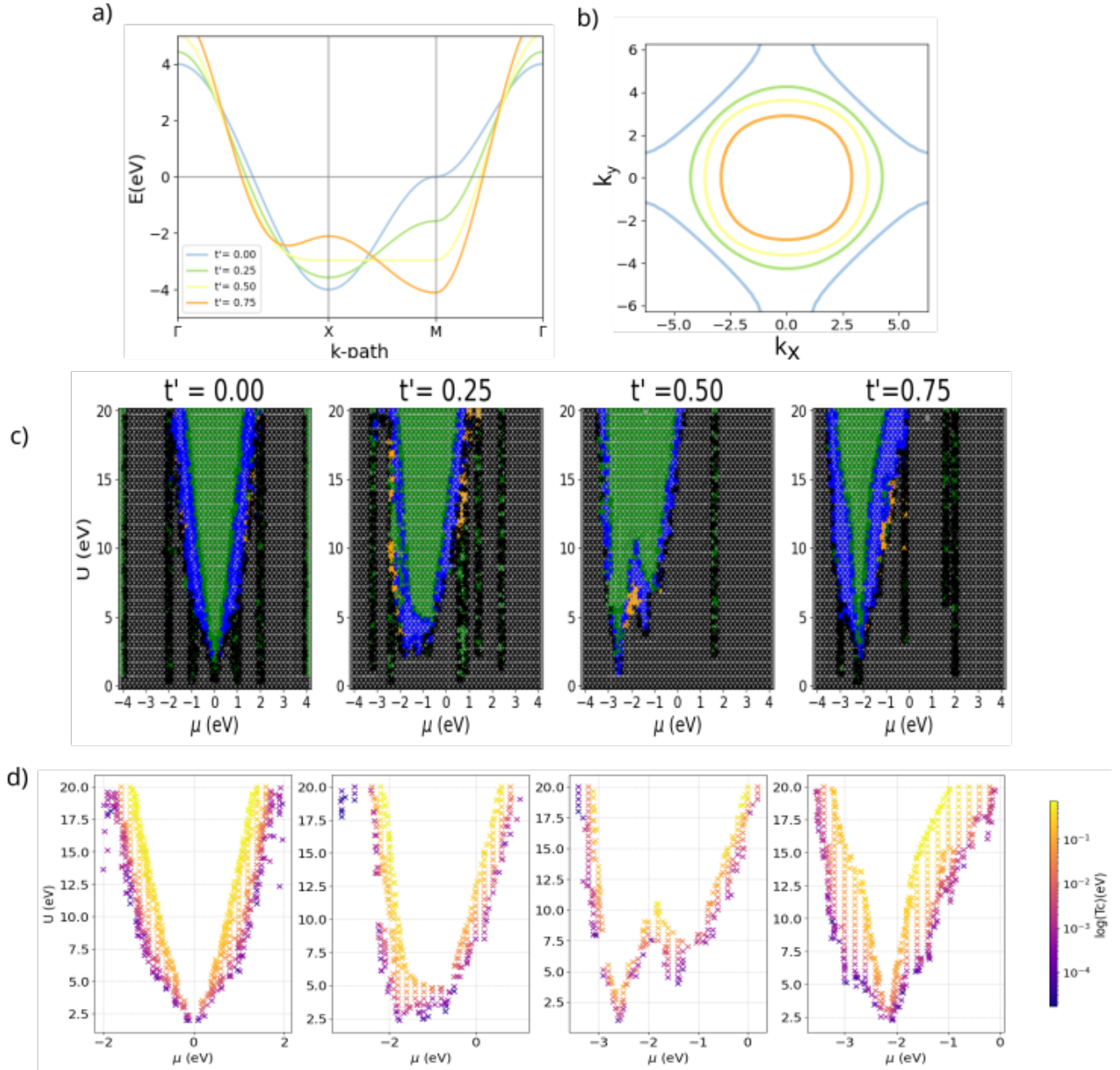


Figure 9: **1NNN model:** a) Single plot of the band structure along high-symmetry path for corresponding values of t' . b) Single plot of the Fermi surface for all values of t' considered. c) Phase diagram for the 1NNN model as a function of Coulomb repulsion U and chemical potential μ ($t = 1\text{eV}$, $n_{kx}n_{ky} = 20 \times 5$, $ff = 4\text{\AA}$) for $t' = 0.00, 0.25, 0.50, 0.75$ eV. d) Transition temperature for the superconducting region (plotted in a logarithmic scale).

5.2.1 Superconductivity in the 1NNN Model

Including a next-nearest neighbour hopping parameter in the 1NN model does not lead to many significant changes in the superconducting properties of the model. The order parameter is predominantly d-wave symmetric and the superconducting temperature (T_c) increases with Coulomb repulsion. Proximity to a Magnetic instability further enhances T_c . Additionally, the same SC-SDW-SC sandwich structure is observed even after breaking particle-hole symmetry, reinforcing the idea that that superconductivity is favoured in the vicinity of a spin density wave (SDW) instability.

While most key features remain unchanged, there is an important difference between the superconducting regions in the 1NN and 1NNN model. When $t' \neq 0$, charge density wave (CDW) patches appear neighbouring some superconducting regions. Specifically, when $\frac{t'}{t} = 0.75$, and for Coulomb repulsion between 8 and 11eV, the superconducting order parameter undergoes a change. Along these horizontal cuts there is a SCI-SDW-SCII-CDW transition. The Superconducting order parameter is always d-wave symmetric in the SCI region and for most of the SCII region, but it abruptly transitions to s-wave symmetric in the vicinity of the CDW region (*See Fig.10*). This behaviour is also observed in the SC regions that neighbour CDW regions for the $t' = 0.25, 0.50eV$ models. To confirm whether this represents a physical phase transition, one would expect to experimentally observe a discontinuity as a result of an additional symmetry breaking when the order parameter shifts from s-wave to d-wave symmetry.

5.2.2 Magnetic stripes in the 1NNN model

The presence of magnetic stripes is another common feature shared by the 1NN and 1NNN models, further supporting its physical origin. A summary of all the stripes and their respective nesting vectors is provided in Table. The locations of these stripes suggest that their formation is a consequence of strong nesting at specific chemical potential values. Notably, the stripe at "magic doping" is the only to undergo a change ordering from ferromagnetic (FM) to antiferromagnetic (AFM) as a result of the strong competition with Superconductivity.

While the transition from a Fermi liquid phase to any of the superconducting (SC), spin density wave (SDW), or charge density wave (CDW) phases is quite abrupt, the critical temperature evolves more smoothly for stripes where there is a strong competition between SC and SDW/CDW instabilities (*see Fig.11*). This is consistent with the discussion in Section 5.1.2. When $\frac{t'}{t} = 0.50$, a magnetic double dome emerges, becoming more pronounced as the Coulomb repulsion increases (*see Fig.12*). This is the pattern one might expect in the superconducting region, as observed in cuprates [53]. However, this trend is only observed in this particular model and phase.

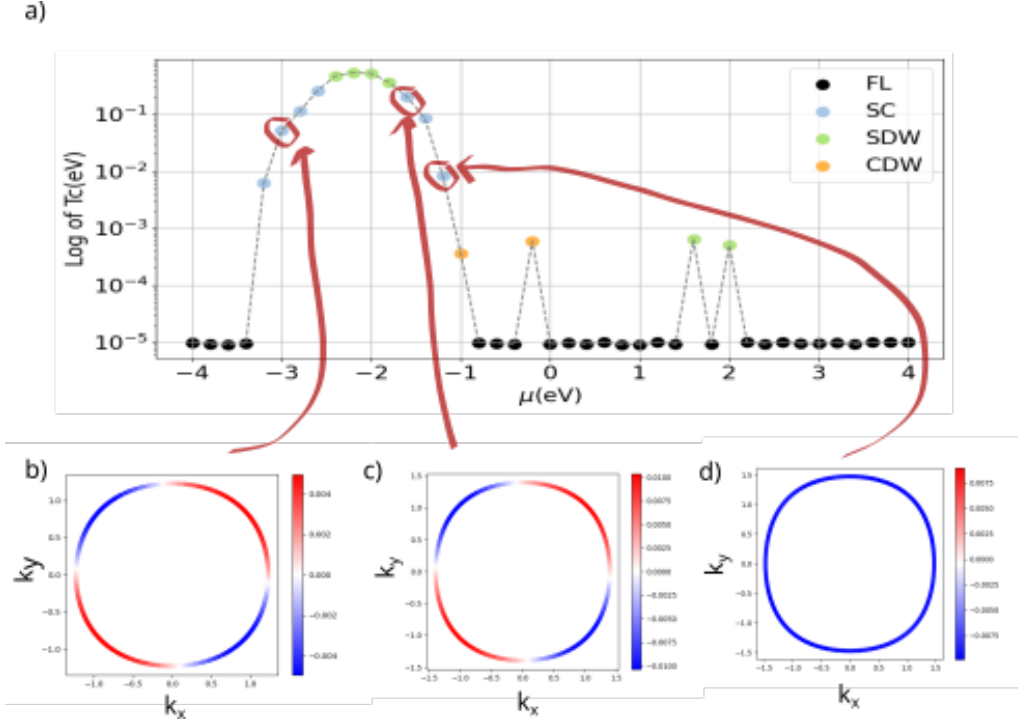


Figure 10: **Change in the superconducting order parameter in the $t' = 0.75$ eV 1NNN model:** Fig a) Critical temperature plotted in a Logarithmic scale as a function of chemical potential μ for $U = 11.50$ eV. The lower panel shows the magnitude of the superconducting order parameter plotted on top of the Fermi surface for $U = 11.50$ eV and $\mu = -3.0$ eV, -1.6 eV and -1.2 eV. These are shown in Figs b) c) and d) respectively.

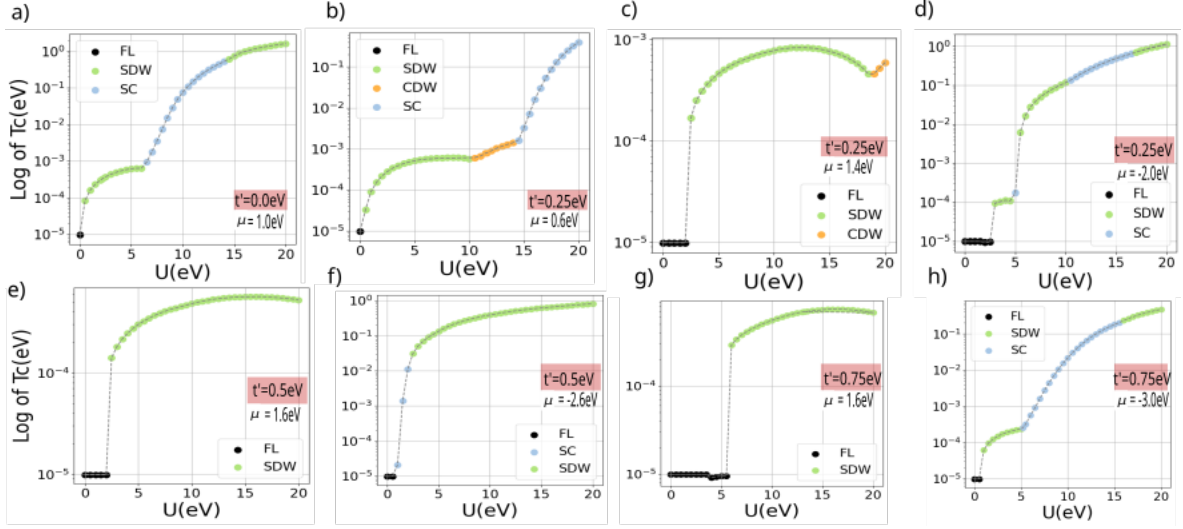


Figure 11: T_c as a function of Coulomb repulsion for a selection of stripes in the **1NNN model**: T_c plotted in a logarithmic scale for stripes at: Fig a) $t' = 0.00\text{eV}$, $\mu = 1.00\text{eV}$, b) $t' = 0.25\text{eV}$, $\mu = 0.60\text{eV}$, c) $t' = 0.25\text{eV}$, $\mu = 1.40\text{eV}$, d) $t' = 0.25\text{eV}$, $\mu = -2.00\text{eV}$, e) $t' = 0.50\text{eV}$, $\mu = 1.60\text{eV}$, f) $t' = 0.50\text{eV}$, $\mu = -2.60\text{eV}$, g) $t' = 0.75\text{eV}$, $\mu = 1.60\text{eV}$, h) $t' = 0.75\text{eV}$, $\mu = -3.00\text{eV}$. Showing abrupt jumps in the critical temperature in FL-(SC,SDW,CDW) phases and a smoother evolution for any SC-SDW/CDW transitions.

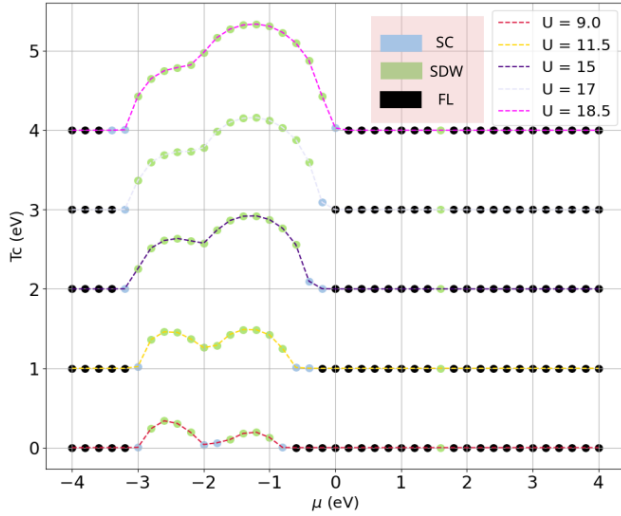


Figure 12: **Magnetic Dome in 1NNN, $t' = 0.50\text{eV}$ model**: T_c as a function of μ for different values of U (offsetted by 1eV). This figure shows how the height of the second magnetic dome increases as a function of U whilst the height of the first remains constant. The turning point of the double dome pattern occurs at $\mu = -2.00\text{eV}$

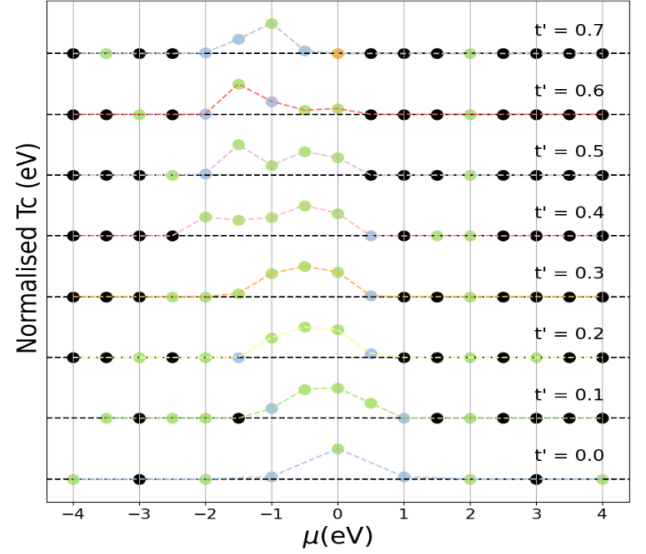


Figure 13: **Continuous variation of t'** : Normalised T_c plotted as a function of chemical potential μ for several values of t' . T_c is normalised separately with respect to the maxima of each plot in order to allow for the clear visualization of the trend as μ is varied.

5.2.3 Continuous variation of next-nearest neighbour hopping

In order to further support the ideas discussed in Section 5.1, the critical temperature is plotted as a function of chemical potential μ for different values of t' at $U=10.00\text{eV}$ (*See Fig.13*). The magnetic region is pushed towards more negative values of the chemical potential as the value of the next-nearest neighbour hopping parameter is increased (and the van Hove singularity is pushed down in energy). The bulk magnetic region remains anti-ferromagnetically ordered and the SC order parameter is predominantly d-wave symmetric. The exception occurs when t' is set to 0.70eV . There, the SC order parameter transitions to s-wave symmetric when it is closest to the boundary with the charge density wave (CDW) phase (*as discussed in Section 5.2.1*).

5.3 Effect of bi-orbital system (1NN2 model)

This project investigates three models: the 1NN, 1NNN and 1NN2 model (*See Fig.1*). For the first two, the hopping parameters in the tight-binding model are treated as free parameters. For the latter, the hopping parameters are determined using the method described below.

Constrained to the case of a single layer, the 1NN model is extended to a multi-orbital system by including two-orbitals per site and investigating the effect of the interorbital hopping. To allow for future comparison with existing literature [54], a choice of $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ orbitals is made. The respective hopping parameters are determined using the table of interatomic matrix elements calculated by J.C. Slater and G.F. Koster [55]. In this calculation, the magnitudes of the σ, π, δ bond strength are approximated to $\approx 1, 0.5, 0.05\text{eV}$ respectively in order to capture their relative values [56–58]. A table summarising the estimated parameters for the models discussed in Section is shown below.

Model	$t_{3z^2-r^2}^{[1,0,0]}$	$t_{3z^2-r^2}^{[0,1,0]}$	$t_{x^2-y^2}$	$t_{x^2-y^2-3z^2-r^2}^{[1,0,0]}$	$t_{x^2-y^2-3z^2-r^2}^{[0,1,0]}$
	-0.781	-0.719	-0.375	-0.402	-0.310
1NN2MN	on	on	on	off	off
1NN2MY	on	on	on	on	on

Table 1: **Nearest neighbour hopping parameters for 2D two-orbital Hubbard models.** First row shows the calculated hopping parameters. These are labelled by a lower and upper index representing the orbital and the direction of hopping respectively. Other rows in the table show which hopping parameters were included in each of the two models from Section 5.3.

The models presented so far were constructed assuming a single orbital per site. This section discusses the effect of incorporating two orbitals per site. The model was calculated using the parameters discussed in Section and with the inclusion of multiple orbitals per site, the Hamiltonian is extended to the Hubbard-Kanamori form (*See Section 3.2.3*). The chemical potential is fixed at both the undoped ($\mu = 0.00\text{eV}$) and doped ($\mu = 1.00\text{eV}$) levels. The Coulomb repulsion and Hunds coupling strengths are varied from $1\text{-}10\text{eV}$ and $0.1\text{-}1.0\text{eV}$, respectively. The calculations were carried out using a form factor of 4\AA and an $n_k \times n_{k_f}$ grid of 20×5 . This section first discusses the 1NN2MY model, where orbital mixing between different orbitals is set to zero, and compares it later with the 1NN2MN model, which includes this orbital mixing.

In the undoped case, the model exhibits an antiferromagnetically ordered spin density wave (SDW) ground state for $U > 3.00eV$. When the coulomb repulsion is set to zero, the groundstate transitions to a charge density wave (CDW) with a (π, π) nesting vector. Doping the system to a chemical potential of $\mu = 1.00eV$ suppresses the SDW, and instead, a small superconducting patch emerges in the boundary of the CDW phase (*See Fig.14*). The magnitude of the Hund's coupling has a minor effect in the dominating phase and its transition temperature (T_c). The Superconducting regions shown in Fig.14.d exhibit different order parameters. The SC region at $U=0.0eV$ is s-wave symmetric whilst the SC region at $U =10.00eV$ is d-wave symmetric. By comparing Figures 14c,d with e,f, it can be concluded that the inclusion of different orbital hopping promotes the emergence of a CDW phase at lower Coulomb repulsion values in the doped case with $\mu = 1.00eV$.

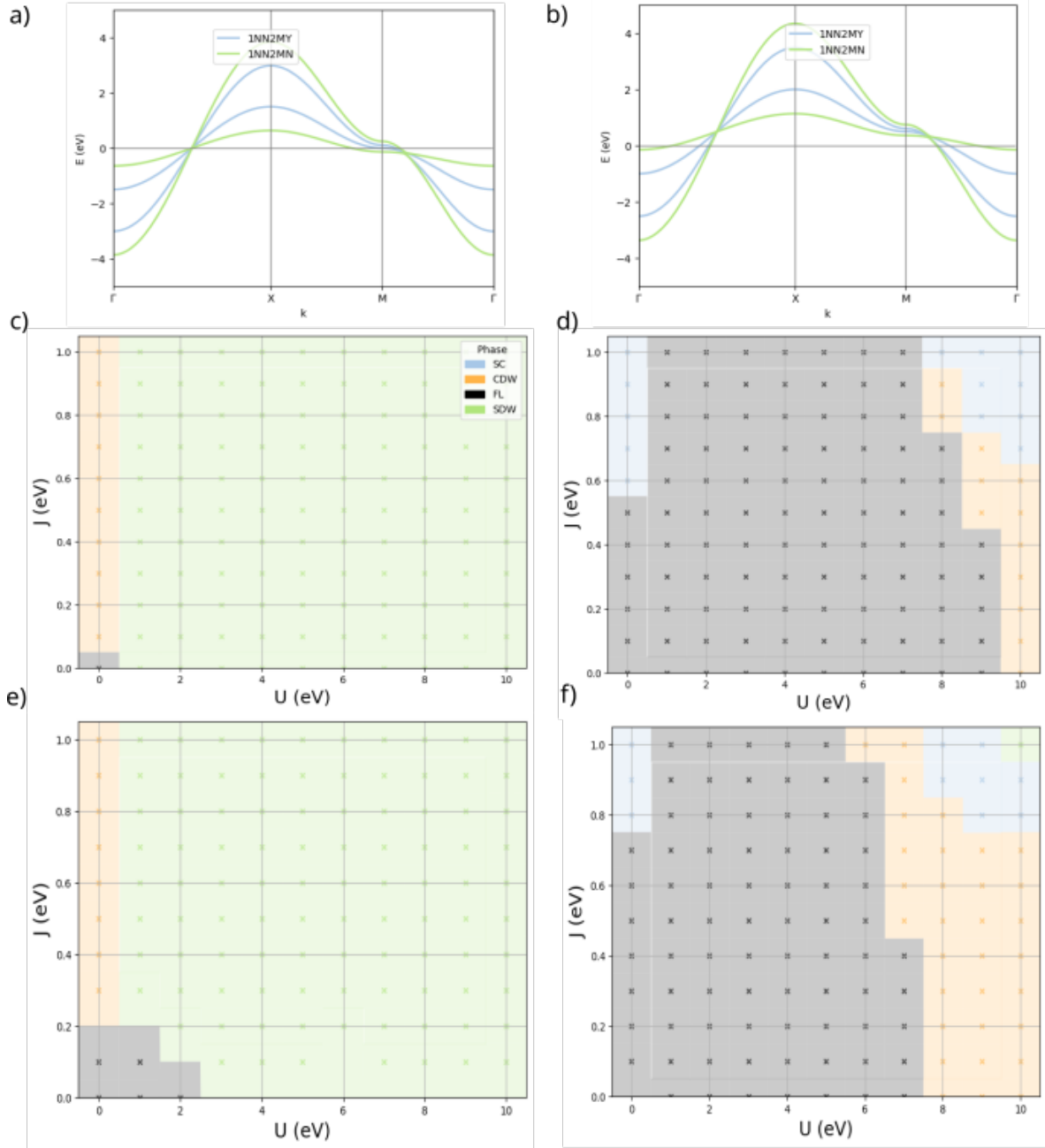


Figure 14: **Phase diagram for the 1NN2 model:** Phase diagram for the 1NN2 model without orbital mixing between different orbitals. Fig a) Band structure for the undoped 1NN2MY/N model. Fig b) Band structure for the 1NN2MY/N model at $\mu = 1.0\text{eV}$. Fig c) Phase diagram for the undoped 1NN2MY model. Fig d) Phase diagram for the 1NN2MY model at $\mu = 1.00\text{eV}$. Fig e) Phase diagram for the undoped 1NN2MN model. Fig f) Phase diagram for the 1NN2MN model at $\mu = 1.00\text{eV}$.

6 Conclusion and Outlook

This project aimed to investigate the interplay between Magnetism and Superconductivity in the 2D Hubbard Model at half-filling. The calculations were carried out in the spin-fluctuation mediated superconductivity framework using the two-particle truncated TU^2FRG scheme in the weak-coupling limit. Although this method fails to capture correlated phases such as Mott-insulating or pseudo-gap phases, it is widely in agreement with previous literature. The results presented here provide a comprehensive study of this model for a uniquely wide range of parameters. A strong competition between an Antiferromagnetically-ordered SDW and d-wave symmetric SC phase is observed. Additionally, several strategies to stabilize and enhance the critical temperature of superconductivity are identified, including increasing the on-site Coulomb repulsion and being near a stabilized SDW region. Narrow magnetic stripes are present, with their ordering changing at the "magical doping" value. The effect of including a next-nearest neighbor hopping parameter is examined in detail. Increasing t' lowers the Van Hove singularity's energy, shifting the region of prominent SDW-SC interplay towards more negative chemical potentials. A magnetic double dome emerges for a ratio of $\frac{t'}{t} = 0.50$. The inclusion of t' also leads to stable charge density wave (CDW) patches surrounding SC regions, where the SC order parameter transitions from d-wave to s-wave symmetry near these patches. Finally, a preliminary analysis is provided on extending these models to a two-orbital-per-site case. The AFM ground state is suppressed as the model is electronically doped, and the magnitude of Hund's coupling has minimal impact on the observed phases.

Future work could involve a more in-depth analysis of the two-orbital-per-site model, potentially exploring broader ranges of chemical potential and Hund's coupling values. Additionally, extending the study to a bi-layer, two-orbital-per-site Hubbard model would be an intriguing direction. One could also investigate the impact of spin-orbit coupling (SOC) on the results obtained. Such extensions would quickly evolve into a multi-dimensional analysis, offering numerous avenues for exploration. However, a particularly relevant direction would be to progressively increase the complexity of these models to better approximate the behavior of unconventional superconductors, such as lanthanum nickelate. This approach would involve a step-by-step examination of how the critical temperature (T_c) and superconducting regions change as model parameters evolve. Ultimately, this could provide valuable insights into the key parameters influencing superconducting phases in unconventional materials.

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A Appendix A

t' (eV)	μ (eV)	Competing with other phase?	Ordering vector	Magnetic ordering
0.00	1.00	Yes (SC)	(0,0)-(π , π)	FM-AFM
0.00	2.00	No	(0,0)-(0, π)	FM-Commensurate
0.25	-3.20	No	(0,0)	FM
0.25	-2.40	No	(0,0)	FM
0.25	-2.00	No	(0,0)-(π , π)	FM - AFM
0.25	0.60	No	(0,0)	FM
0.25	1.40	Yes (CDW)	(0,0)	FM
0.25	2.40	No	(0,0)	FM
0.50	-2.60	No	(0,0)	FM
0.50	1.60	No	(0,0)	FM
0.75	-3.00	Yes(SC)	(0,0)	FM
0.75	-2.20	Yes(SC)	(0,0)-inc.	FM- Incommensurate
0.75	2.00	No	(0,0).	FM

Table 2: **Survey of stripes in the 1NNN model.** Table summarising the location and magnetic ordering of the Stripes in the 1NNN model .