

CDMFT+HFD : an extension of dynamical mean field theory for non-local interactions applied to the single band extended Hubbard model

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Abstract

We examine the phase diagram of the extended Hubbard model on a square lattice, for both attractive and repulsive nearest-neighbor interactions, using CDMFT+HFD, a combination of Cluster Dynamical Mean Field theory (CDMFT) and a Hartree-Fock mean-field decoupling of the inter-cluster extended interaction. For attractive non-local interactions, this model exhibits a region of phase separation near half-filling, in the vicinity of which we find islands of d -wave superconductivity, decaying rapidly as a function of doping, with disconnected regions of extended s -wave order at smaller (higher) electron densities. On the other hand, when the extended interaction is repulsive, a Mott insulating state at half-filling is destabilized by hole doping, in the strong-coupling limit, in favor of d -wave superconductivity. At the particle-hole invariant chemical potential, we find a first-order phase transition from antiferromagnetism (AF) to d -wave superconductivity as a function of the attractive nearest-neighbor interaction, along with a deviation of the density from the half-filled limit. A repulsive extended interaction instead favors charge-density wave (CDW) order at half-filling.

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20 1 Introduction

21 The single-band Hubbard model has long served as a useful platform for studying the effect of
22 strong electronic correlations [1–6]. In particular, it explains many of the experimental obser-
23 vations in the high- T_c cuprate superconductors [2, 7–16], providing an approximate picture for
24 the description of these materials [17–25]. More recently, there have been numerous studies
25 on extensions of this model with nearest-neighbor interactions, known as the extended Hub-
26 bard model (EHM) [26–90]. There are several reasons for the continuing interest of the com-
27 munity in exploring the effect of non-local interactions. In actual materials, the interactions
28 between neighboring sites may not be completely screened, necessitating a more careful treat-
29 ment of longer-range interactions. The model with an attractive nearest-neighbor interaction
30 provides an effective representation of the attractive interactions mediated by electron-phonon
31 coupling, and may be realized in ultra-cold atom systems. The relevance of studying such a
32 model is further emphasized by recent ARPES studies on the one-dimensional cuprate chain
33 compound $\text{Ba}_{2-x}\text{Sr}_x\text{CuO}_{3+\delta}$ [91], where the observations can be explained using a Hubbard
34 model with an attractive extended interaction. On the other hand, the model with repulsive
35 non-local interactions provides an ideal playground for studying the interplay of charge and
36 spin fluctuations, since the relative magnitude of the charge fluctuations can be controlled by
37 the strength of the extended interaction [26, 30, 34, 35]. The EHM at quarter-filling has proven
38 useful for describing the charge ordering transition due to inter-site Coulomb interactions in
39 a variety of materials [28, 48, 49, 79, 83]. Both the Hubbard model and its extension with
40 longer-range interactions have contributed significantly to the methodological development
41 in the field of strongly correlated systems, and in particular high- T_c superconductors, which is
42 essential for obtaining results that can be quantitatively compared with experiments.

43 In recent years, the properties of the EHM have been analyzed using a variety of ap-
44 proaches, including, among others, mean-field theory [50–52, 72], functional renormalization
45 group (fRG) [39], exact diagonalization (ED) [29, 32, 55, 61], density-matrix renormalization
46 group (DMRG) [57, 63], Quantum Monte Carlo (QMC) [70, 87, 89, 92] and the fluctuation-
47 exchange approximation (FLEX) [56]. However, many of the approaches used are best suited
48 for studying the weak-coupling or the strong-coupling limit, and there are few that can de-
49 scribe the intermediate-coupling regime equally well. Even among those that can, each has its
50 own limitations. For instance, simple exact diagonalizations are restricted to small systems,
51 quantum Monte Carlo methods suffer from the fermion sign problem in many applications
52 of interest, the density-matrix renormalization group (DMRG) applies to one-dimensional or
53 ribbon-like systems, etc. In addition, certain aspects of the model with repulsive interactions
54 have been studied in detail using the so-called extended dynamical mean-field theory (EDMFT)
55 approach [93–95], in which the local density fluctuations together with the local self-energy
56 are propagated on the whole lattice using the known dispersion and density-density extended
57 interactions. Other variations of this method, such as a combination of EDMFT with the GW

58 approximation [27, 96–98], which perturbatively includes non-local self-energy corrections,
 59 and the dual boson method [81, 82, 99], which constructs a diagrammatic expansion about
 60 the extended DMFT, have likewise contributed to its understanding. More recently, cluster
 61 methods [26, 38, 76–78, 100, 101], which capture short-range correlations non-perturbatively
 62 within periodic clusters, have also been applied to this model. However, such studies have
 63 largely been limited to fixed densities and repulsive interactions. Overall, there have been
 64 fewer studies that consider both an extensive range of interaction couplings and band fillings,
 65 and relatively less focus on the case of attractive extended interactions.

66 In this paper, we study the phase diagram of the extended Hubbard model on a square
 67 lattice, for both attractive and repulsive nearest-neighbor interactions, using CDMFT+HFD,
 68 an extension of the Cluster Dynamical Mean Field Theory (CDMFT) [100, 102] approach with
 69 a Hartree-Fock decoupling of the inter-cluster interactions. CDMFT belongs to a class of meth-
 70 ods called Quantum Cluster Methods [103–109]. This is a set of approaches that consider a
 71 finite cluster of sites embedded in an infinite lattice, and introduce additional fields or “bath”
 72 degrees of freedom, determined by variational or self-consistency principles, to best represent
 73 the effect of the surrounding infinite lattice. These methods have proven useful for interpola-
 74 tion between results obtained in the weak- and strong-coupling regimes, since their accuracy
 75 is controlled by the size of the clusters used, rather than the strength of the couplings. Fur-
 76 ther, we treat the inter-cluster interactions within a Hartree-Fock mean-field decoupling, which
 77 generates additional Hartree, Fock and anomalous contributions to the cluster Hamiltonian.
 78 While a similar treatment has been used to study the model at quarter-filling [48] for the case
 79 of repulsive interactions, with the objective of understanding the electronic properties of met-
 80 als close to a Coulomb-driven charge ordered insulator transition, this analysis was focused
 81 on a specific parameter regime, and did not include superconducting orders.

82 This work constitutes a test of the CDMFT+HFD method, described in Sect. 2 below. Our
 83 main findings are as follows. For a weak repulsive local interaction U and an attractive ex-
 84 tended interaction V , the system undergoes a transition towards a phase separated (PS) state
 85 when the chemical potential lies in the vicinity of its particle-hole symmetric value, $U/2 + 4V$.
 86 The exact region of phase separation is identified by using the hysteresis in the behavior of the
 87 electron density as a function of the chemical potential, which corresponds to the coexistence
 88 of two different uniform-density solutions. As a function of doping away from the half-filled
 89 point, symmetrical and sharply decaying regions of $d_{x^2-y^2}$ -wave superconducting order are
 90 observed, followed by disconnected regions of extended s -wave order near quarter-filling, as
 91 well as at very small (large) densities. A stronger attractive extended interaction tends to fa-
 92 vor phase separation as well as superconductivity, whereas the repulsive on-site interaction
 93 U is found to be detrimental to both. At the particle-hole symmetric chemical potential, we
 94 detect a first-order phase transition from antiferromagnetism (AF) to d -wave superconductiv-
 95 ity as the attractive V becomes stronger, which is accompanied by a gradual deviation of the
 96 density from its half-filled limit, induced by phase separation. For repulsive nearest-neighbor
 97 interactions in the strong-coupling regime $U \gg t$, the Mott insulating state at half-filling is
 98 destabilized, upon hole doping, in favor of a dome-shaped region of d -wave superconducting
 99 order. This order is found to be remarkably stable in the presence of a non-local interaction,
 100 and slightly suppressed by it. At half-filling, a repulsive non-local interaction induces a first-
 101 order phase transition from antiferromagnetism (AF) to a charge-density wave (CDW) order.
 102 Our results are qualitatively in agreement with the existing literature on the phase diagram
 103 of the EHM, with some notable differences in the region of attractive interactions. An im-
 104 portant difference is that intra-cluster fluctuations are treated exactly, which tends to make
 105 superconducting orders somewhat weaker in this approach.

106 The paper is organized as follows. In Sect. 2, we introduce the model Hamiltonian, and
 107 provide a brief overview of the CDMFT approach that we use for our analysis, as well as the

108 Hartree-Fock mean-field decoupling of the inter-cluster interactions. In Sect. 3, we describe
 109 the phase diagram obtained as a function of the interaction strength and doping, and the phase
 110 transitions observed at half-filling. Finally, in Sect. 4, we summarize our results, discuss some
 111 relevant observations and present the conclusions of our study.

112 2 Model and method

113 2.1 Model Hamiltonian

114 The general form of the extended Hubbard model Hamiltonian is

$$H = \sum_{\mathbf{r}, \mathbf{r}', \sigma} t_{\mathbf{r}\mathbf{r}'} c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'} n_{\mathbf{r}\sigma} n_{\mathbf{r}'\sigma'} \quad (1)$$

115 where \mathbf{r}, \mathbf{r}' label lattice sites, $t_{\mathbf{r}\mathbf{r}'}$ are the hopping amplitudes, U the on-site Hubbard interaction,
 116 and $V_{\mathbf{r}\mathbf{r}'}$ the nearest-neighbor interaction (each bond counted once, hence the factor $\frac{1}{2}$).

117 For the purpose of our analysis, we study the following model on a square lattice:

$$H = -t \sum_{\mathbf{r}} (c_{\mathbf{r}}^\dagger c_{\mathbf{r}+\mathbf{x}} + c_{\mathbf{r}}^\dagger c_{\mathbf{r}+\mathbf{y}} + \text{H.c.}) + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} - \mu \sum_{\mathbf{r}} (n_{\mathbf{r}\uparrow} + n_{\mathbf{r}\downarrow}) + V \sum_{\mathbf{r}, \sigma, \sigma'} (n_{\mathbf{r}\sigma} n_{\mathbf{r}+\mathbf{x}, \sigma'} + n_{\mathbf{r}\sigma} n_{\mathbf{r}+\mathbf{y}, \sigma'}) \quad (2)$$

118 where \mathbf{x}, \mathbf{y} are the lattice unit vectors along the x and y directions, and the operator $c_{\mathbf{r}\alpha}$ an-
 119 nihilates a particle with spin $\alpha = \uparrow, \downarrow$ at site \mathbf{r} . The occupation number is $n_{\mathbf{r}\alpha} = c_{\mathbf{r}\alpha}^\dagger c_{\mathbf{r}\alpha}$. We
 120 consider a range of values for the chemical potential μ , corresponding to a continuous range
 121 of densities, from $n = 0$ to 2, along with a repulsive local interaction $U > 0$, and a nearest-
 122 neighbor interaction V that can be positive or negative. The particle-hole symmetric value of
 123 the chemical potential, $\mu = U/2 + 4V$, which corresponds to a half-filled band in the absence
 124 of phase separation, features prominently in our analysis. The unit of energy is taken to be
 125 the nearest-neighbor hopping amplitude $t = 1.0$, with the lattice constant $a = 1$. Note that
 126 in the absence of longer-range hopping terms, beyond the nearest-neighbor bonds, the model
 127 respects particle-hole symmetry $n \rightarrow 2 - n$.

128 We examine the possibility of superconducting as well as density-wave orders. For this
 129 purpose, the anomalous operators are defined on the lattice using a d -vector, as

$$\Delta_{\mathbf{r}\mathbf{r}', b} c_{\mathbf{r}\sigma} (i\sigma_b \sigma_2)_{\sigma\sigma'} c_{\mathbf{r}'\sigma'} + \text{H.c.} \quad (3)$$

130 where $b = 0, 1, 2, 3$, and σ_b are the Pauli matrices. The case $b = 0$ corresponds to singlet
 131 superconductivity, in which case $\Delta_{\mathbf{r}\mathbf{r}', 0} = \Delta_{\mathbf{r}'\mathbf{r}, 0}$ and the cases $b = 1, 2, 3$ correspond to triplet
 132 superconductivity, in which case, $\Delta_{\mathbf{r}\mathbf{r}', b} = -\Delta_{\mathbf{r}'\mathbf{r}, b}$. In practice, these operators are defined by
 133 specifying b and the relative position $\mathbf{r} - \mathbf{r}'$.

134 Density wave operators are defined with a spatial modulation characterized by a wave
 135 vector \mathbf{Q} , and can be based on sites or on bonds. In our analysis, we focus on site density
 136 waves, defined as

$$\sum_{\mathbf{r}} A_{\mathbf{r}} \cos(\mathbf{Q} \cdot \mathbf{r} + \phi) \quad (4)$$

137 where $A_{\mathbf{r}} = n_{\mathbf{r}}, S_{\mathbf{r}}^x, S_{\mathbf{r}}^z$ corresponds to charge- or spin-density wave orders, and ϕ is a sliding
 138 phase. We probe the presence of density-wave orders with $\mathbf{Q} = (\pi, \pi)$ and $\phi = 0$.

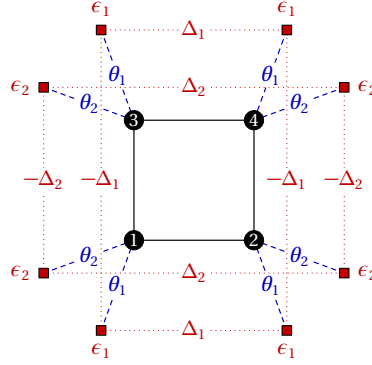


Figure 1: Schematic representation of the first (“simple”) impurity problem used in our analysis, with bath energies ϵ_i , cluster-bath hybridization parameters θ_i and anomalous bath parameters Δ_i . Physical sites are marked by numbered black dots and bath orbitals by red squares. We choose the bath parameters such that the environment of each cluster site is identical. This impurity model has reflection symmetry with respect to horizontal and vertical mirror planes (C_{2v} symmetry), and typically involves only spin-independent hopping terms. Pairing terms $\Delta_{1,2}$ are introduced between bath orbitals, with signs adapted to the SC order probed (shown here for a d -wave order, but all positive for an extended s -wave order). The number of independent bath parameters is 6.

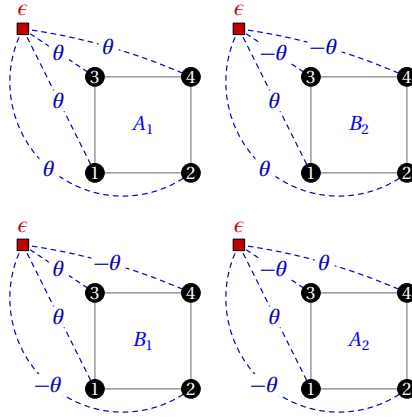


Figure 2: Schematic representation of the second (“general”) impurity problem used in our analysis. Each representation of the point group C_{2v} ($A_{1,2}$ and $B_{1,2}$) corresponds to a set of phases (± 1), and each of the 8 bath orbitals belongs to one of these four representations (two bath orbitals per representation). The different bath orbitals are independent (the bath system is diagonal) and we only show here a view of each of the four representations with the corresponding signs associated to each cluster site (black dots). The hybridization parameters θ are shown, and corresponding pairing operators (or anomalous hybridizations) between each bath orbital and each site also exist, with the same relative phases. We have 3 parameters per bath orbital, which leads to a total of 24 bath parameters, and subtracting six constraints due to a C_{4v} rotational symmetry, we obtain 18 independent bath parameters for the general model.

139 2.2 Method: CDMFT+HFD

140 Let us briefly describe the method used in our analysis, Cluster dynamical mean-field theory
 141 (CDMFT). For a detailed discussion of the basic principles of such Quantum Cluster Methods,
 142 please see Ref. [103, 105, 110].

143 This approach is an extension of dynamical mean-field theory (DMFT) [111–114], which
 144 accounts for short-range spatial correlations, by considering a cluster of sites with open bound-
 145 ary conditions, instead of a single-site impurity. The effect of the cluster’s environment is taken
 146 into account by introducing a set of uncorrelated “bath” orbitals hybridized with it. In this man-
 147 ner, the infinite lattice is tiled into identical clusters coupled to a bath of auxiliary, uncorrelated
 148 orbitals, with energy levels $\epsilon_{i\sigma}$, which may or may not be spin dependent, and hybridized with
 149 the cluster sites (labeled r) with amplitudes $\theta_{ir\sigma}$. In addition, for studying superconducting
 150 orders, different types of anomalous pairings $\Delta_{ij\sigma\sigma'}$ may be introduced between bath orbitals
 151 i, j or $\Delta_{ir\sigma\sigma'}$ between bath orbital i and cluster site r .

152 The cluster and bath size is limited by the exact diagonalization solver: the practical upper
 153 limit for the total number of cluster and bath orbitals is $4+8=12$, given that the ground state
 154 and Green function must be computed repeatedly in this approach. A true finite-size analysis
 155 is impossible here, for the next cluster size of the same square geometry would be 9, and the
 156 number of bath orbitals would need to grow accordingly. Even in a one-dimensional model,
 157 analyzing finite-size effects in CDMFT is challenging, because of the combined effects of cluster
 158 size and bath size [115].

159 We use two types of bath models. In the simple model (Fig. 1), the environment of each
 160 cluster is identical, and we introduce two bath orbitals per cluster site. Parameters of the impu-
 161 rity model include bath orbital energy levels ($\epsilon_{1,2}$), hybridization between each cluster site and
 162 the corresponding bath orbitals ($\theta_{1,2}$), and pairings between the bath orbitals ($\Delta_{1,2}$). The pre-
 163 cise form of $\Delta_{1,2}$, including their relative phases between different bath orbitals, depends on
 164 whether we probe extended s -wave, d -wave, or triplet superconductivity. This simple impurity
 165 model involves 6 independent parameters to be determined self-consistently. At half-filling,
 166 we introduce bath energies as well as hoppings, that are consistent with the appearance of a
 167 density-wave order, and additionally spin-dependent in the presence of antiferromagnetism.
 168 This increases the number of independent parameters. However, imposing particle-hole sym-
 169 metry at half-filling once again reduces this number to 6. For $V < 0$, we do not impose
 170 particle-hole symmetry on the bath parameters due to the possibility of phase separation, and
 171 the number then increases to 10.

172 We also use a more general bath model (Fig. 2). While the total number of bath orbitals
 173 is unchanged, every bath orbital is connected to every cluster site (with distinct combinations
 174 of relative phases), and we define bath energies, cluster-bath hybridizations and anomalous
 175 pairings between the cluster and the bath sites. In this model the bath is diagonal, i.e., the
 176 different bath orbitals are not directly coupled between themselves. We have 3 parameters
 177 per bath orbital, and taking into account six constraints due to rotation symmetry, there are
 178 18 independent bath parameters to set. At the particle-hole symmetric chemical potential,
 179 we introduce bath energies, hybridizations and anomalous pairings that have two different
 180 values for alternative sites. This gives us a total of 42 independent parameters in the absence
 181 of particle-hole symmetry for $V < 0$ and 15 independent parameters when superconductivity
 182 is absent (i.e. for $V > 0$) and particle-hole symmetry is taken into account.

183 All bath parameters are determined by a self-consistency condition (see Ref. [103, 105, 110]
 184 for details). The simple bath model is expected to be easier to converge than the general bath
 185 model, because of the smaller set of parameters. While we expect the results obtained from the
 186 general bath model to be more reliable, we do find most of the results to be qualitatively similar
 187 in the two cases. Once the bath parameters are converged, the self-energy $\Sigma(\omega)$ associated

188 with the cluster is applied to the whole lattice, so that the lattice Green function is

$$\mathbf{G}^{-1}(\tilde{\mathbf{k}}, \omega) = \mathbf{G}_0^{-1}(\tilde{\mathbf{k}}, \omega) - \Sigma(\omega) \quad (5)$$

189 Here, $\tilde{\mathbf{k}}$ denotes a reduced wave vector (defined in the Brillouin zone of the super-lattice
190 of clusters defined by the tiling) and \mathbf{G}_0 is the non-interacting Green function. The Green-
191 function-like objects \mathbf{G} , \mathbf{G}_0 and Σ are $L \times L$ matrices, L being the number of physical degrees
192 of freedom on the cluster (here $L = 8$ because of spin and the four cluster sites). The aver-
193 age values of one-body operators defined on the lattice are obtained using the lattice Green
194 function \mathbf{G} determined from the solution for the optimum values of the bath parameters. An
195 exact-diagonalization solver (the Lanczos method or variants thereof) is used at zero temper-
196 ature. The computational size of the problem increases exponentially with the total number
197 of cluster and bath orbitals.

198 In the presence of extended interactions, we also perform a Hartree-Fock mean-field de-
199 composition of the interaction terms defined between different clusters, while the interactions
200 within a cluster are treated exactly. The inter-cluster interactions are decoupled in the Hartree,
201 Fock and anomalous channels, which contribute to the number density, the hopping and the
202 pairing operators, respectively. Moreover, we only retain those combinations of the site/bond
203 operators that are physically relevant in the regions we work in (such as d -wave or extended
204 s -wave), and discard the rest. The mean-field values of the relevant combinations are deter-
205 mined self-consistently, within the CDMFT loop that optimizes the bath parameters. For the
206 details of this procedure, please refer to Appendix A. For a comparison of different methods
207 used for solving the self-consistent nonlinear equations involved in the CDMFT procedure,
208 please refer to Appendix B.

209 3 Results

210 In this section, we discuss the salient features of the phase diagram obtained from our analysis,
211 for both attractive and repulsive nearest-neighbor interactions. The dominant superconduct-
212 ing and density-wave orders are identified by computing the corresponding order parameters
213 using the optimum values of the CDMFT (bath and mean-field) parameters, as a function of
214 electron density, as well as at half-filling. In the following analysis, we focus our attention on
215 the strong coupling limit $U \gg t$ for $V > 0$, which is a regime well-understood on physical
216 grounds. For $V < 0$, we consider relatively weak interactions $U \sim t$, far from the Mott insu-
217 lating regime, which primarily serve the purpose of controlling the extent of phase separation
218 when the interaction V becomes sufficiently attractive. At half-filling, we confirm the nature
219 of the phase transitions, by plotting the relevant order parameters both as a function of $U > 0$,
220 for fixed values of $V > 0$ or $V < 0$, and as a function of V for fixed values of U .

221 3.1 Phase diagram at the particle-hole symmetric chemical potential

222 Here, we fix the chemical potential to $\mu = U/2 + 4V$, corresponding to a half-filled band, and
223 examine the behavior of different superconducting and density-wave orders, as a function of
224 the local repulsion U as well as attractive/repulsive V . While antiferromagnetism is favored
225 at half-filling, in both weak- and strong-coupling regimes, an attractive non-local interaction
226 is expected to drive the system towards a superconducting instability, and eventually phase
227 separation. On the other hand, repulsive interactions V would typically foster competition
228 between charge and spin fluctuations, and favor a charge-ordered state. Below, we discuss the
229 results obtained using the simple bath model (Fig. 1).

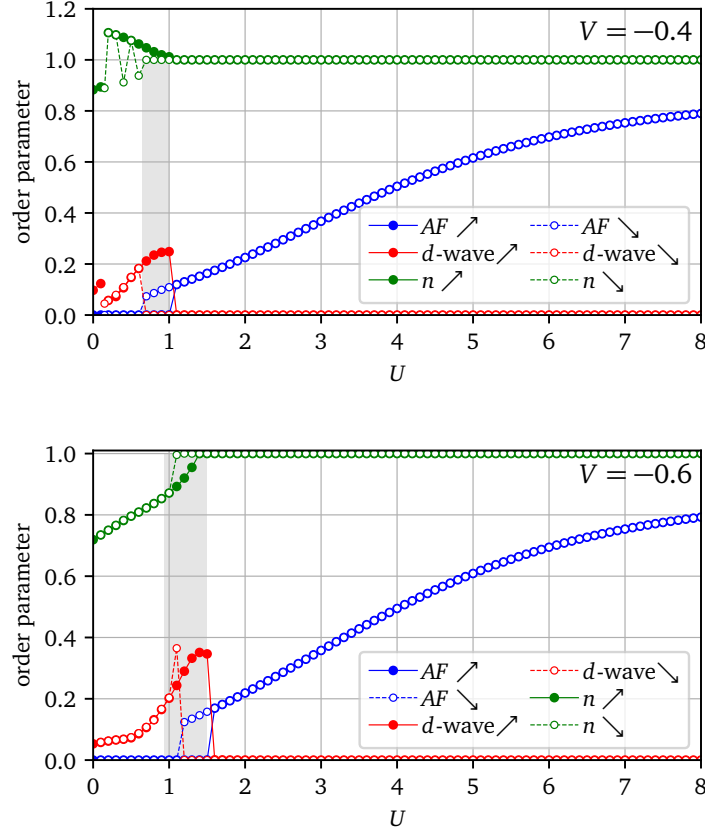


Figure 3: First-order phase transition from d -wave superconductivity (indicated by filled/open red circles) to antiferromagnetism (AF, indicated by filled/open blue circles), as a function of the repulsive local interaction U , at fixed $V = -0.4$ (top) and $V = -0.6$ (bottom), and fixed chemical potential $\mu = U/2 + 4V$ (particle-hole symmetric point). The simple impurity model (Fig. 1) is used. The transition is accompanied by a deviation in the number density (indicated by filled/open green circles) from the half-filled value $n = 1$, meaning that we are entering a phase separated regime. The dashed (solid) curves of each color depict the behavior of the different quantities for decreasing (increasing) U , respectively. The prominent region of hysteresis between the two curves confirms the order of the transition. The small jump/discontinuity observed in the d -wave order parameter for increasing U for $V = -0.4$ results from issues with the convergence of the CDMFT procedure at that point. On the other hand, for $V = -0.6$, we observe a jump in the d -wave order parameter for decreasing U , which appears to signal a transition from a d -wave order at half-filling to one coexisting with phase separation, rather than being a numerical error. Likewise, for increasing U , we observe a nontrivial d -wave order parameter both in the presence and absence of phase separation for $V = -0.6$ (for more details, see Appendix B).

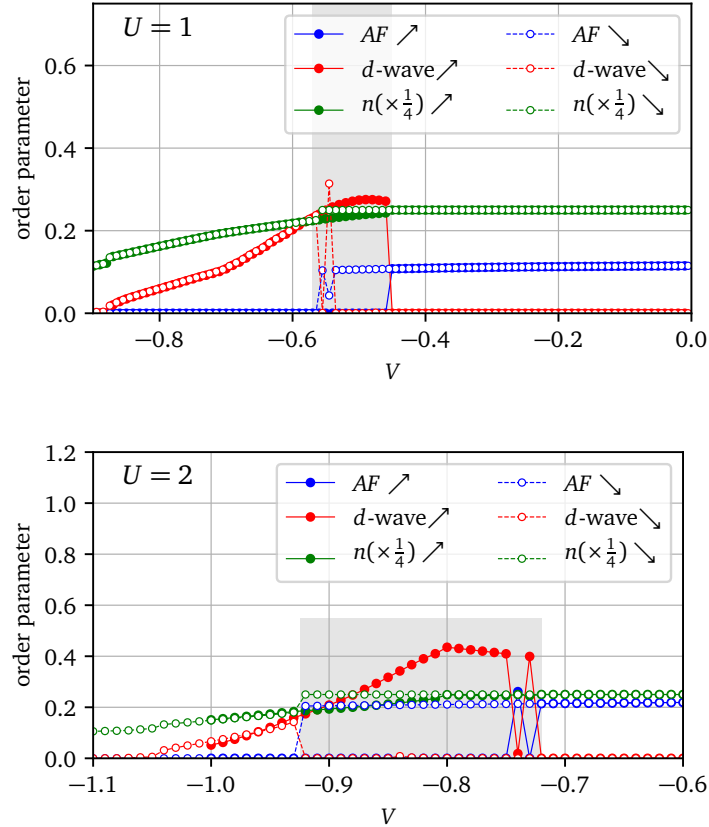


Figure 4: First-order phase transition from antiferromagnetism (AF) (indicated by filled/open blue circles) to d -wave superconductivity (indicated by filled/open red circles), for increasingly attractive V , followed by a rapid suppression in the superconducting order parameter, for on-site interaction $U = 1$ (top) and $U = 2$ (bottom). The simple impurity model (Fig. 1) is used. The transition is accompanied by a deviation in the number density (indicated by filled/open green circles) from the half-filled value $n = 1$. The dashed (solid) curves of each color depict the behavior of different quantities for decreasing/more negative (increasing/less negative) V , and we find significant hysteresis. For larger repulsive interactions U , the transition is found to occur at a critical value of V that is more attractive. For $U = 1$, we observe oscillations between the d -wave and AF orders at half-filling, close to the transition for decreasing/more negative V , while for $U = 2$, we see a significant region of d -wave superconductivity close to half-filling for increasing/less negative V , as well as similar oscillations between the d -wave and AF orders at half-filling, close to the transition between the two states for increasing/less negative V .

230 3.1.1 $V < 0$:

231 For a fixed attractive nearest-neighbor interaction V , as the strength of the local repulsive
 232 interaction U decreases, the system undergoes a first-order phase transition from antiferro-
 233 magnetism to d -wave superconductivity. This is accompanied by a deviation in the electron
 234 density from its half-filled limit, which can be attributed to the effects of phase separation, dis-
 235 cussed in more detail in the next subsection. Each of the order parameters is plotted for both
 236 increasing and decreasing U , and the region of hysteresis between the two curves indicates
 237 that the transition is first-order in nature. We have verified that other pairing symmetries,
 238 such as extended s -wave and p -wave, do not compete with $d_{x^2-y^2}$ pairing in this regime. The
 239 results of our analysis are shown in Fig. 3. Likewise, an antiferromagnetic order is destabilized
 240 in favor of d -wave superconductivity for an attractive V , at a fixed repulsive $U \sim t$, with signif-
 241 icant hysteresis between the curves obtained for increasing/decreasing V . The latter state is
 242 then rapidly suppressed due to the effect of phase separation. The results are shown in Fig. 4.

243 3.1.2 $V > 0$:

244 For repulsive nearest-neighbor interactions V , we do not expect to find any superconducting
 245 orders at half-filling in the strong-coupling limit $U \gg t$, and instead focus on studying the
 246 competition between charge- and spin-density-wave orders. At fixed $V > 0$, we observe a
 247 first-order phase transition from a charge-density wave (CDW) to an antiferromagnetic (AF)
 248 state, as a function of increasing U . Likewise, for a large repulsive U , the system undergoes
 249 a phase transition from antiferromagnetism to CDW, as a function of the repulsive V . In both
 250 cases, a large region of hysteresis is observed between the results obtained for increasing and
 251 decreasing values of the respective interaction couplings. The results of our analysis are shown
 252 in Figs 5 and 6, respectively.

253 We do not present the corresponding results for the more general bath model (Fig. 2) here,
 254 as they are found to be qualitatively similar to those obtained for the simple model. The key
 255 differences, that are sometimes observed, include a) an increase/decrease in the strength of
 256 the d -wave order parameter close to the transition, b) a smaller region of hysteresis, c) a small
 257 shift in the position of the transition, particularly as a function of V for fixed U .

258 3.2 Phase diagram as a function of density

259 Next, we examine the phase diagram of the model over a continuous range of densities, for
 260 $U > 0$ and attractive/repulsive V . For $V > 0$, we once again limit ourselves to the strong-
 261 coupling limit $U \gg t$. For $V < 0$, we focus on studying the effect of an attractive extended
 262 interaction, with a local repulsion U controlling the extent of phase separation.

263 3.2.1 $V < 0$:

264 Let us now discuss the different phases that are supported by the model as a function of den-
 265 sity. Close to half-filling, we find a region of phase separation, indicated by a jump in the
 266 density, flanked by symmetrical islands of $d_{x^2-y^2}$ pairing, which decay rapidly as a function of
 267 density. For further smaller (larger) fillings, an extended s -wave order appears in the form of
 268 disconnected regions, near quarter-filling and at very small (large) densities. Interestingly, the
 269 variation of the extended s -wave order parameter as a function of U and V are found to be dif-
 270 ferent for the simple bath model and the more general one. In the case of the simple model (see
 271 Fig. 7), we find small regions of extended s -wave superconductivity near quarter-filling, that
 272 vary non-monotonously as a function of U . Only for sufficiently attractive V , nearly symmetri-
 273 cal regions of extended s -wave order also appear close to the band edges. The corresponding
 274 results for the general bath model are illustrated in Fig. 8. While the overall magnitude of the

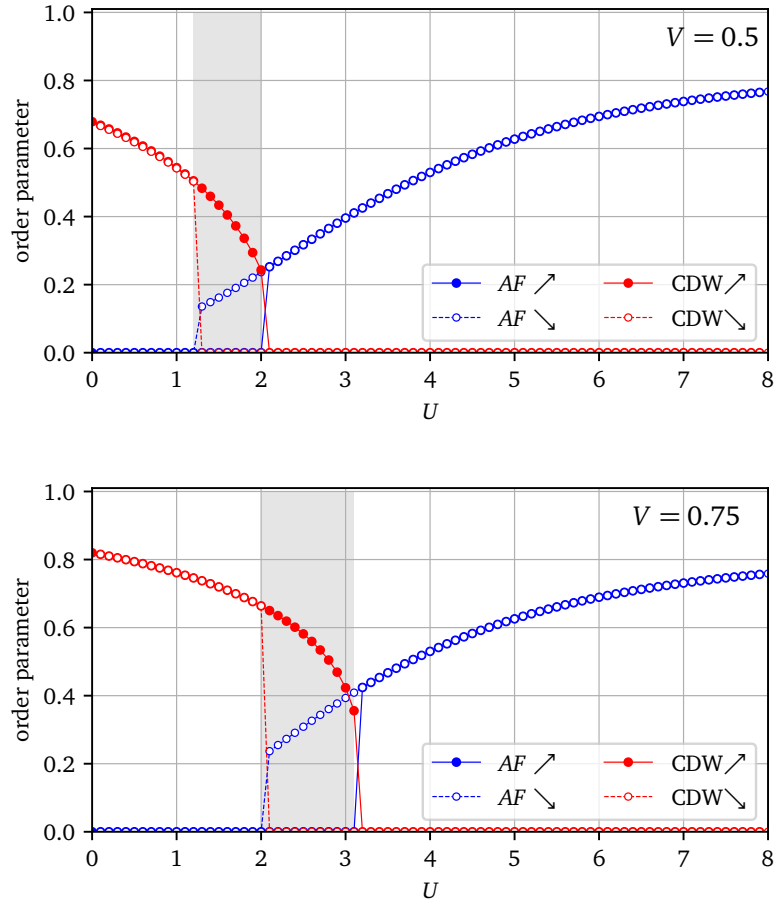


Figure 5: First-order phase transition from a charge-density wave (CDW) order (indicated by filled/open red circles) to antiferromagnetism (indicated by filled/open blue circles), at half-filling, as a function of the local repulsive interaction U , for $V = 0.5$ (top) and $V = 0.75$ (bottom). The simple impurity model (Fig. 1) is used. The dashed (solid) curves of each color depict the behavior of the order parameters for decreasing (increasing) U , and exhibit significant hysteresis. As the repulsive V becomes stronger, the transition is found to occur at a larger value of U , the CDW order parameter increases considerably in magnitude, and the region of hysteresis is somewhat enhanced.

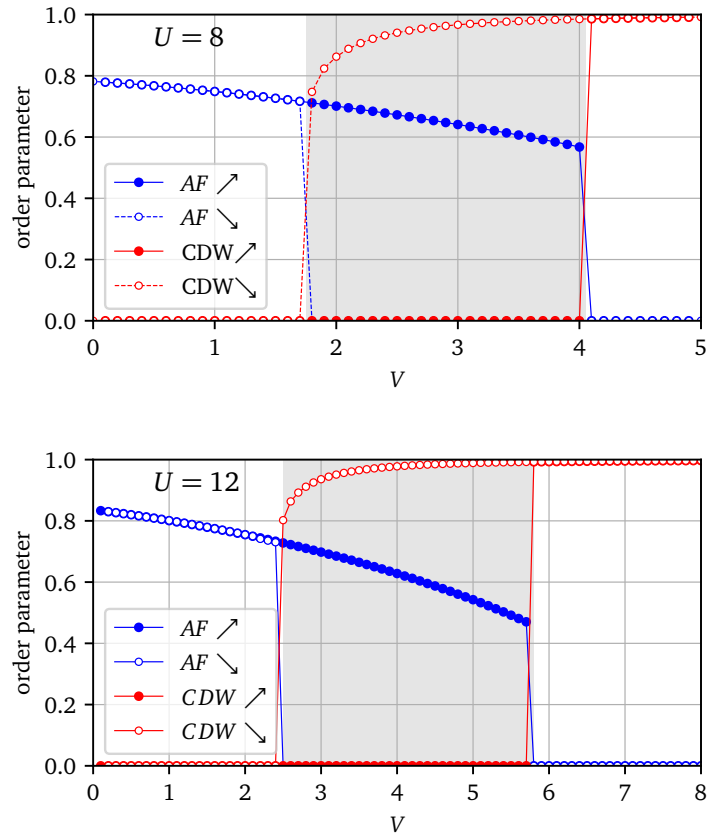


Figure 6: First-order phase transition from antiferromagnetism (indicated by filled/open blue circles) to charge-density wave (CDW) order (indicated by filled/open red circles), at half-filling, as a function of the repulsive interaction V for fixed U , with $U = 8$ (top) and $U = 12$ (bottom). The simple impurity model (Fig. 1) is used. The dashed (solid) curves of each color depict the behavior of the order parameters for decreasing (increasing) V , and exhibit considerable hysteresis. As U increases, the transition occurs at a larger critical value of V , and the antiferromagnetic order parameter increases in magnitude.

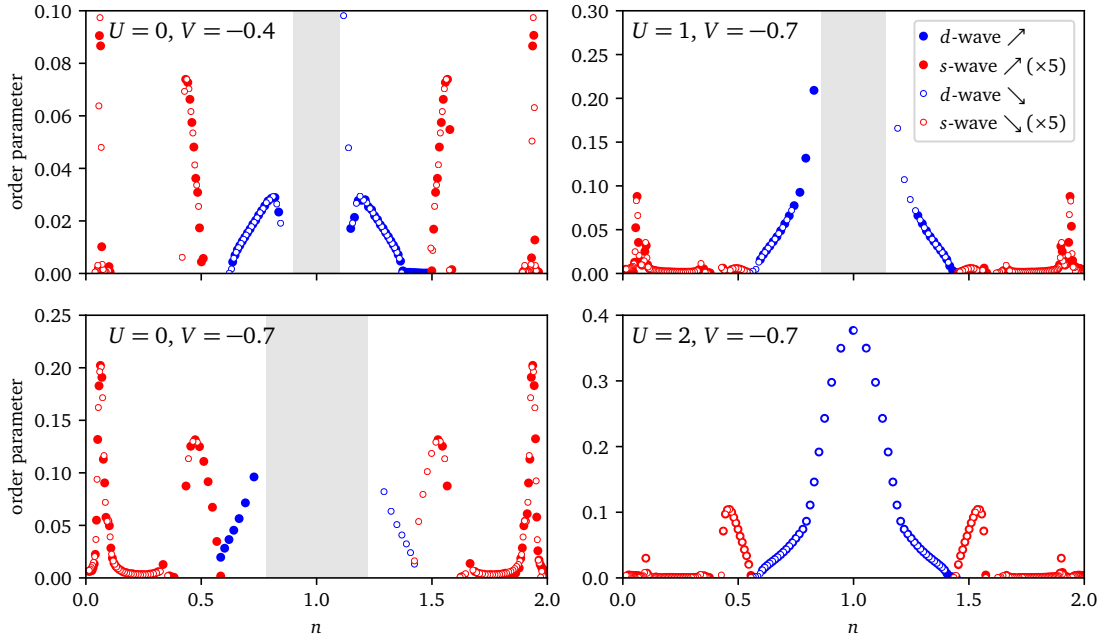


Figure 7: Superconducting order parameter of the EHM with attractive nearest-neighbor interactions, as a function of density n , from $n = 0$ to 2 for the simple bath model (Fig. 1). Close to the half-filled value $n = 1$, we find signatures of phase separation, indicated by a gap in the curve over a range of densities, caused by a jump in the compressibility $\partial n / \partial \mu$ (as shown in Fig. 9). For smaller (larger) fillings, nearly symmetrical and sharply defined regions of d -wave superconductivity (represented by filled/open blue circles) are followed by disconnected patches of extended s -wave order (represented by filled/open red circles), which appear only beyond a critical attractive value of V . Note that the asymmetry between either the d -wave regions or the extended s -wave regions near the band edges, especially evident for $V = -0.4$, is a numerical artefact owing to insufficient accuracy in the CDMFT procedure and has no physical consequence.

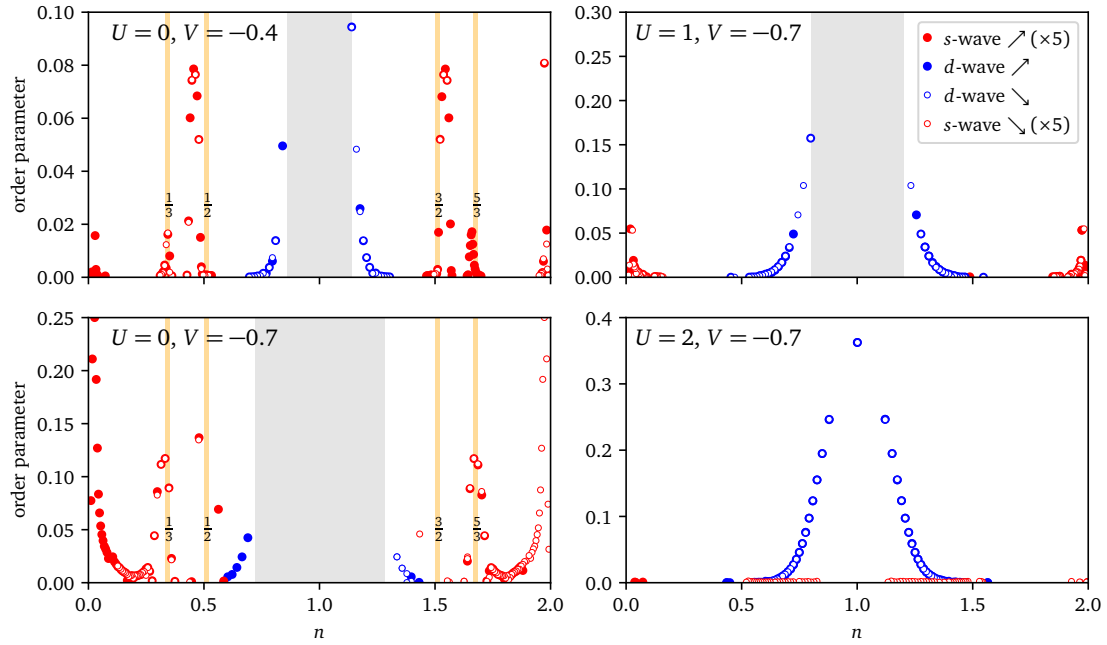


Figure 8: Superconducting order parameter of the EHM with attractive nearest-neighbor interactions, as a function of density n , from $n = 0$ to 2 for the general bath model (Fig. 2). The overall behavior of the d - and extended s -wave patches are similar to the corresponding result for the simple bath model. However, note that the structure of the s -wave order parameter has changed, with a more extended region near quarter-filling, and an additional patch near $1/3$ -filling. For $U = 0, V = -0.7$, the phase separation region extends all the way to quarter-filling, and the corresponding superconducting patches are almost absent, and asymmetric about $n = 1$. Moreover, the new s -wave order parameter becomes unambiguously weaker as the repulsive U increases, and is completely absent for $U = 1$ and $U = 2$, thus resolving the question of the non-monotonous behavior of the s -wave order parameter in the simple bath model.

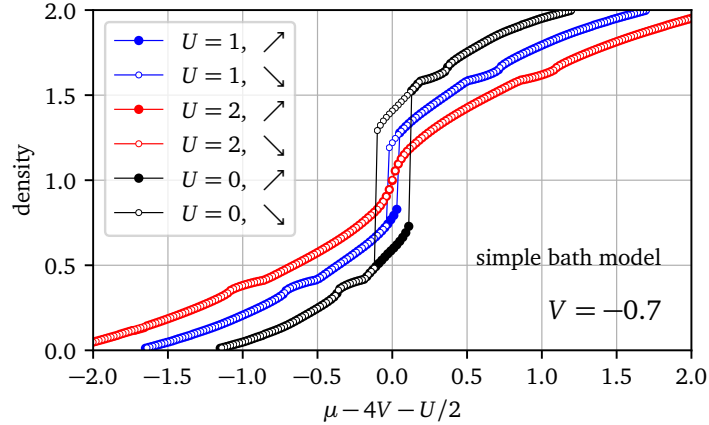


Figure 9: Number density n as a function of the chemical potential μ (measured with respect to its particle-hole invariant value, $\mu_c = U/2 + 4V$) for an EHM with attractive nearest-neighbor interactions, over a range of values of $U \geq 0$ and $V < 0$ for the simple bath model (Fig. 1). On either side of half-filling ($\mu = \mu_c$), we find symmetrical jumps in the compressibility $\partial n / \partial \mu$ enclosing a region of hysteresis, which corresponds to the coexistence of two different uniform-density solutions. This is interpreted as the region of phase separation. The red, blue and black filled/open circles represent the behavior for various values of U for $V = -0.7$, and demonstrate that while a sufficiently attractive interaction V favors phase separation, a stronger on-site repulsion U is detrimental to it.

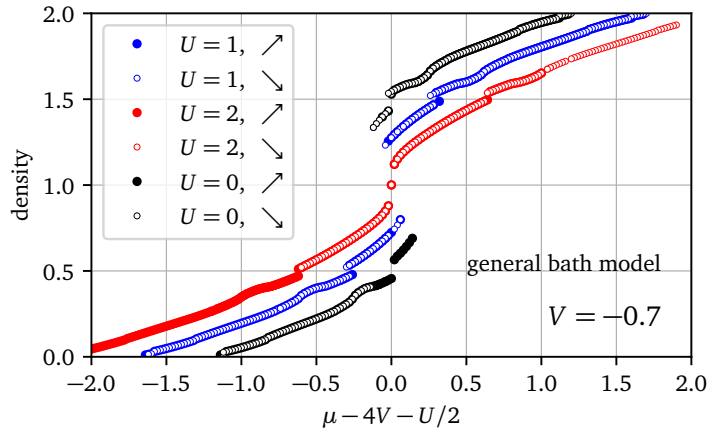


Figure 10: Number density n as a function of the chemical potential μ (measured with respect to its particle-hole invariant value, $\mu_c = U/2 + 4V$) for the EHM with attractive nearest-neighbor interactions, over a range of values of $U \geq 0$ and $V < 0$ for the general bath model (Fig. 2). The behavior is very similar to that observed in the simple bath model, with the most notable difference being the appearance of symmetric jumps in the number density n , close to quarter-filling, for each of the curves.

275 s -wave order parameter turns out to be smaller than in the previous case, its shape is more
 276 extended at quarter-filling, with two patches appearing next to each other, which, interest-
 277 ingly, appear close to fillings of $1/3$ and $1/2$, respectively. While it is tempting to blame the
 278 $n = 1/2$ feature on a commensurate finite-size effect on a 4-site cluster, this is less obvious
 279 for the $n = 1/3$ feature. The superconductivity also clearly becomes stronger as a function of
 280 $V < 0$. Notably, the s -wave order is clearly absent for both $U = 1$ and $U = 2$, thus eliminating
 281 the confusion caused by the aforementioned non-monotonous variation in the case of the sim-
 282 ple model, and illustrating the advantage of considering a larger number of bath parameters
 283 in the CDMFT procedure. This being said, the conclusions from the two bath models are very
 284 similar. Using two different bath models provides us with an order-of-magnitude estimate of
 285 the error caused by the discreteness of the bath.

286 To better characterize the region of phase separation, we examine the behavior of the num-
 287 ber density n as a function of the chemical potential μ , measured with respect to its particle-
 288 hole symmetric value $\mu_c = U/2 + 4V$. On either side of $\mu = \mu_c$, we find symmetrical jumps
 289 in the compressibility $\partial n / \partial \mu$, enclosing a region of hysteresis in the $\mu - n$ curve, depicted in
 290 Fig. 9, where two uniform-density solutions coexist. Within our approach, this is interpreted
 291 as the region of phase separation, and is found to shrink under the influence of stronger local
 292 repulsive interactions U , and expand when V becomes more attractive. The corresponding re-
 293 sults for the general bath model are depicted in Fig. 10. The two sets of results are qualitatively
 294 similar, except for symmetric jumps observed in the number density n near quarter-filling in
 295 the latter case. We note that the jumps occur only for the model with the larger number of
 296 bath parameters, and are the most prominent for $U = 0, V = -0.7$, where the phase separa-
 297 tion region extends all the way to quarter-filling, becoming progressively smaller for $U = 1$
 298 and 2. It is plausible that phase separation might lead to the appearance of multiple jumps in
 299 the density, at half-filling as well as quarter-filling. Moreover, a finite-size effect would have
 300 been even more obvious in the simple bath model, where these jumps are found to be absent.
 301 The origin of the jumps is currently unclear to us.

302 The appearance of a phase separated state for sufficiently attractive interactions is a famil-
 303 iar result [32, 52, 71, 81, 87, 116], which has received attention from other groups, including
 304 very recently [70], but the characterization of the region of phase separation tends to depend
 305 on the method used for the analysis, and whether it is capable of handling a nonuniform
 306 distribution of particles.

307 3.2.2 $V > 0$:

308 At half-filling, for $U = 8t$, the large on-site interaction freezes the charge degree of freedom,
 309 and the ground state is a Mott insulator. Hole doping is found to destabilize the magnetic
 310 order, and drive the system towards a d -wave superconducting phase. We encounter a dome-
 311 shaped region of d -wave superconductivity for $V = 0$, which is suppressed at smaller densities,
 312 where no competing superconducting orders are found to be stabilized in our analysis. Upon
 313 introducing a repulsive $V \sim t$, the superconducting order remains stable, but is somewhat
 314 suppressed. The results are depicted in Fig. 11. The corresponding results for the general bath
 315 model are depicted in Fig. 12. The two sets of results are qualitatively similar, with the most
 316 noticeable difference being the relatively sharper transition to and from the d -wave ordered
 317 state in the latter case. These results are consistent with the picture of superconductivity
 318 mediated by short-range spin fluctuations in a doped Mott insulator [117–119].

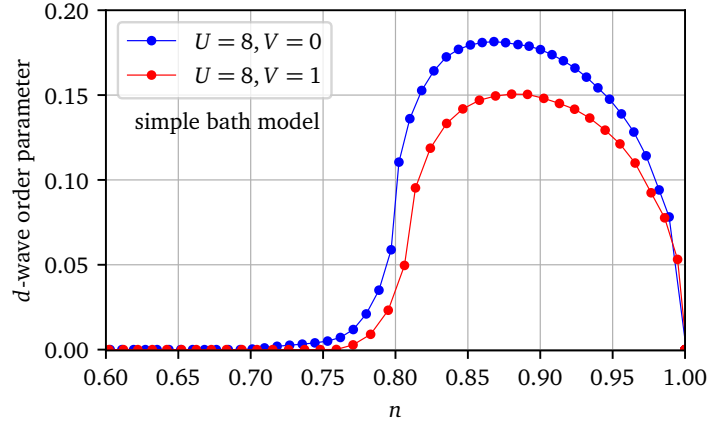


Figure 11: Superconducting d -wave order parameter of the EHM with repulsive nearest-neighbor interactions in the strong-coupling limit, i.e., at $U = 8t$, using the simple bath model (Fig. 1). The Mott insulating state at half-filling is destabilized in favor of $d_{x^2-y^2}$ pairing, upon hole doping. The dome-like region of d -wave superconducting order is observed for $V = 0$ (indicated by the solid blue curve) and is somewhat suppressed for nonzero repulsive V (indicated by the solid red curve). No other superconducting orders are found to be stabilized in this region.

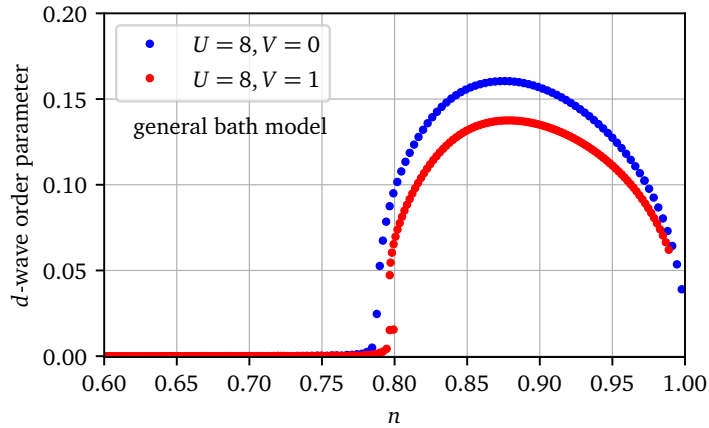


Figure 12: Superconducting d -wave order parameter of the EHM with repulsive nearest-neighbor interactions in the strong-coupling limit ($U = 8t$) using the general bath model (Fig. 2). The behavior is qualitatively similar to that obtained in the simple model, with a slight difference in the magnitudes of the d -wave order parameter. The most noticeable difference between the two bath models is the relatively sharp transition into and out of the d -wave superconducting phase.

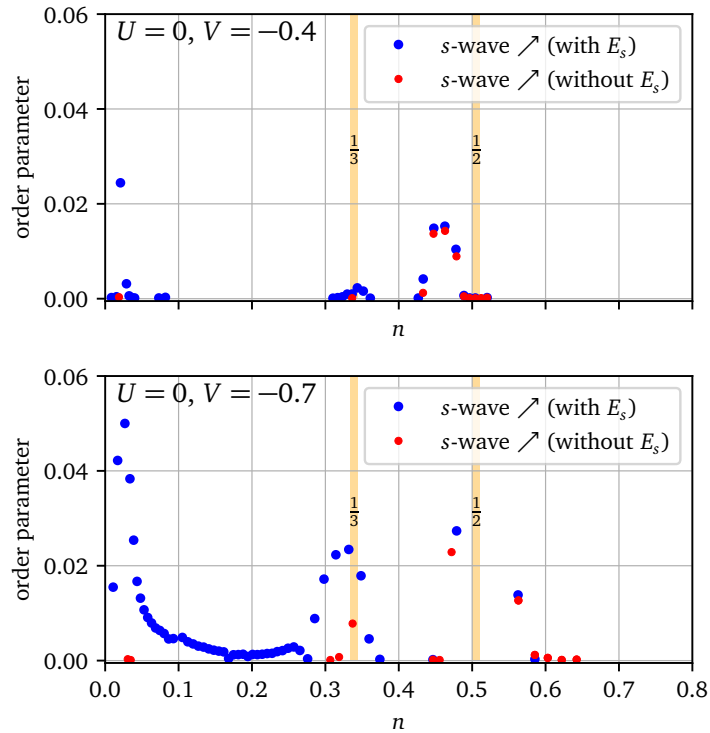


Figure 13: The figure shows the behavior of the extended s -wave order parameter as a function of the number density n , with and without the inclusion of the self-consistent anomalous mean-field parameter E_s (see Appendix A), for $U = 0, V = -0.4$ (above) and $U = 0, V = -0.7$ (below). Clearly, some of the regions with a nontrivial s -wave order parameter are found to be absent when E_s is not included. For $U = 0, V = -0.7$, the most prominent among these appears to be the region with density in the range $0 < n < 0.3$. Upon considering a stronger attractive V , these regions tend to reappear, but are suppressed in magnitude in the absence of E_s .

319 4 Discussion and conclusions

320 In summary, we have studied the phase diagram of the extended Hubbard model, for both
 321 attractive and repulsive nearest-neighbor interactions, using a combination of Cluster Dynam-
 322 ical Mean Field Theory (CDMFT), with a dynamical Hartree-Fock approximation for treating
 323 inter-cluster interactions. We examine possible phase transitions at half-filling, as well as the
 324 dominant phases that are stabilized as a function of density. At the particle-hole invariant
 325 chemical potential, which corresponds to a half-filled band in the absence of phase separation,
 326 the antiferromagnetically ordered state undergoes a first-order phase transition to d -wave su-
 327 perconductivity for a critical attractive interaction V . Stronger attractive extended interactions
 328 also tend to induce phase separation, which manifests itself in the form of a gradual deviation
 329 of the density from its half-filled limit, for a fixed chemical potential. For a sufficiently strong
 330 repulsive interaction V , a charge-density wave order is stabilized at half-filling.

331 As a function of density, a phase separated state near the half-filled point is flanked by
 332 symmetrical regions of d -wave superconductivity, that decay sharply as a function of density,
 333 and islands of extended s -wave order at smaller (larger) band fillings. For the case of repulsive
 334 non-local interactions, in the strongly coupled limit, the Mott insulator at half-filling gives way
 335 to a dome-shaped region of d -wave superconductivity, upon hole doping, which is expected
 336 on physical grounds. No other competing superconducting orders are found to be stabilized
 337 in this region of parameter space.

338 For the most part, our results are found to be qualitatively consistent with the existing
 339 literature. The transition between antiferromagnetism and CDW at half-filling, for repulsive
 340 interactions, has been predicted by several previous studies [26,31,54,58,62,65,70,76–78,87],
 341 although the critical interaction strength typically depends on the method of analysis. For
 342 densities away from half-filling, there have also been some predictions of d_{xy} pairing, that
 343 appears beyond the region of $d_{x^2-y^2}$ pairing, for repulsive extended interactions [39,56]. We
 344 do not find such a state in our analysis. The phase diagrams obtained from self-consistent
 345 mean-field theory based analyses tend to prominently feature d -wave superconductivity at
 346 half-filling, with a continuous region of extended s -wave order at smaller densities, along
 347 with a region of coexistence between the two, i.e., $s + id$ pairing [50,51]. In our analysis,
 348 we do not usually see a coexistence between d - and extended s -wave orders. In the simple
 349 model, such a coexistence is observed only in those regimes where both interactions $U > 0$
 350 and $V < 0$ are sufficiently strong, and comparable in magnitude. This may be due to the
 351 fact that the superconducting orders found in our analysis are fairly weak, and the significant
 352 attractive interactions that are, therefore, needed for stabilizing overlapping regions of d -
 353 and extended s -wave orders, would also lead to a larger region of phase separation. This
 354 effect can only be compensated by including a sufficiently large repulsive local interaction.
 355 On the other hand, we have not been able to verify a similar coexistence of the orders for the
 356 general bath model, due to the rapid suppression of the extended s -wave order, near quarter-
 357 filling, with an increase in U . Some studies have also suggested the possibility of p -wave
 358 superconductivity, especially at half-filling [32], and for intermediate hole doping, beyond
 359 the region of d -wave superconducting order [39,50,51]. We do not find signatures of p -
 360 wave superconductivity in the parameter regimes that we study. Some of our results at half-
 361 filling are found to be qualitatively consistent with a recent study on the extended Hubbard
 362 model using the determinantal Quantum Monte Carlo technique [70], which also reports the
 363 transitions between d -wave superconductivity and AFM, as well as between phase separation
 364 and d -wave, that we observe in our analysis. In addition, the authors of the aforementioned
 365 paper also explore other quadrants of the $U - V$ phase diagram, including the case where
 366 $U < 0$, which we do not take into account, since the repulsive component of the Coulomb
 367 interaction is always expected to be present in a realistic situation.

368 In contrast to ordinary mean-field theory, our approach takes the intra-cluster fluctuations
 369 into account exactly, and is therefore expected to give more reliable quantitative results. In par-
 370 ticular, ordered phases are weaker in this approach than in ordinary mean-field theory. At the
 371 same time, it should be noted that we only take into account spatial fluctuations within small
 372 clusters, and the accuracy of the method is controlled by the size of the clusters used. To illus-
 373 trate the importance of including the effect of the inter-cluster interactions self-consistently,
 374 which are usually disregarded in cluster-based approaches, we have compared the behavior of
 375 the superconducting d - and extended s -wave orders as a function of density n , for an attractive
 376 V (see Fig. 13) in the presence and absence of the anomalous mean-field parameters (which we
 377 refer to as E_d and E_s respectively). Certain regions of the extended s -wave order, that we ob-
 378 serve in our analysis, disappear entirely in the absence of the self-consistent anomalous mean
 379 field parameter E_s . These regions tend to reappear, but with a smaller amplitude, when the at-
 380 tractive V is sufficiently strong. Likewise, in the case of d -wave superconductivity, we find that
 381 the superconducting order parameter is negligible when E_d is absent, and tends to reappear,
 382 with a much smaller amplitude, when the repulsive U is increased. Our approach is more suit-
 383 able for making predictions about the thermodynamic limit than exact diagonalization studies
 384 on finite-sized clusters, since only the self-energy is limited by the cluster size. Some recent
 385 studies have explored the possibility of magnetic states characterized by ordering wave vectors
 386 that are incommensurate with the lattice periodicity [120] in the two-dimensional Hubbard
 387 model, for electron densities below half-filling, where the antiferromagnetic state becomes
 388 unstable. Our approach is unsuitable for identifying such incommensurate charge and spin
 389 orders. Our method does not suffer from fundamental restrictions on its applicability in any
 390 particular parameter regime, and allows us to study the behavior of the model as a continuous
 391 function of doping, rather than by focusing on specific densities, as has been done in many
 392 previous studies. In the future, this method could be potentially useful for analyzing more
 393 complicated models, including those with spin-orbit interactions. It can also be applied to the
 394 single-band Hubbard model on a triangular lattice, in which the importance of non-local inter-
 395 actions has been pointed out in the literature [121]. It would also be interesting to explore the
 396 regime of non-perturbative repulsive local interactions and attractive extended interactions, to
 397 observe their combined effect on driving or suppressing phase separation [122, 123]. Longer-
 398 range hopping terms can also be included within our exact diagonalization implementation,
 399 which give rise to geometric frustration, making the analysis more relevant for the physics of
 400 the cuprates.

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407 A The inter-cluster mean-field procedure

408 The extended interaction term can be rewritten as

$$\frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'} n_{\mathbf{r}\sigma} n_{\mathbf{r}'\sigma'} = \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^c n_{\mathbf{r}\sigma} n_{\mathbf{r}'\sigma'} + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^{\text{ic}} n_{\mathbf{r}\sigma} n_{\mathbf{r}'\sigma'}$$

409 where \mathbf{r}, \mathbf{r}' refer to the lattice sites, and $n_{\mathbf{r}\sigma}$ is the number of particles at site \mathbf{r} with spin σ .
 410 Here $V_{\mathbf{r}\mathbf{r}'}^c$ and $V_{\mathbf{r}\mathbf{r}'}^{\text{ic}}$ refer to the intra-cluster and inter-cluster parts of the interaction. Inspired

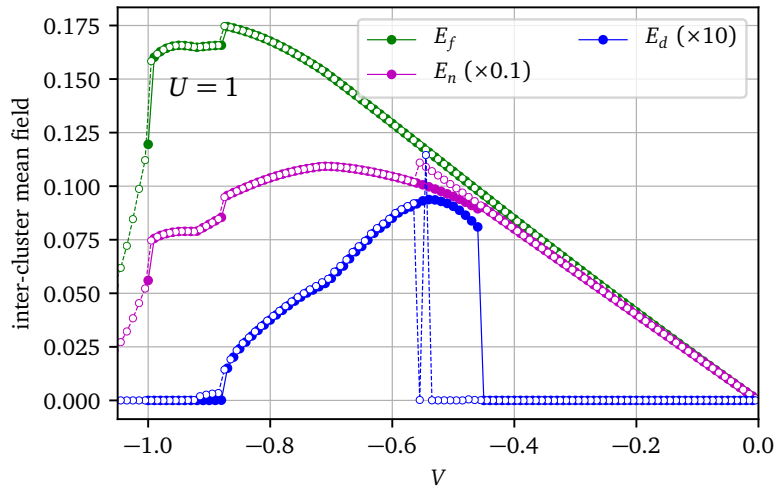


Figure 14: Inter-cluster Hartree-Fock mean fields for the solutions shown in the top panel of Fig. 4. E_d is the eigen-operator associated with d -wave superconductivity, E_f with the nearest-neighbor kinetic operator $f_{\mathbf{r}\mathbf{r}'\sigma\sigma}$ and E_n with the density n (basically a shift in the chemical potential induced by V). The mean-field E_s associated with extended s -wave superconductivity is negligible over almost the entire range of V , since this is at half-filling, except at significantly attractive V (due to phase separation). Note the very different scales (the superconducting mean field is much magnified). The filled and empty circles denote the results for increasing (less negative) and decreasing (more negative) V , respectively. The oscillations in the d -wave order parameters observed close to the transition are also reflected in the corresponding mean-field parameter.

411 by Wick's theorem, we decompose the inter-cluster part of the interaction into Hartree, Fock
412 and anomalous channels, as follows:

$$\begin{aligned} \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^{\text{ic}} n_{\mathbf{r}\sigma} n_{\mathbf{r}'\sigma'} &= \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^{\text{ic}} \left(n_{\mathbf{r}\sigma} \bar{n}_{\mathbf{r}'\sigma'} - \frac{1}{2} \bar{n}_{\mathbf{r}\sigma} \bar{n}_{\mathbf{r}'\sigma'} \right) \\ &\quad - \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^{\text{ic}} \left(f_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \bar{f}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}^* - \frac{1}{2} \bar{f}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}^* \bar{f}_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \right) \\ &\quad + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^{\text{ic}} \left(\Delta_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \bar{\Delta}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}^* + \Delta_{\mathbf{r}\mathbf{r}'\sigma\sigma'}^\dagger \bar{\Delta}_{\mathbf{r}\mathbf{r}'\sigma\sigma'} - \bar{\Delta}_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \bar{\Delta}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}^* \right) \quad (\text{A.1}) \end{aligned}$$

413 where the operators are defined as $n_{\mathbf{r}\sigma} \equiv c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}\sigma}$, $f_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \equiv c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma'}$ and $\Delta_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \equiv c_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma'}$. Note
414 that the applicability of Wick's theorem is not exact in this case, as we are considering a model
415 which already includes on-site interactions, but must be considered as an *ad hoc* Ansatz. In
416 other words, at a fundamental level, we are not assuming that the ground state of the system is
417 a Slater determinant. We are rather resting on a variational principle for the self-energy [124]
418 on which CDMFT is formally based.

419 The sum over sites \mathbf{r}, \mathbf{r}' is taken over the whole lattice. But the average $\bar{n}_{\mathbf{r}\sigma}$ will be assumed
420 to have the periodicity of the cluster, i.e., $\bar{n}_{\mathbf{r}+\mathbf{R}\sigma} = \bar{n}_{\mathbf{r}\sigma}$ where \mathbf{R} belongs to the super-lattice. In
421 addition, the two-site averages $\bar{f}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}$ and $\bar{\Delta}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}$ are assumed to depend only on the relative
422 position $\mathbf{r} - \mathbf{r}'$. The mean-field inter-cluster interaction (A.1) is then a one-body contribution
423 to the Hamiltonian with the periodicity of the super-lattice, and contains both intra-cluster
424 and inter-cluster terms, whereas the purely intra-cluster part $V_{\mathbf{r}\mathbf{r}'}^{\text{C}}$ retains its fully correlated
425 character.

426 For a four-site cluster, we have a total of eight bonds between neighboring clusters, along
427 the x and y directions, with two spin combinations (σ, σ') per bond, where we consider spin-
428 parallel combinations for the Fock terms (in the absence of spin-dependent hopping) and spin-
429 antiparallel combinations for the anomalous terms. In practice, we only consider physically
430 relevant combinations of operators defined on different sites/bonds for our analysis (such as
431 those compatible with a d -wave or an extended s -wave order). As an illustration of this, let
432 us consider the pairing fields Δ defined on all of these bonds, which we denote by the labels
433 $i = 1 - 16$ (including different bond and spin combinations).

434 The mean-field Hamiltonian can be written as

$$\frac{V}{2} \sum_{i,j} (\bar{\Delta}_i^* M_{ij} \Delta_j + \Delta_i^\dagger M_{ij} \bar{\Delta}_j - \bar{\Delta}_i^* M_{ij} \bar{\Delta}_j) \quad (\text{A.2})$$

435 where $i, j = (\mathbf{r}, \mathbf{r}', \sigma, \sigma')$ and the matrix M_{ij} describes the combinations of the pairing fields
436 defined on different bonds which appear in the Hartree-Fock decomposition of the inter-cluster
437 interactions. The matrix M turns out to be an identity matrix for the Fock and pairing fields f
438 and Δ respectively, but the corresponding matrix for the Hartree fields n is off-diagonal.

439 Defining the eigen-combinations of the pairing fields by

$$E_\alpha = U_{\alpha i} \Delta_i \quad (\text{A.3})$$

440 and the eigenvalues of the matrix M by λ_α , such that

$$M_{ij} = \sum_{\alpha, \beta} U_{\alpha i}^* \lambda_\alpha \delta_{\alpha\beta} U_{\beta j}$$

441 we can rewrite Eq. (A.2), above, as

$$\frac{V}{2} \sum_{\alpha} \lambda_\alpha (\bar{E}_\alpha^* E_\alpha + E_\alpha^\dagger \bar{E}_\alpha - \bar{E}_\alpha^* \bar{E}_\alpha) \quad (\text{A.4})$$

442 The mean-field values \bar{E}_α of the relevant eigen-combinations E_α of the pairing operators de-
 443 fined on different nearest-neighbor bonds are obtained self-consistently within the CDMFT
 444 loop, and likewise for the other mean fields that are the appropriate eigen-combinations of
 445 $\bar{n}_{r\sigma}$ and $\bar{f}_{rr'\sigma\sigma'}$.

446 B CDMFT convergence

447 The CDMFT procedure is iterative and aims at finding a solution to a set of nonlinear equations
 448 that can be schematically expressed as

$$\mathbf{x} = \mathbf{f}(\mathbf{x}) , \quad (\text{B.1})$$

449 where \mathbf{x} stands for the set of bath and inter-cluster Hartree-Fock parameters and \mathbf{f} is an equally
 450 large set of functions that returns the next set of parameters from the current set, following
 451 a procedure that combines the CDMFT update with the inter-cluster mean-field one. The
 452 canonical way to solve Eqs (B.1) is the fixed-point method: the map $\mathbf{x}_{n+1} = \mathbf{f}(\mathbf{x}_n)$ is iterated
 453 until the difference $\Delta\mathbf{x}_{n+1} = \mathbf{x}_{n+1} - \mathbf{x}_n$ is smaller than some preset accuracy.

454 However, if the purpose is to find a solution to (B.1), there are more efficient and stable
 455 alternatives. Specifically, one could use the classic Broyden method for finding roots of sets
 456 of nonlinear equations, a generalization to many variables of Newton’s root-finding method.
 457 Broyden’s method relies on a computation of the Jacobian matrix $\mathbf{J} = \partial\mathbf{f}/\partial\mathbf{x}$ that is improved
 458 at each iteration. It typically finds a solution with fewer iterations than the fixed-point method,
 459 and with greater accuracy. In addition, it is “stickier”, meaning that upon performing an exter-
 460 nal loop over model parameters, it will “stick” to the current solution (or the current phase),
 461 whereas the fixed-point method will be prone to instabilities and will more likely switch to
 462 more stable solutions.

463 This means that the fixed-point method, although less efficient, is more appropriate to
 464 detect phase transitions, whereas the Broyden method is better at keeping the current solution
 465 into its metastable regime. Hence the Broyden method will typically result in wider hysteresis
 466 loops than the fixed-point method when the external parameter is cycled in both directions
 467 (ascending and descending).

468 In practice, we can converge the CDMFT-DHF procedure on the difference $\Delta\mathbf{x}_{n+1}$, but we
 469 can also ask for the convergence of physical quantities, such as the cluster self-energy $\Sigma(\omega)$, or
 470 relevant order parameters. It may happen that physical quantities converge even though bath
 471 parameters do not, because the latter are sometimes subject to discrete “gauge” symmetries
 472 that do not affect physical observables. But even though convergence criteria may be based
 473 on physical quantities, the iteration $\mathbf{x}_n \rightarrow \mathbf{x}_{n+1}$ is still based on either the fixed point or the
 474 Broyden method. In this work, we used the self-energy and relevant order parameters as
 475 convergence criteria, with accuracies of the order of 10^{-4} .

476 As an illustration, we compare the behavior of the relevant order parameters for the phases
 477 observed at the particle-hole symmetric chemical potential as a function of $U > 0$ for $V = -0.6$
 478 in Fig. 15 and as a function of $V < 0$ for $U = 2$ in Fig. 16, using the fixed-point and the
 479 Broyden methods for obtaining the optimal set of CDMFT parameters. As expected, the region
 480 of hysteresis is found to be much larger when the Broyden method is used, consistent with
 481 the tendency of this method to stick to the current solution. Interestingly, we find that the
 482 existence of d -wave order does not necessarily coincide with phase separation, and there may
 483 be a region with a nontrivial d -order parameter even at half-filling. However, such a region is
 484 not easily observed with the fixed-point method and is usually significantly amplified when the
 485 Broyden method is used, as illustrated in the lower plot of Fig. 15. We also observe oscillations
 486 between the d -wave solutions obtained in the presence and absence of phase separation within

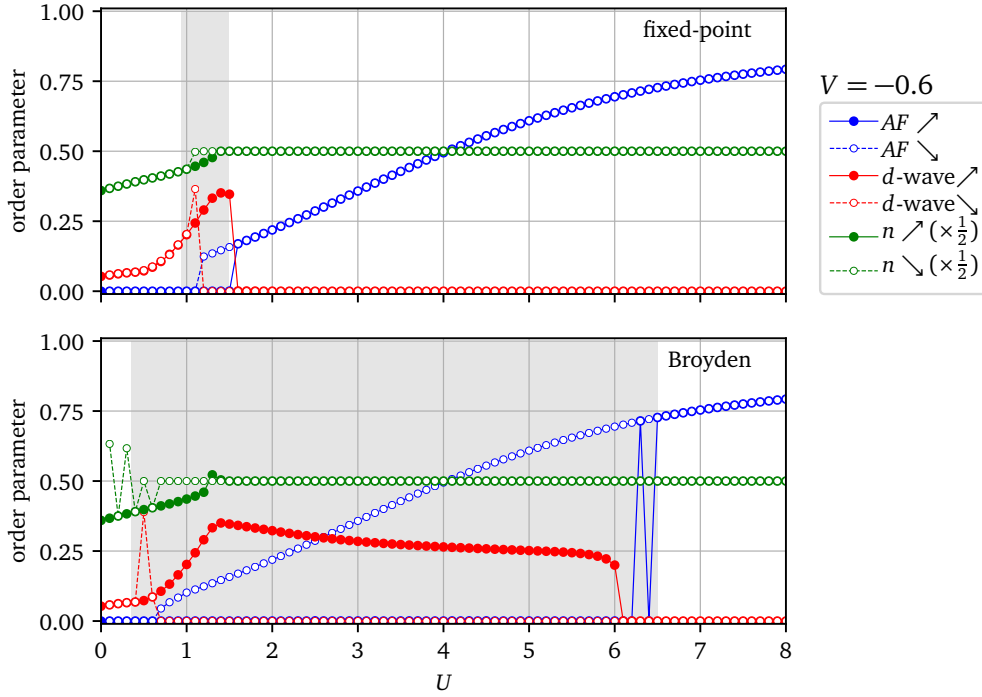


Figure 15: Order parameters for the different phases observed at the particle-hole symmetric chemical potential for $V = -0.6$, as a function of U , using the fixed-point method (above) and the Broyden method (below) for obtaining the optimal set of bath and mean-field parameters. The hysteresis loop obtained for increasing and decreasing U is found to be much larger for the Broyden method, indicating that it has a tendency to stick to the current solution. A prominent region with a nontrivial d -wave superconducting order parameter is observed at half-filling for the Broyden method (indicated by the region with filled red circles in the lower plot). The transition from the phase-separated to the half-filled state is indicated by a shoulder-like feature in the corresponding d -wave order parameter. Oscillations are observed between the d -wave solutions with and without phase separation, within the hysteresis region, for both methods. In the presence of phase separation, the density is found to oscillate between values greater than and less than 1, when the Broyden method is used, and sometimes also with the fixed-point method. Moreover, some oscillations are also observed between the AF and normal states, close to the phase transition towards AF for increasing U (see open blue circles in the lower plot).

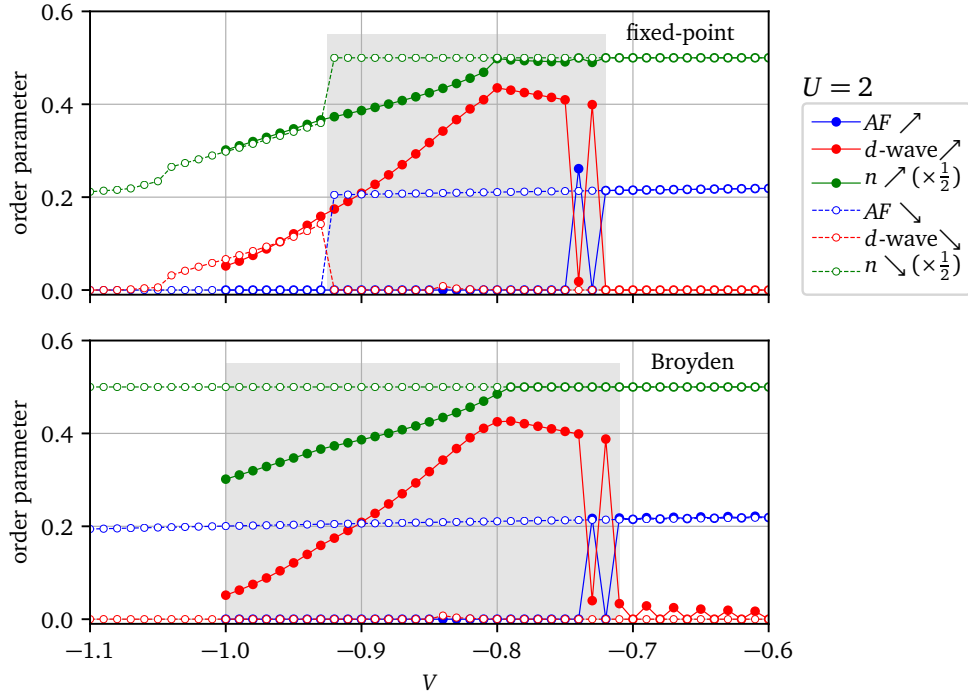


Figure 16: Order parameters corresponding to the different phases observed at the particle-hole symmetric chemical potential for $U = 2$, as a function of V , using the fixed-point method (above) and the Broyden method (below) for obtaining the optimal bath and mean-field parameters. Once again, the hysteresis region between increasing and decreasing negative V is found to be much larger when the Broyden method is employed. Interestingly, the AF region is found to persist all the way to $V = -1.8$ for decreasing (more negative) V with the Broyden method (not shown in the figure), beyond which the system directly undergoes a transition to the normal state, and the intervening d -wave superconducting region is found to be absent (the open blue circles in the lower plot depict the behavior up till $V = -1.1$). For increasing (less negative) V , a part of the d -wave superconducting phase observed is found to be very close to half-filling for both methods (indicated by the filled red circles). Moreover, oscillations are observed between the d -wave and AF phases, which are found to occur more frequently when the Broyden method is used. Note that the results for increasing V have been plotted starting from $V = -1.0$ in both cases for convenience, but may be smoothly extrapolated to more negative values of V .

487 the gray hysteresis region, for both the methods. Although the Broyden method converges
488 faster even with a higher accuracy, we obtain more oscillatory solutions in general with this
489 method, which includes oscillations between densities greater than and less than 1 in the
490 phase-separated region for small U , as well as between the normal state and the AF state,
491 close to the transition from d -wave to antiferromagnetism for increasing U . In Fig. 16, we see
492 that d -wave superconducting state persists well into the region of half-filling as V becomes
493 less negative, for both methods. When the Broyden method is used, we find that the system
494 continues in the AF state down to $V = -1.8$ and then undergoes a transition to the normal
495 state, without the appearance of a d -wave order or phase separation. This is an extreme
496 example of the tendency of this method to preserve the existing solution. In contrast, the
497 fixed-point method gives rise to a phase transition towards the d -wave superconducting state,
498 close to $V=-0.9$. Therefore, for most situations, it is more convenient for us to employ the
499 fixed-point method for our computations.

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CDMFT+HFD : an extension of dynamical mean field theory for non-local interactions applied to the single band extended Hubbard model

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Abstract

We examine the phase diagram of the extended Hubbard model on a square lattice, for both attractive and repulsive nearest-neighbor interactions, using CDMFT+HFD, a combination of Cluster Dynamical Mean Field theory (CDMFT) and a Hartree-Fock mean-field decoupling of the inter-cluster extended interaction. For attractive non-local interactions, this model exhibits a region of phase separation near half-filling, in the vicinity of which we find **pockets-islands** of d -wave superconductivity, decaying rapidly as a function of doping, with disconnected **patches-regions** of extended s -wave order at smaller (higher) electron densities. On the other hand, when the extended interaction is repulsive, a Mott insulating state at half-filling is destabilized by hole doping, in the strong-coupling limit, in favor of d -wave superconductivity. At the particle-hole invariant chemical potential, we find a first-order phase transition from antiferromagnetism (AF) to d -wave superconductivity as a function of the attractive nearest-neighbor interaction, along with a deviation of the density from the half-filled limit. A repulsive extended interaction instead favors charge-density wave (CDW) order at half-filling.

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21 1 Introduction

22 The single-band Hubbard model has long served as a useful platform for studying the effect of
23 strong electronic correlations [1–6]. In particular, it explains many of the experimental obser-
24 vations in the high- T_c cuprate superconductors [2, 7–16], providing an approximate picture for
25 the description of these materials [17–25]. More recently, there have been numerous studies
26 on extensions of this model with nearest-neighbor interactions, known as the extended Hub-
27 bard model (EHM) [26–90]. There are several reasons for the continuing interest of the com-
28 munity in exploring the effect of non-local interactions. In actual materials, the interactions
29 between neighboring sites may not be completely screened, necessitating a more careful treat-
30 ment of longer-range interactions. The model with an attractive nearest-neighbor interaction
31 provides an effective representation of the attractive interactions mediated by electron-phonon
32 coupling, and may be realized in ultra-cold atom systems. The relevance of studying such a
33 model is further emphasized by recent ARPES studies on the one-dimensional cuprate chain
34 compound $\text{Ba}_{2-x}\text{Sr}_x\text{CuO}_{3+\delta}$ [91], where the observations can be explained using a Hubbard
35 model with an attractive extended interaction. On the other hand, the model with repulsive
36 non-local interactions provides an ideal playground for studying the interplay of charge and
37 spin fluctuations, since the relative magnitude of the charge fluctuations can be controlled by
38 the strength of the extended interaction [26, 30, 34, 35]. The EHM at quarter-filling has proven
39 useful for describing the charge ordering transition due to inter-site Coulomb interactions in
40 a variety of materials [28, 48, 49, 79, 83]. Both the Hubbard model and its extension with
41 longer-range interactions have contributed significantly to the methodological development
42 in the field of strongly correlated systems, and in particular high- T_c superconductors, which is
43 essential for obtaining results that can be quantitatively compared with experiments.

44 In recent years, the properties of the EHM have been analyzed using a variety of ap-
45 proaches, including, among others, mean-field theory [50–52, 72], functional renormalization
46 group (fRG) [39], exact diagonalization (ED) [29, 32, 55, 61], density-matrix renormalization
47 group (DMRG) [57, 63], Quantum Monte Carlo (QMC) [70, 87, 89, 92] and the fluctuation-
48 exchange approximation (FLEX) [56]. However, many of the approaches used are best suited
49 for studying the weak-coupling or the strong-coupling limit, and there are few that can de-
50 scribe the intermediate-coupling regime equally well. Even among those that can, each has its
51 own limitations. For instance, simple exact diagonalizations are restricted to small systems,
52 quantum Monte Carlo methods suffer from the fermion sign problem in many applications
53 of interest, the density-matrix renormalization group (DMRG) applies to one-dimensional or
54 ribbon-like systems, etc. In addition, certain aspects of the model with repulsive interactions
55 have been studied in detail using the so-called extended dynamical mean-field theory (EDMFT)
56 approach [93–95], in which the local density fluctuations together with the local self-energy

57 are propagated on the whole lattice using the known dispersion and density-density extended
 58 interactions. Other variations of this method, such as a combination of EDMFT with the GW
 59 approximation [27, 96–98], which perturbatively includes non-local self-energy corrections,
 60 and the dual boson method [81, 82, 99], which constructs a diagrammatic expansion about
 61 the extended DMFT, have likewise contributed to its understanding. More recently, cluster
 62 methods [26, 38, 76–78, 100, 101], which capture short-range correlations non-perturbatively
 63 within periodic clusters, have also been applied to this model. However, such studies have
 64 largely been limited to fixed densities and repulsive interactions. Overall, there have been
 65 fewer studies that consider both an extensive range of interaction couplings and band fillings,
 66 and relatively less focus on the case of attractive extended interactions.

67 In this paper, we study the phase diagram of the extended Hubbard model on a square
 68 lattice, for both attractive and repulsive nearest-neighbor interactions, using CDMFT+HFD,
 69 an extension of the Cluster Dynamical Mean Field Theory (CDMFT) [100, 102] approach with
 70 a Hartree-Fock decoupling of the inter-cluster interactions. CDMFT belongs to a class of meth-
 71 ods called Quantum Cluster Methods [103–109]. This is a set of approaches that consider a
 72 finite cluster of sites embedded in an infinite lattice, and introduce additional fields or “bath”
 73 degrees of freedom, determined by variational or self-consistency principles, to best represent
 74 the effect of the surrounding infinite lattice. These methods have proven useful for interpola-
 75 tion between results obtained in the weak- and strong-coupling regimes, since their accuracy
 76 is controlled by the size of the clusters used, rather than the strength of the couplings. Fur-
 77 ther, we treat the inter-cluster interactions within a Hartree-Fock mean-field decoupling, which
 78 generates additional Hartree, Fock and anomalous contributions to the cluster Hamiltonian.
 79 While a similar treatment has been used to study the model at quarter-filling [48] for the case
 80 of repulsive interactions, with the objective of understanding the electronic properties of met-
 81 als close to a Coulomb-driven charge ordered insulator transition, this analysis was focused
 82 on a specific parameter regime, and did not include superconducting orders.

83 This work constitutes a test of the CDMFT+HFD method, described in Sect. H-2 below. Our
 84 main findings are as follows. For a weak repulsive local interaction U and an attractive ex-
 85 tended interaction V , the system undergoes a transition towards a phase separated (PS) state
 86 when the chemical potential lies in the vicinity of its particle-hole symmetric value, $U/2 + 4V$.
 87 The exact region of phase separation is identified by using the hysteresis in the behavior of
 88 the electron density as a function of the chemical potential, which corresponds to the coex-
 89 istence of two different uniform-density solutions. As a function of doping away from the
 90 half-filled point, symmetrical and sharply decaying regions of $d_{x^2-y^2}$ -wave superconducting
 91 order are observed, followed by disconnected **pockets regions** of extended s -wave order near
 92 quarter-filling, as well as at very small (large) densities. A stronger attractive extended in-
 93 teraction tends to favor phase separation as well as superconductivity, whereas the repulsive
 94 on-site interaction U is found to be detrimental to both. At the particle-hole symmetric chemi-
 95 cal potential, we detect a first-order phase transition from antiferromagnetism (AF) to d -wave
 96 superconductivity as the attractive V becomes stronger, which is accompanied by a gradual
 97 deviation of the density from its half-filled limit, induced by phase separation. For repulsive
 98 nearest-neighbor interactions in the strong-coupling regime $U \gg t$, the Mott insulating state
 99 at half-filling is destabilized, upon hole doping, in favor of a dome-shaped region of d -wave
 100 superconducting order. This order is found to be remarkably stable in the presence of a non-
 101 local interaction, and slightly suppressed by it. At half-filling, a repulsive non-local interaction
 102 induces a first-order phase transition from antiferromagnetism (AF) to a charge-density wave
 103 (CDW) order. Our results are qualitatively in agreement with the existing literature on the
 104 phase diagram of the EHM, with some notable differences in the region of attractive interac-
 105 tions. An important difference is that intra-cluster fluctuations are treated exactly, which tends
 106 to make superconducting orders somewhat weaker in this approach.

107 The paper is organized as follows. In Sect. H2, we introduce the model Hamiltonian, and
 108 provide a brief overview of the CDMFT approach that we use for our analysis, as well as the
 109 Hartree-Fock mean-field decoupling of the [intercluster-inter-cluster](#) interactions. In Sect. H3,
 110 we describe the phase diagram obtained as a function of the interaction strength and doping,
 111 and the phase transitions observed at half-filling. Finally, in Sect. IV4, we summarize our
 112 results, discuss some relevant observations and present the conclusions of our study.

113 2 Model and method

114 2.1 Model Hamiltonian

115 The general form of the extended Hubbard model Hamiltonian is

$$H = \sum_{\mathbf{r}, \mathbf{r}', \sigma} t_{\mathbf{r}\mathbf{r}'} c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'} n_{\mathbf{r}\sigma} n_{\mathbf{r}'\sigma'} \quad (1)$$

116 where \mathbf{r}, \mathbf{r}' label lattice sites, $t_{\mathbf{r}\mathbf{r}'}$ are the hopping amplitudes, U the on-site Hubbard interaction,
 117 and $V_{\mathbf{r}\mathbf{r}'}$ the nearest-neighbor interaction (each bond counted once, hence the factor $\frac{1}{2}$).

118 For the purpose of our analysis, we study the following model on a square lattice:

$$H = -t \sum_{\mathbf{r}} (c_{\mathbf{r}}^\dagger c_{\mathbf{r}+\mathbf{x}} + c_{\mathbf{r}}^\dagger c_{\mathbf{r}+\mathbf{y}} + \text{H.c.}) + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} - \mu \sum_{\mathbf{r}} (n_{\mathbf{r}\uparrow} + n_{\mathbf{r}\downarrow}) + V \sum_{\mathbf{r}, \sigma, \sigma'} (n_{\mathbf{r}\sigma} n_{\mathbf{r}+\mathbf{x}, \sigma'} + n_{\mathbf{r}\sigma} n_{\mathbf{r}+\mathbf{y}, \sigma'}) \quad (2)$$

119 where \mathbf{x}, \mathbf{y} are the lattice unit vectors along the x and y directions, and the operator $c_{\mathbf{r}\alpha}$ an-
 120 nihilates a particle with spin $\alpha = \uparrow, \downarrow$ at site \mathbf{r} . The occupation number is $n_{\mathbf{r}\alpha} = c_{\mathbf{r}\alpha}^\dagger c_{\mathbf{r}\alpha}$. We
 121 consider a range of values for the chemical potential μ , corresponding to a continuous range
 122 of densities, from $n = 0$ to 2, along with a repulsive local interaction $U > 0$, and a nearest-
 123 neighbor interaction V that can be positive or negative. The particle-hole symmetric value of
 124 the chemical potential, $\mu = U/2 + 4V$, which corresponds to a half-filled band in the absence
 125 of phase separation, features prominently in our analysis. The unit of energy is taken to be
 126 the nearest-neighbor hopping amplitude $t = 1.0$, with the lattice constant $a = 1$. Note that
 127 in the absence of longer-range hopping terms, beyond the nearest-neighbor bonds, the model
 128 respects particle-hole symmetry $n \rightarrow 2 - n$.

129 We examine the possibility of superconducting as well as density-wave orders. For this
 130 purpose, the anomalous operators are defined on the lattice using a d -vector, as

$$\Delta_{\mathbf{r}\mathbf{r}', b} c_{\mathbf{r}\sigma} (i\sigma_b \sigma_2)_{\sigma\sigma'} c_{\mathbf{r}'\sigma'} + \text{H.c.} \quad (3)$$

131 where $b = 0, 1, 2, 3$, and σ_b are the Pauli matrices. The case $b = 0$ corresponds to singlet
 132 superconductivity, in which case $\Delta_{\mathbf{r}\mathbf{r}', 0} = \Delta_{\mathbf{r}'\mathbf{r}, 0}$ and the cases $b = 1, 2, 3$ correspond to triplet
 133 superconductivity, in which case, $\Delta_{\mathbf{r}\mathbf{r}', b} = -\Delta_{\mathbf{r}'\mathbf{r}, b}$. In practice, these operators are defined by
 134 specifying b and the relative position $\mathbf{r} - \mathbf{r}'$.

135 Density wave operators are defined with a spatial modulation characterized by a wave
 136 vector \mathbf{Q} , and can be based on sites or on bonds. In our analysis, we focus on site density
 137 waves, defined as

$$\sum_{\mathbf{r}} A_{\mathbf{r}} \cos(\mathbf{Q} \cdot \mathbf{r} + \phi) \quad (4)$$

138 where $A_{\mathbf{r}} = n_{\mathbf{r}}, S_{\mathbf{r}}^x, S_{\mathbf{r}}^z$ corresponds to charge- or spin-density wave orders, and ϕ is a sliding
 139 phase. We probe the presence of density-wave orders with $\mathbf{Q} = (\pi, \pi)$ and $\phi = 0$.

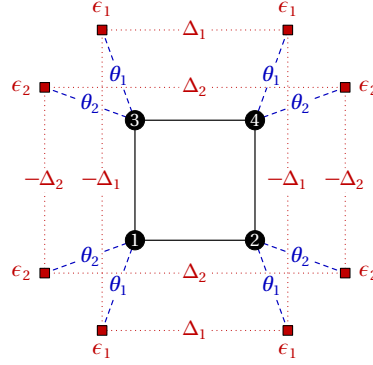


Figure 1: Schematic representation of the first (“simple”) impurity problem used in our analysis, with bath energies ϵ_i , cluster-bath hybridization parameters θ_i and anomalous bath parameters Δ_i . Physical sites are marked by numbered black dots and bath orbitals by red squares. We choose the bath parameters such that the environment of each cluster site is identical. This impurity model has reflection symmetry with respect to horizontal and vertical mirror planes (C_{2v} symmetry), and typically involves only spin-independent hopping terms. Pairing terms $\Delta_{1,2}$ are introduced between bath orbitals, with signs adapted to the SC order probed (shown here for a d -wave order, but all positive for an extended s -wave order). The number of independent bath parameters is 6.

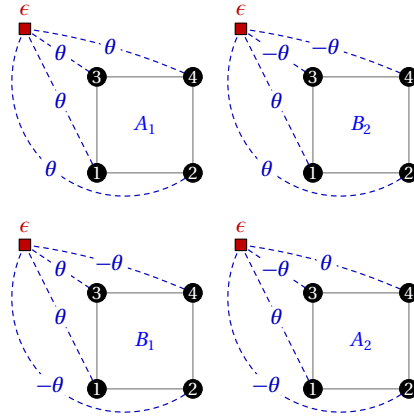


Figure 2: Schematic representation of the second (“general”) impurity problem used in our analysis. Each representation of the point group C_{2v} ($A_{1,2}$ and $B_{1,2}$) corresponds to a set of phases (± 1), and each of the 8 bath orbitals belongs to one of these four representations (two bath orbitals per representation). The different bath orbitals are independent (the bath system is diagonal) and we only show here a view of each of the four representations with the corresponding signs associated to each cluster site (black dots). The hybridization parameters θ are shown, and corresponding pairing operators (or anomalous hybridizations) between each bath orbital and each site also exist, with the same relative phases. The number We have 3 parameters per bath orbital, which leads to a total of 24 bath parameters, and subtracting six constraints due to a C_{4v} rotational symmetry, we obtain 18 independent bath parameters is 18.

140 2.2 Method: CDMFT+HFD

141 Let us briefly describe the method used in our analysis, Cluster dynamical mean-field theory
 142 (CDMFT). For a detailed discussion of the basic principles of such Quantum Cluster Methods,
 143 please see Ref. [103, 105, 110].

144 This approach is an extension of dynamical mean-field theory (DMFT) [111–114], which
 145 accounts for short-range spatial correlations, by considering a cluster of sites with open bound-
 146 ary conditions, instead of a single-site impurity. The effect of the cluster’s environment is taken
 147 into account by introducing a set of uncorrelated “bath” “bath” orbitals hybridized with it. In
 148 this manner, the infinite lattice is tiled into identical clusters coupled to a bath of auxiliary,
 149 uncorrelated orbitals, with energy levels $\epsilon_{i\sigma}$, which may or may not be spin dependent, and
 150 hybridized with the cluster sites (labeled r) with amplitudes $\theta_{ir\sigma}$. In addition, for studying
 151 superconducting orders, different types of anomalous pairings $\Delta_{ij\sigma\sigma'}$ may be introduced be-
 152 tween bath orbitals i, j or $\Delta_{ir\sigma\sigma'}$ between bath orbital i and cluster site r .

153 ~~In our analysis, we~~ The cluster and bath size is limited by the exact diagonalization solver:
 154 the practical upper limit for the total number of cluster and bath orbitals is 4+8=12, given that
 155 the ground state and Green function must be computed repeatedly in this approach. A true
 156 finite-size analysis is impossible here, for the next cluster size of the same square geometry
 157 would be 9, and the number of bath orbitals would need to grow accordingly. Even in a
 158 one-dimensional model, analyzing finite-size effects in CDMFT is challenging, because of the
 159 combined effects of cluster size and bath size [115].

160 We use two types of bath models. In the simple model (Fig. 1), the environment of each
 161 cluster is identical, and we introduce two bath orbitals per cluster site. Parameters of the
 162 impurity model include bath orbital energy levels ($\epsilon_{1,2}$), hybridization between each cluster
 163 site and the corresponding bath orbitals ($\theta_{1,2}$), and pairings between the bath orbitals ($\Delta_{1,2}$).
 164 The precise form of $\Delta_{1,2}$, including their relative phases between different bath orbitals, de-
 165 pends on whether we probe extended s -wave, d -wave, or triplet superconductivity. This sim-
 166 ple impurity model involves 6 independent parameters to be determined self-consistently. At
 167 half-filling, we introduce bath energies as well as hoppings, that are consistent with the ap-
 168 pearance of a density-wave order, and additionally spin-dependent in the presence of anti-
 169 ferromagnetism. This increases the number of independent parameters. However, imposing
 170 particle-hole symmetry at half-filling once again reduces this number to 6. For $V < 0$, we
 171 do not impose particle-hole symmetry on the bath parameters due to the possibility of phase
 172 separation, and the number then increases to 10.

173 We also use a more general bath model (Fig. 2). While the total number of bath orbitals
 174 is unchanged, every bath orbital is connected to every cluster site (with distinct combinations
 175 of relative phases), and we define bath energies, cluster-bath hybridizations and anomalous
 176 pairings between the cluster and the bath sites. In this model the bath is diagonal, i.e., the dif-
 177 ferent bath orbitals are not directly coupled between themselves, ~~and,~~ We have 3 parameters
 178 per bath orbital, and taking into account six constraints due to rotation symmetry, there are
 179 18 independent bath parameters to set. At the particle-hole symmetric chemical potential, we
 180 introduce bath energies, hybridizations and anomalous pairings that have two different values
 181 for alternative sites. ~~Even upon taking into account particle-hole symmetry, this~~ This gives us
 182 a total of ~~52~~ 42 independent parameters in the ~~presence of superconductivity, and 20~~ absence
 183 of particle-hole symmetry for $V < 0$ and 15 independent parameters when superconductivity
 184 is absent (i.e. for $V > 0$) and particle-hole symmetry is taken into account.

185 All bath parameters are determined by a self-consistency condition (see Ref. [103, 105, 110]
 186 for details). The simple bath model is expected to be easier to converge than the general bath
 187 model, because of the smaller set of parameters. While we expect the results obtained from the
 188 general bath model to be more reliable, we do find most of the results to be qualitatively similar
 189 in the two cases. Once the bath parameters are converged, the self-energy $\Sigma(\omega)$ associated

190 with the cluster is applied to the whole lattice, so that the lattice Green function is

$$\mathbf{G}^{-1}(\tilde{\mathbf{k}}, \omega) = \mathbf{G}_0^{-1}(\tilde{\mathbf{k}}, \omega) - \Sigma(\omega) \quad (5)$$

191 Here, $\tilde{\mathbf{k}}$ denotes a reduced wave vector (defined in the Brillouin zone of the super-lattice
192 of clusters defined by the tiling) and \mathbf{G}_0 is the non-interacting Green function. The Green-
193 function-like objects \mathbf{G} , \mathbf{G}_0 and Σ are $L \times L$ matrices, L being the number of physical degrees
194 of freedom on the cluster (here $L = 8$ because of spin and the four cluster sites). The aver-
195 age values of one-body operators defined on the lattice are obtained using the lattice Green
196 function \mathbf{G} determined from the solution for the optimum values of the bath parameters. An
197 exact-diagonalization solver (the Lanczos method or variants thereof) is used at zero temper-
198 ature. The computational size of the problem increases exponentially with the total number
199 of cluster and bath orbitals.

200 In the presence of extended interactions, we also perform a Hartree-Fock mean-field de-
201 composition of the interaction terms defined between different clusters, while the interactions
202 within a cluster are treated exactly. The inter-cluster interactions are decoupled in the Hartree,
203 Fock and anomalous channels, which contribute to the number density, the hopping and the
204 pairing operators, respectively. Moreover, we only retain those combinations of the site/bond
205 operators that are physically relevant in the regions we work in (such as ~~*d-wave or extended*~~
206 ~~*s-waved-wave or extended s-wave*~~), and discard the rest. The mean-field values of the rele-
207 vant combinations are determined self-consistently, within the CDMFT loop that optimizes the
208 bath parameters. For the details of this procedure, please refer to [the Appendix Appendix A.](#)
209 [For a comparison of different methods used for solving the self-consistent nonlinear equations](#)
210 [involved in the CDMFT procedure, please refer to Appendix B.](#)

211 3 Results

212 In this section, we discuss the salient features of the phase diagram obtained from our analysis,
213 for both attractive and repulsive nearest-neighbor interactions. The dominant superconduct-
214 ing and density-wave orders are identified by computing the corresponding order parameters
215 using the optimum values of the CDMFT (bath and mean-field) parameters, as a function of
216 electron density, as well as at half-filling. In the following analysis, we focus our attention on
217 the strong coupling limit $U \gg t$ for $V > 0$, which is a regime well-understood on physical
218 grounds. For $V < 0$, we consider relatively weak interactions $U \sim t$, far from the Mott insu-
219 lating regime, which primarily serve the purpose of controlling the extent of phase separation
220 when the interaction V becomes sufficiently attractive. At half-filling, we confirm the nature
221 of the phase transitions, by plotting the relevant order parameters both as a function of $U > 0$,
222 for fixed values of $V > 0$ or $V < 0$, and as a function of V for fixed values of U .

223 3.1 Phase diagram at the particle-hole symmetric chemical potential

224 Here, we fix the chemical potential to $\mu = U/2 + 4V$, corresponding to a half-filled band, and
225 examine the behavior of different superconducting and density-wave orders, as a function of
226 the local repulsion U as well as attractive/repulsive V . While antiferromagnetism is favored at
227 half-filling, in both ~~the~~ weak- and strong-coupling regimes, an attractive non-local interaction
228 is expected to drive the system towards a superconducting instability, and eventually phase
229 separation. On the other hand, repulsive interactions V would typically foster competition
230 between charge and spin fluctuations, and favor a charge-ordered state. Below, we discuss the
231 results obtained using the simple bath model (Fig. 1).

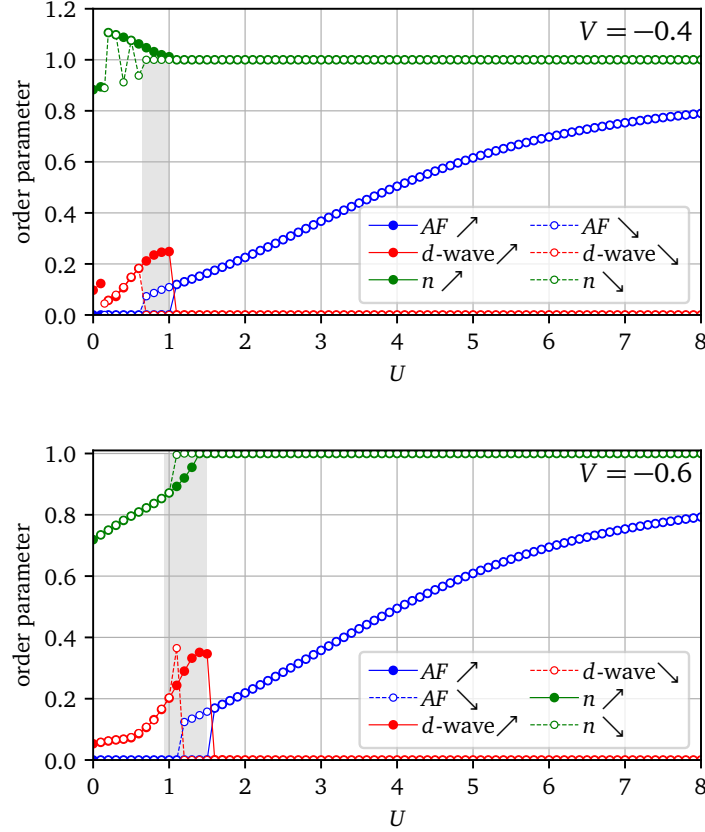


Figure 3: First-order phase transition from d -wave superconductivity (indicated by filled/open red circles) to antiferromagnetism (AF, indicated by filled/open blue circles), as a function of the repulsive local interaction U , at fixed $V = -0.4$ (top) and $V = -0.6$ (bottom), and fixed chemical potential $\mu = U/2 + 4V$ (particle-hole symmetric point). The simple impurity model (Fig. 1) is used. The transition is accompanied by a deviation in the number density (indicated by filled/open green circles) from the half-filled value $n = 1$, meaning that we are entering a phase separated regime. **This may also explain the rapid suppression of superconductivity for smaller values of U for a more negative interaction V .** The dashed (solid) curves of each color depict the behavior of the different quantities for decreasing (increasing) U , respectively. The prominent region of hysteresis between the two curves confirms the order of the transition. The small jump/discontinuity observed in the d -wave order parameter for increasing U for $V = -0.4$ results from issues with the convergence of the CDMFT procedure at that point. On the other hand, for $V = -0.6$, we observe a jump in the d -wave order parameter for decreasing U , which appears to signal a transition from a d -wave order at half-filling to one coexisting with phase separation, rather than being a numerical error. Likewise, for increasing U , we observe a nontrivial d -wave order parameter both in the presence and absence of phase separation for $V = -0.6$ (for more details, see Appendix B).

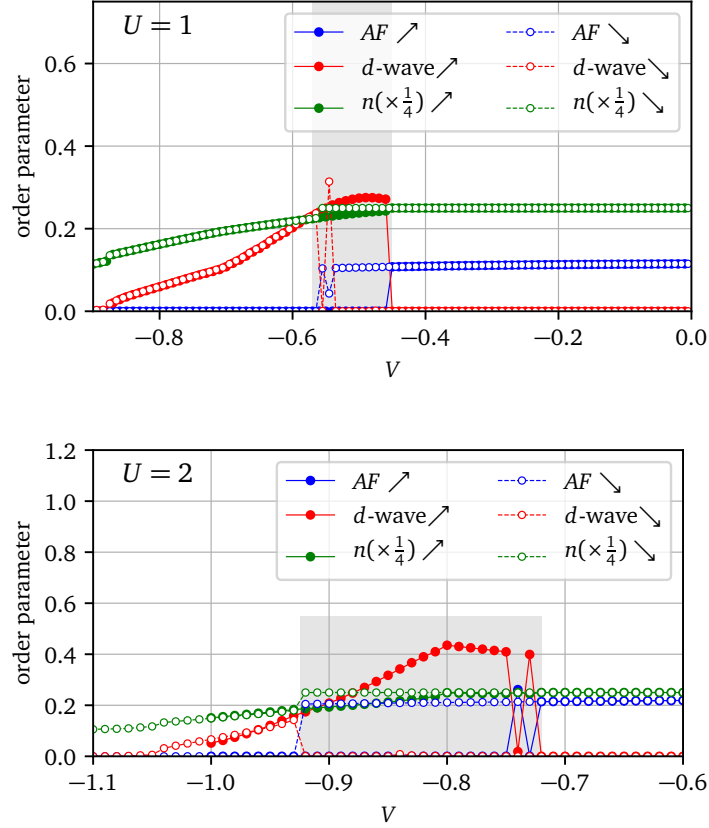


Figure 4: First-order phase transition from antiferromagnetism (AF) (indicated by filled/open blue circles) to d -wave superconductivity (indicated by filled/open red circles), for increasingly attractive V , followed by a rapid suppression in the superconducting order parameter, for on-site interaction $U = 1$ (top) and $U = 2$ (bottom). The simple impurity model (Fig. 1) is used. The transition is accompanied by a deviation in the number density (indicated by filled/open green circles) from the half-filled value $n = 1$. The dashed (solid) curves of each color depict the behavior of different quantities for decreasing/more negative (increasing/less negative) V , and we find significant hysteresis. For larger repulsive interactions U , the transition is found to occur at a critical value of V that is more attractive. For $U = 1$, we observe oscillations between the d -wave and AF orders at half-filling, close to the transition for decreasing/more negative V , while for $U = 2$, we see a significant region of d -wave superconductivity close to half-filling for increasing/less negative V , as well as similar oscillations between the d -wave and AF orders at half-filling, close to the transition between the two states for increasing/less negative V .

232 3.1.1 $V < 0$:

233 For a fixed attractive nearest-neighbor interaction V , as the strength of the local repulsive
 234 interaction U decreases, the system undergoes a first-order phase transition from antiferro-
 235 magnetism to d -wave superconductivity. This is accompanied by a deviation in the electron
 236 density from its half-filled limit, which can be attributed to the effects of phase separation, dis-
 237 cussed in more detail in the next subsection. Each of the order parameters is plotted for both
 238 increasing and decreasing U , and the region of hysteresis between the two curves indicates
 239 that the transition is first-order in nature. We have verified that other pairing symmetries,
 240 such as extended s -wave and p -wave, do not compete with $d_{x^2-y^2}$ pairing in this regime. The
 241 results of our analysis are shown in Fig. 3. Likewise, an antiferromagnetic order is destabi-
 242 lized in favor of ~~d -wave~~ d -wave superconductivity for an attractive V , at a fixed repulsive
 243 $U \sim t$, with significant hysteresis between the curves obtained for increasing/decreasing V .
 244 The latter state is then rapidly suppressed due to the effect of phase separation. The results
 245 are shown in Fig. 4.

246 3.1.2 $V > 0$:

247 For repulsive nearest-neighbor interactions V , we do not expect to find any superconducting
 248 orders at half-filling in the strong-coupling limit $U \gg t$, and instead focus on studying the
 249 competition between charge- and spin-density-wave orders. At fixed $V > 0$, we observe a
 250 first-order phase transition from a charge-density wave (CDW) to an antiferromagnetic (AF)
 251 state, as a function of increasing U . Likewise, for a large repulsive U , the system undergoes
 252 a phase transition from antiferromagnetism to CDW, as a function of the repulsive V . In both
 253 cases, a large region of hysteresis is observed between the results obtained for increasing and
 254 decreasing values of the respective interaction couplings. The results of our analysis are shown
 255 in Figs 5 and 6, respectively.

256 We do not present the corresponding results for the more general bath model (Fig. 2) here,
 257 as they are found to be qualitatively similar to those obtained for the simple model. The key
 258 differences, that are sometimes observed, include a) an increase/decrease in the strength of
 259 the ~~d -wave~~ d -wave order parameter close to the transition, b) a smaller region of hysteresis,
 260 c) a small shift in the position of the transition, particularly as a function of V for fixed U .

261 3.2 Phase diagram as a function of density

262 Next, we examine the phase diagram of the model over a continuous range of densities, for
 263 $U > 0$ and attractive/repulsive V . For $V > 0$, we once again limit ourselves to the strong-
 264 coupling limit $U \gg t$. For $V < 0$, we focus on studying the effect of an attractive extended
 265 interaction, with a local repulsion U controlling the extent of phase separation.

266 3.2.1 $V < 0$:

267 Let us now discuss the different phases that are supported by the model as a function of density.
 268 Close to half-filling, we find a region of phase separation, indicated by a jump in the density,
 269 flanked by symmetrical ~~pockets~~ islands of $d_{x^2-y^2}$ pairing, which decay rapidly as a function of
 270 density. For further smaller (larger) fillings, an extended s -wave order appears in the form of
 271 disconnected ~~patches~~ regions, near quarter-filling and at very small (large) densities. Interest-
 272 ingly, the variation of the extended ~~s -wave~~ s -wave order parameter as a function of U and V
 273 are found to be different for the simple bath model and the more general one. In the case of
 274 the simple model (see Fig. 7), we find small regions of extended ~~s -wave~~ s -wave superconduc-
 275 tivity near quarter-filling, that vary non-monotonously as a function of U . Only for sufficiently
 276 attractive V , nearly symmetrical ~~patches~~ regions of extended s -wave order also appear close to

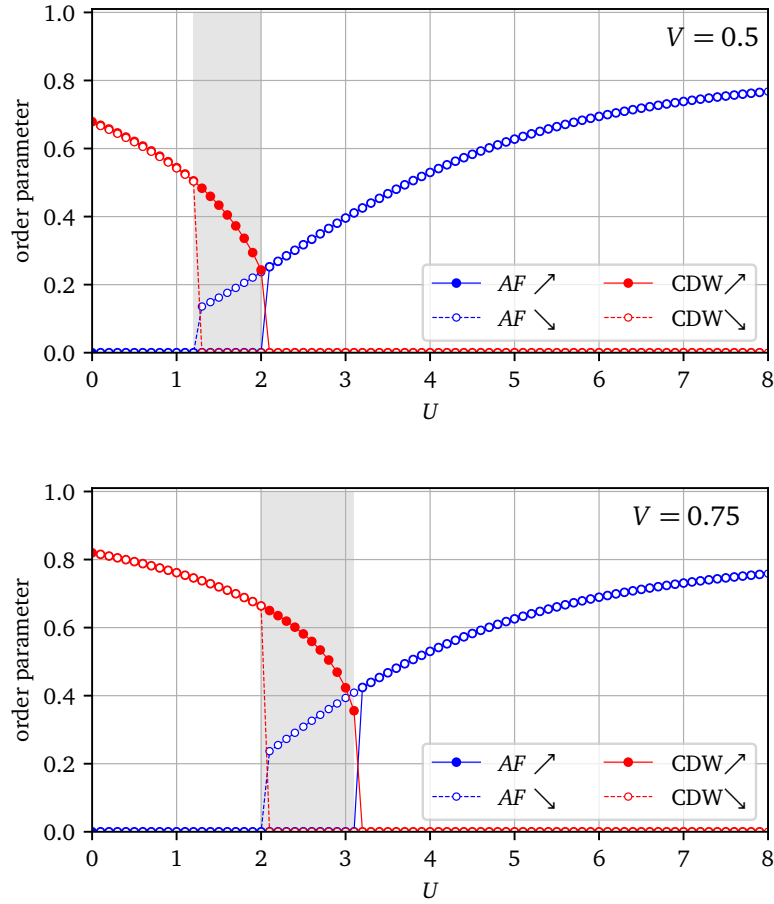


Figure 5: First-order phase transition from a charge-density wave (CDW) order (indicated by filled/open red circles) to antiferromagnetism (indicated by filled/open blue circles), at half-filling, as a function of the local repulsive interaction U , for $V = 0.5$ (top) and $V = 0.75$ (bottom). The simple impurity model (Fig. 1) is used. The dashed (solid) curves of each color depict the behavior of the order parameters for decreasing (increasing) U , and exhibit significant hysteresis. As the repulsive V becomes stronger, the transition is found to occur at a larger value of U , the CDW order parameter increases considerably in magnitude, and the region of hysteresis is somewhat enhanced.

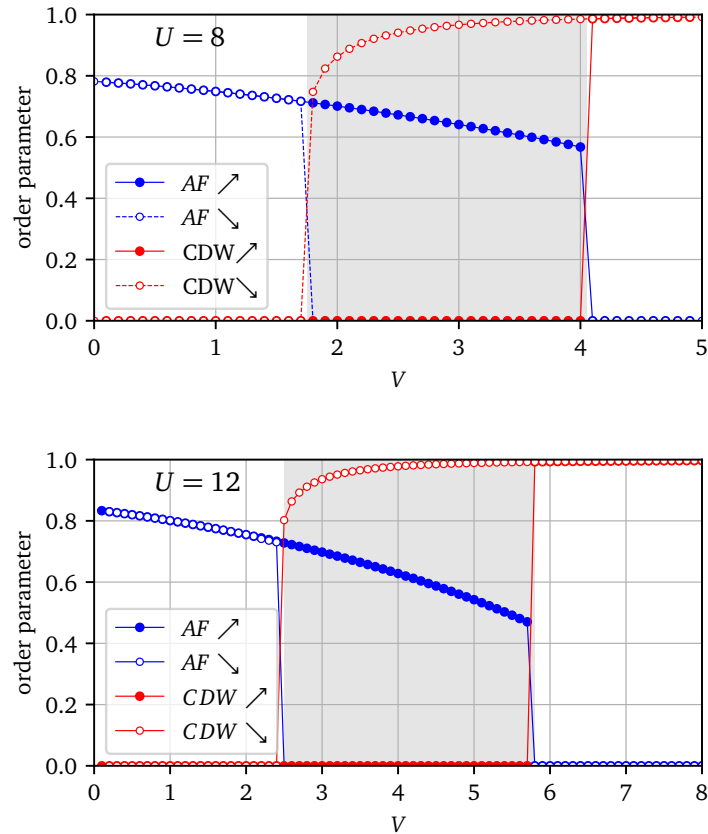


Figure 6: First-order phase transition from antiferromagnetism (indicated by filled/open blue circles) to charge-density wave (CDW) order (indicated by filled/open red circles), at half-filling, as a function of the repulsive interaction V for fixed U , with $U = 8$ (top) and $U = 12$ (bottom). The simple impurity model (Fig. 1) is used. The dashed (solid) curves of each color depict the behavior of the order parameters for decreasing (increasing) V , and exhibit considerable hysteresis. As U increases, the transition occurs at a larger critical value of V , and the antiferromagnetic order parameter increases in magnitude.

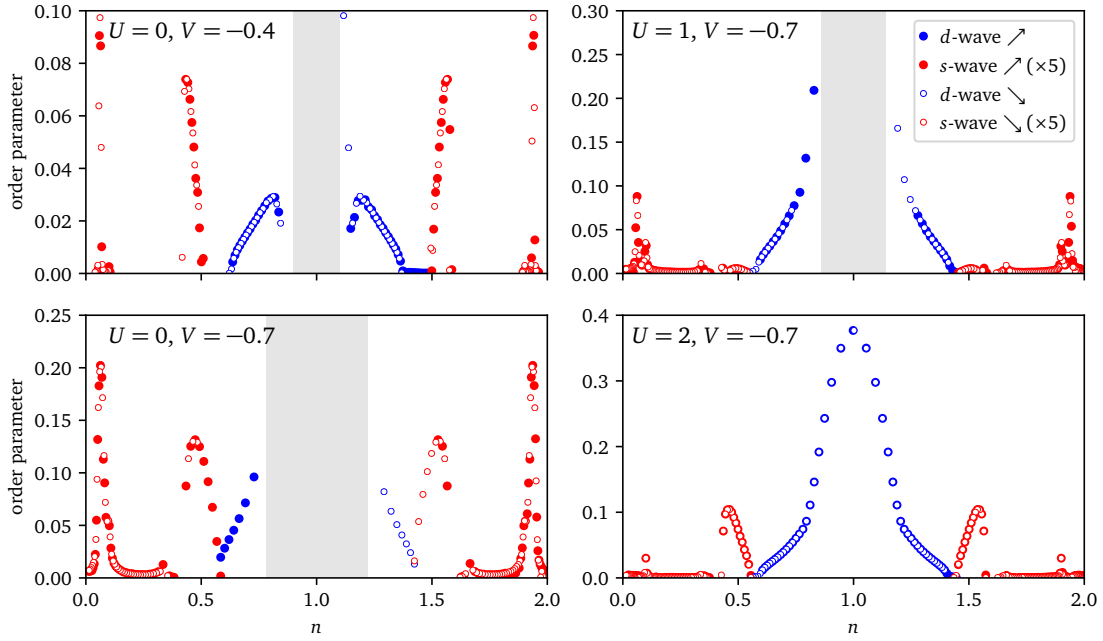


Figure 7: Superconducting order parameter of the EHM with attractive nearest-neighbor interactions, as a function of density n , from $n = 0$ to 2 for the simple bath model (Fig. 1). Close to the half-filled value $n = 1$, we find signatures of phase separation, indicated by a gap in the curve over a range of densities, caused by a jump in the compressibility $\partial n / \partial \mu$ (as shown in Fig. 9). For smaller (larger) fillings, nearly symmetrical and sharply defined regions of d -wave superconductivity (represented by filled/open blue circles) are followed by disconnected patches of extended s -wave order (represented by filled/open red circles), which appear only beyond a critical attractive value of V . Note that the asymmetry between either the d -wave regions or the extended s -wave regions near the band edges, especially evident for $V = -0.4$, is a numerical artefact owing to insufficient accuracy in the CDMFT procedure and has no physical consequence.

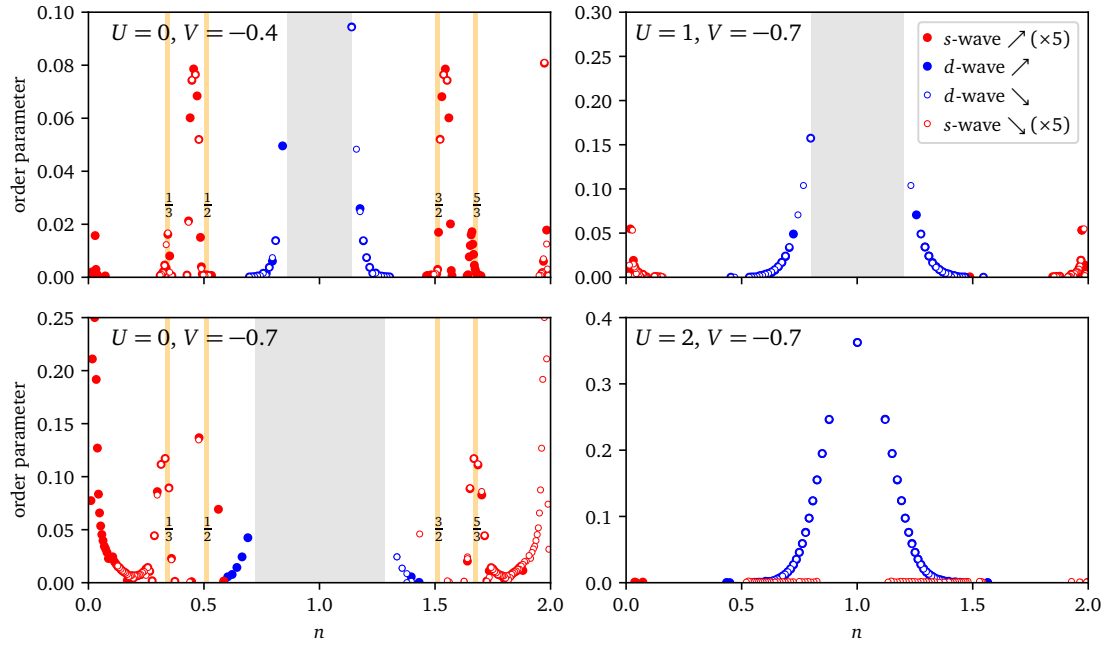


Figure 8: Superconducting order parameter of the EHM with attractive nearest-neighbor interactions, as a function of density n , from $n = 0$ to 2 for the general bath model (Fig. 2). The overall behavior of the d - and extended s -wave patches are similar to the corresponding result for the simple bath model. However, note that the structure of the s -wave order parameter has changed, with a more extended region near quarter-filling, and an additional patch near $1/3$ -filling. For $U = 0, V = -0.7$, the phase separation region extends all the way to quarter-filling, and the corresponding superconducting patches are almost absent, and asymmetric about $n = 1$. Moreover, the new s -wave order parameter becomes unambiguously weaker as the repulsive U increases, and is completely absent for $U = 1$ and $U = 2$, thus resolving the question of the ~~nonmonotonous~~ non-monotonous behavior of the s -wave order parameter in the simple bath model.

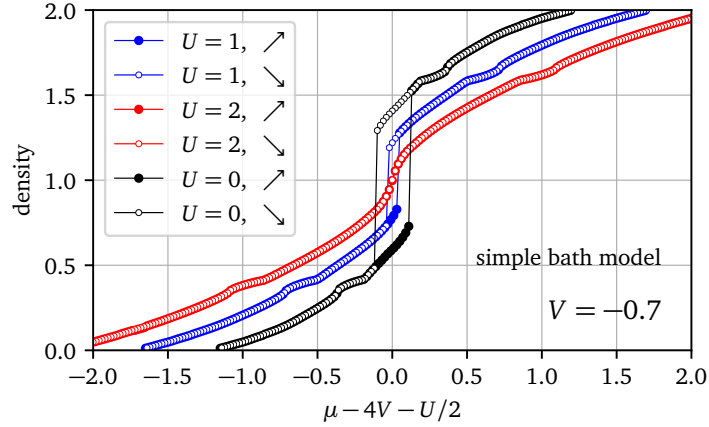


Figure 9: Number density n as a function of the chemical potential μ (measured with respect to its particle-hole invariant value, $\mu_c = U/2 + 4V$) for an EHM with attractive nearest-neighbor interactions, over a range of values of $U \geq 0$ and $V < 0$ for the simple bath model (Fig. 1). On either side of half-filling ($\mu = \mu_c$), we find symmetrical jumps in the compressibility $\partial n / \partial \mu$ enclosing a region of hysteresis, which corresponds to the coexistence of two different uniform-density solutions. This is interpreted as the region of phase separation. The red, blue and black filled/open circles represent the behavior for various values of U for $V = -0.7$, and demonstrate that while a sufficiently attractive interaction V favors phase separation, a stronger on-site repulsion U is detrimental to it.

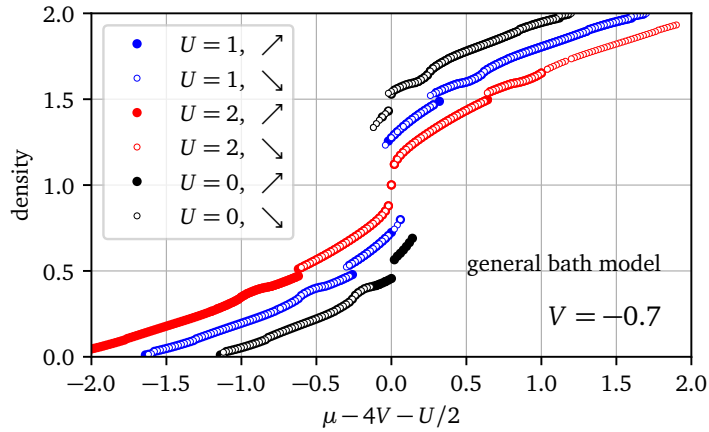


Figure 10: Number density n as a function of the chemical potential μ (measured with respect to its particle-hole invariant value, $\mu_c = U/2 + 4V$) for the EHM with attractive nearest-neighbor interactions, over a range of values of $U \geq 0$ and $V < 0$ for the general bath model (Fig. 2). The behavior is very similar to that observed in the simple bath model, with the most notable difference being the appearance of symmetric jumps in the number density n , close to quarter-filling, for each of the curves.

277 the band edges. The corresponding results for the general bath model are illustrated in Fig. 8.
 278 While the overall magnitude of the s -wave order parameter turns out to be smaller than in
 279 the previous case, its shape is more extended at quarter-filling, with two patches appearing
 280 next to each other, which, interestingly, appear close to fillings of $1/3$ and $1/2$, respectively.
 281 While it is tempting to blame the $n = 1/2$ feature on a commensurate finite-size effect on a
 282 4-site cluster, this is less obvious for the $n = 1/3$ feature. The superconductivity also clearly
 283 becomes stronger as a function of $V < 0$. Notably, the ~~s -wave~~ s -wave order is clearly absent
 284 for both $U = 1$ and $U = 2$, thus eliminating the confusion caused by the aforementioned
 285 non-monotonous variation in the case of the simple model—, and illustrating the advantage
 286 of considering a larger number of bath parameters in the CDMFT procedure. This being said,
 287 the conclusions from the two bath models are very similar. Using two different bath models
 288 provides us with an order-of-magnitude estimate of the error caused by the discreteness of the
 289 bath.

290 To better characterize the region of phase separation, we examine the behavior of the num-
 291 ber density n as a function of the chemical potential μ , measured with respect to its particle-
 292 hole symmetric value $\mu_c = U/2 + 4V$. On either side of $\mu = \mu_c$, we find symmetrical jumps
 293 in the compressibility $\partial n / \partial \mu$, enclosing a region of hysteresis in the $\mu - n$ curve, depicted in
 294 Fig. 9, where two uniform-density solutions coexist. Within our approach, this is interpreted
 295 as the region of phase separation, and is found to shrink under the influence of stronger local
 296 repulsive interactions U , and expand when V becomes more attractive. The corresponding re-
 297 sults for the general bath model are depicted in Fig. 10. The two sets of results are qualitatively
 298 similar, except for symmetric jumps observed in the number density n near quarter-filling in
 299 the latter case. We note that the jumps occur only for the model with the larger number of
 300 bath parameters, and are the most prominent for $U = 0, V = -0.7$, where the phase separa-
 301 tion region extends all the way to quarter-filling, becoming progressively smaller for $U = 1$
 302 and 2. It is plausible that phase separation might lead to the appearance of multiple jumps in
 303 the density, at half-filling as well as quarter-filling. Moreover, a finite-size effect would have
 304 been even more obvious in the simple bath model, where these jumps are found to be absent.
 305 The origin of the jumps is currently unclear to us.

306 The appearance of a phase separated state for sufficiently attractive interactions is a famil-
 307 iar result [32, 52, 71, 81, 87, 116], which has received attention from other groups, including
 308 very recently [70], but the characterization of the region of phase separation tends to depend
 309 on the method used for the analysis, and whether it is capable of handling a ~~non-uniform~~
 310 nonuniform distribution of particles.

311 3.2.2 $V > 0$:

312 At half-filling, for $U = 8t$, the large on-site interaction freezes the charge degree of freedom,
 313 and the ground state is a Mott insulator. Hole doping is found to destabilize the magnetic
 314 order, and drive the system towards a d -wave superconducting phase. We encounter a dome-
 315 shaped region of d -wave superconductivity for $V = 0$, which is suppressed at smaller densities,
 316 where no competing superconducting orders are found to be stabilized in our analysis. Upon
 317 introducing a repulsive $V \sim t$, the superconducting order remains stable, but is somewhat
 318 suppressed. The results are depicted in Fig. 11. The corresponding results for the general bath
 319 model are depicted in Fig. 12. The two sets of results are qualitatively similar, with the most
 320 noticeable difference being the relatively sharper transition to and from the d -wave ordered
 321 state in the latter case. These results are consistent with the picture of superconductivity
 322 mediated by short-range spin fluctuations in a doped Mott insulator [117–119].

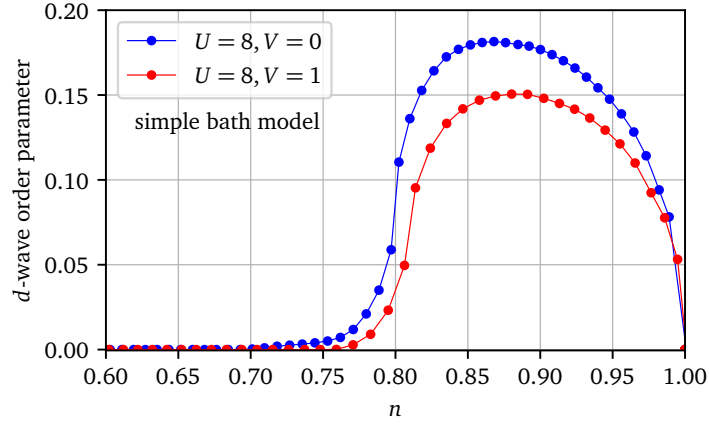


Figure 11: Superconducting d -wave order parameter of the EHM with repulsive nearest-neighbor interactions in the strong-coupling limit, i.e., at $U = 8t$, using the simple bath model (Fig. 1). The Mott insulating state at half-filling is destabilized in favor of $d_{x^2-y^2}$ pairing, upon hole doping. The dome-like region of d -wave superconducting order is observed for $V = 0$ (indicated by the solid blue curve) and is somewhat suppressed for non-zero repulsive V (indicated by the solid red curve). No other superconducting orders are found to be stabilized in this region.

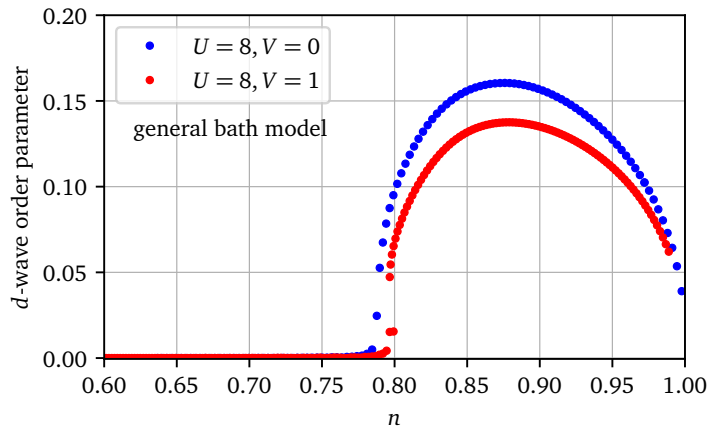


Figure 12: Superconducting d -wave order parameter of the EHM with repulsive nearest-neighbor interactions in the strong-coupling limit ($U = 8t$) using the general bath model (Fig. 2). The behavior is qualitatively similar to that obtained in the simple model, with a slight difference in the magnitudes of the d -wave order parameter. The most noticeable difference between the two bath models is the relatively sharp transition into and out of the d -wave superconducting phase.

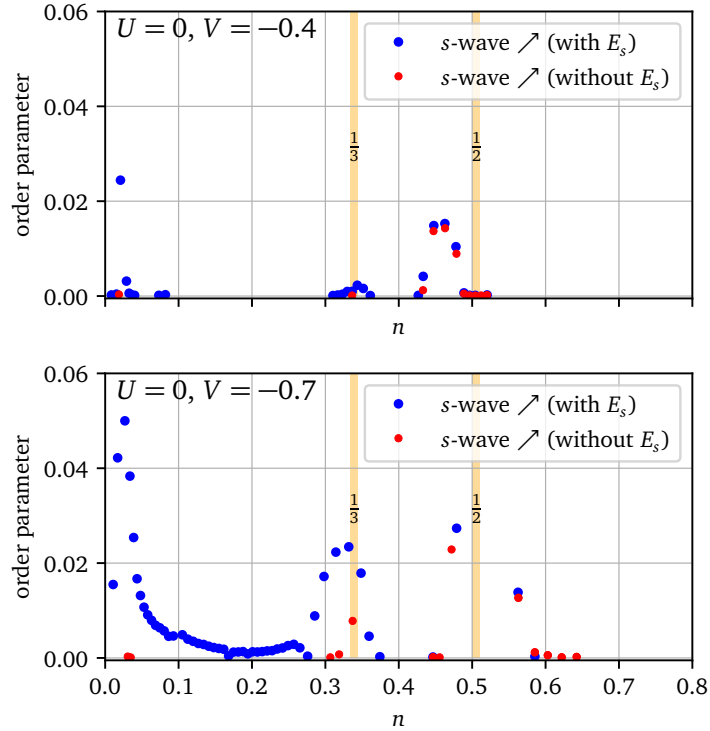


Figure 13: The figure shows the behavior of the extended ~~s-wave~~ ~~s-wave~~ order parameter as a function of the number density n , with and without the inclusion of the self-consistent anomalous mean-field parameter E_s (see Appendix A), for $U = 0, V = -0.4$ (above) and $U = 0, V = -0.7$ (below). Clearly, some of the regions with a nontrivial ~~s-wave~~ ~~s-wave~~ order parameter are found to be absent when E_s is not included. For $U = 0, V = -0.7$, the most prominent among these appears to be the region with density in the range $0 < n < 0.3$. Upon considering a stronger attractive V , these regions tend to reappear, but are suppressed in magnitude in the absence of E_s .

323 4 Discussion and conclusions

324 In summary, we have studied the phase diagram of the extended Hubbard model, for both
 325 attractive and repulsive nearest-neighbor interactions, using a combination of Cluster Dynam-
 326 ical Mean Field Theory (CDMFT), with a dynamical Hartree-Fock approximation for treating
 327 inter-cluster interactions. We examine possible phase transitions at half-filling, as well as the
 328 dominant phases that are stabilized as a function of density. At the particle-hole invariant
 329 chemical potential, which corresponds to a half-filled band in the absence of phase separation,
 330 the antiferromagnetically ordered state undergoes a first-order phase transition to d -wave su-
 331 perconductivity for a critical attractive interaction V . Stronger attractive extended interactions
 332 also tend to induce phase separation, which manifests itself in the form of a gradual deviation
 333 of the density from its half-filled limit, for a fixed chemical potential. For a sufficiently strong
 334 repulsive interaction V , a charge-density wave order is stabilized at half-filling.

335 As a function of density, a phase separated state near the half-filled point is flanked by
 336 symmetrical regions of d -wave superconductivity, that decay sharply as a function of density,
 337 and ~~disconnected patches~~ ~~islands~~ of extended s -wave order at smaller (larger) band fillings.
 338 For the case of repulsive non-local interactions, in the strongly coupled limit, the Mott insula-
 339 tor at half-filling gives way to a dome-shaped region of d -wave superconductivity, upon hole

340 doping, which is expected on physical grounds. No other competing superconducting orders
 341 are found to be stabilized in this region of parameter space.

342 For the most part, our results are found to be qualitatively consistent with the existing
 343 literature. The transition between antiferromagnetism and CDW at half-filling, for repulsive
 344 interactions, has been predicted by several previous studies [26,31,54,58,62,65,70,76–78,87],
 345 although the critical interaction strength typically depends on the method of analysis. For
 346 densities away from half-filling, there have also been some predictions of d_{xy} pairing, that
 347 appears beyond the region of $d_{x^2-y^2}$ pairing, for repulsive extended interactions [39,56]. We
 348 do not find such a state in our analysis. The phase diagrams obtained from self-consistent
 349 mean-field theory based analyses tend to prominently feature d -wave superconductivity at
 350 half-filling, with a continuous region of extended s -wave order at smaller densities, along with
 351 a region of coexistence between the two, i.e., $s + id$ pairing [50,51]. In our analysis, we do
 352 not usually see a coexistence between d - and extended s -wave orders. In the simple model,
 353 such a coexistence is observed only in those regimes where both ~~the~~ interactions $U > 0$ and
 354 $V < 0$ are sufficiently strong, and comparable in magnitude. This may be due to the fact
 355 that the superconducting orders found in our analysis are fairly weak, and the significant
 356 attractive interactions that are, therefore, needed for stabilizing overlapping regions of d -
 357 and extended s -wave orders, would also lead to a larger region of phase separation. This
 358 effect can only be compensated by including a sufficiently large repulsive local interaction.
 359 On the other hand, we have not been able to verify a similar coexistence of the orders for
 360 the general bath model, due to the rapid suppression of the extended ~~s -wave~~ s -wave order,
 361 near quarter-filling, with an increase in U . Some studies have also suggested the possibility
 362 of p -wave superconductivity, especially at half-filling [32], and for intermediate hole doping,
 363 beyond the region of d -wave superconducting order [39,50,51]. We do not find signatures of
 364 p -wave superconductivity in the parameter regimes that we study. Some of our results at half-
 365 filling are found to be qualitatively consistent with a recent study on the extended Hubbard
 366 model using the determinantal Quantum Monte Carlo technique [70], which also reports the
 367 transitions between d -wave superconductivity and AFM, as well as between phase separation
 368 and d -wave, that we observe in our analysis. In addition, the authors of the aforementioned
 369 paper also explore other quadrants of the $U - V$ phase diagram, including the case where
 370 $U < 0$, which we do not take into account, since the repulsive component of the Coulomb
 371 interaction is always expected to be present in a realistic situation.

372 In contrast to ordinary mean-field theory, our approach takes the intra-cluster fluctuations
 373 into account exactly, and is therefore expected to give more reliable quantitative results. In par-
 374 ticular, ordered phases are weaker in this approach than in ordinary mean-field theory. At the
 375 same time, it should be noted that we only take into account spatial fluctuations within small
 376 clusters, and the accuracy of the method is controlled by the size of the clusters used. To illus-
 377 trate the importance of including the effect of the inter-cluster interactions self-consistently,
 378 which are usually disregarded in cluster-based approaches, we have compared the behavior of
 379 the superconducting ~~d - and extended s -wave~~ d - and extended s -wave orders as a function
 380 of density n , for an attractive V (see Fig. 13) in the presence and absence of the anomalous
 381 mean-field parameters (which we refer to as E_d and E_s respectively). Certain regions of the ex-
 382 tended ~~s -wave~~ s -wave order, that we observe in our analysis, disappear entirely in the absence
 383 of the self-consistent anomalous mean field parameter E_s . These regions tend to reappear, but
 384 with a smaller amplitude, when the attractive V is sufficiently strong. Likewise, in the case
 385 of ~~d -wave~~ d -wave superconductivity, we find that the superconducting order parameter is
 386 negligible when E_d is absent, and tends to reappear, with a much smaller amplitude, when
 387 the repulsive U is increased. Our approach is more suitable for making predictions about the
 388 thermodynamic limit than exact diagonalization studies on finite-sized clusters, since only the
 389 self-energy is limited by the cluster size. Some recent studies have explored the possibility

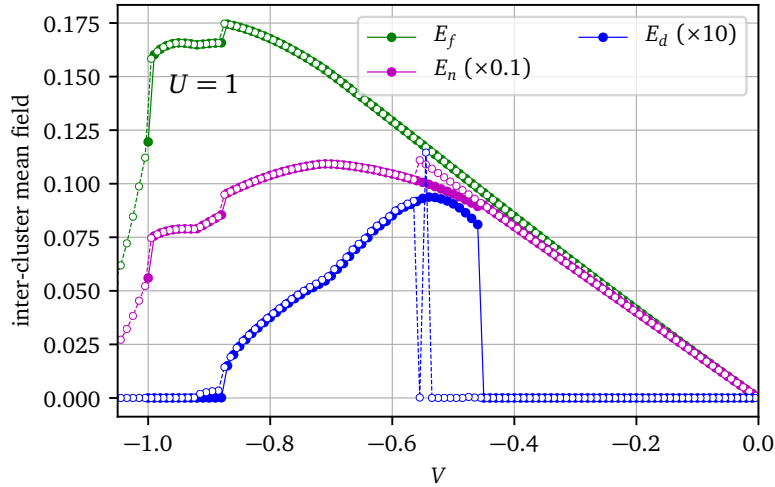


Figure 14: Inter-cluster Hartree-Fock mean fields for the solutions shown in the top panel of Fig. 4. E_d is the eigen-operator associated with d -wave superconductivity, E_f with the nearest-neighbor kinetic operator $f_{\text{tr}'\sigma\sigma}$ and E_n with the density n (basically a shift in the chemical potential induced by V). The mean-field E_s associated with extended s -wave superconductivity is negligible over almost the entire range of V , since this is at half-filling, except at significantly attractive V (due to phase separation). Note the very different scales (the superconducting mean field is much magnified). The filled and empty circles denote the results for increasing (less negative) and decreasing (more negative) V , respectively. [The oscillations in the \$d\$ -wave order parameters observed close to the transition are also reflected in the corresponding mean-field parameter.](#)

390 of magnetic states characterized by ordering wave vectors that are incommensurate with the
 391 lattice periodicity [120] in the two-dimensional Hubbard model, for electron densities below
 392 half-filling, where the antiferromagnetic state becomes unstable. Our approach is unsuitable
 393 for identifying such incommensurate charge and spin orders. Our method does not suffer from
 394 fundamental restrictions on its applicability in any particular parameter regime, and allows us
 395 to study the behavior of the model as a continuous function of doping, rather than by focusing
 396 on specific densities, as has been done in many previous studies. In the future, this method
 397 could be potentially useful for [analysing-analyzing](#) more complicated models, including those
 398 with spin-orbit interactions. [It can also be applied to the single-band Hubbard model on a](#)
 399 [triangular lattice, in which the importance of non-local interactions has been pointed out in](#)
 400 [the literature \[121\]. It would also be interesting to explore the regime of non-perturbative](#)
 401 [repulsive local interactions and attractive extended interactions, to observe their combined](#)
 402 [effect on driving or suppressing phase separation \[122, 123\]. Longer-range hopping terms can](#)
 403 [also be included within our exact diagonalization implementation, which give rise to geometric](#)
 404 [frustration, making the analysis more relevant for the physics of the cuprates.](#)

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411 A Appendix

412 A The inter-cluster mean-field procedure

413 The extended interaction term can be rewritten as

$$\frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'} n_{\mathbf{r}\sigma} n_{\mathbf{r}'\sigma'} = \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^c n_{\mathbf{r}\sigma} n_{\mathbf{r}'\sigma'} + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^{\text{ic}} n_{\mathbf{r}\sigma} n_{\mathbf{r}'\sigma'}$$

414 where \mathbf{r}, \mathbf{r}' refer to the lattice sites, and $n_{\mathbf{r}\sigma}$ is the number of particles at site \mathbf{r} with spin σ .
 415 Here $V_{\mathbf{r}\mathbf{r}'}^c$ and $V_{\mathbf{r}\mathbf{r}'}^{\text{ic}}$ refer to the intra-cluster and inter-cluster parts of the interaction. Inspired
 416 by Wick's theorem, we decompose the inter-cluster part of the interaction into Hartree, Fock
 417 and anomalous channels, as follows:

$$\begin{aligned} \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^{\text{ic}} n_{\mathbf{r}\sigma} n_{\mathbf{r}'\sigma'} &= \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^{\text{ic}} \left(n_{\mathbf{r}\sigma} \bar{n}_{\mathbf{r}'\sigma'} - \frac{1}{2} \bar{n}_{\mathbf{r}\sigma} \bar{n}_{\mathbf{r}'\sigma'} \right) \\ &\quad - \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^{\text{ic}} \left(f_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \bar{f}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}^* - \frac{1}{2} \bar{f}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}^* \bar{f}_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \right) \\ &\quad + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} V_{\mathbf{r}\mathbf{r}'}^{\text{ic}} \left(\Delta_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \bar{\Delta}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}^* + \Delta_{\mathbf{r}\mathbf{r}'\sigma\sigma'}^\dagger \bar{\Delta}_{\mathbf{r}\mathbf{r}'\sigma\sigma'} - \bar{\Delta}_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \bar{\Delta}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}^* \right) \quad (\text{A.1}) \end{aligned}$$

418 where the operators are defined as $n_{\mathbf{r}\sigma} \equiv c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}\sigma}$, $f_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \equiv c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma'}$ and $\Delta_{\mathbf{r}\mathbf{r}'\sigma\sigma'} \equiv c_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma'}$. Note
 419 that the applicability of Wick's theorem is not exact in this case, as we are considering a model
 420 which already includes on-site interactions, but must be considered as an *ad hoc* Ansatz. In
 421 other words, at a fundamental level, we are not assuming that the ground state of the system is
 422 a Slater determinant. We are rather resting on a variational principle for the self-energy [124]
 423 on which CDMFT is formally based.

424 The sum over sites \mathbf{r}, \mathbf{r}' is taken over the whole lattice. But the average $\bar{n}_{\mathbf{r}\sigma}$ will be assumed
 425 to have the periodicity of the cluster, i.e., $\bar{n}_{\mathbf{r}+\mathbf{R}\sigma} = \bar{n}_{\mathbf{r}\sigma}$ where \mathbf{R} belongs to the super-lattice. In
 426 addition, the two-site averages $\bar{f}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}$ and $\bar{\Delta}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}$ are assumed to depend only on the relative
 427 position $\mathbf{r} - \mathbf{r}'$. The mean-field inter-cluster interaction (A.1) is then a one-body contribution
 428 to the Hamiltonian with the periodicity of the super-lattice, and contains both intra-cluster
 429 and inter-cluster terms, whereas the purely intra-cluster part $V_{\mathbf{r}\mathbf{r}'}^c$ retains its fully correlated
 430 character.

431 For a four-site cluster, we have a total of eight bonds between neighboring clusters, along
 432 the x and y directions, with two spin combinations (σ, σ') per bond, where we consider
 433 spin-parallel combinations for the Fock terms (in the absence of spin-dependent hopping)
 434 and spin-antiparallel combinations for the anomalous terms. In practice, we only consider
 435 physically relevant combinations of operators defined on different sites/bonds for our analysis
 436 (such as those compatible with a ~~d -wave~~ d -wave or an extended ~~s -wave~~ s -wave order). As
 437 an illustration of this, let us consider the pairing fields Δ defined on all of these bonds, which
 438 we denote by the labels $i = 1 - 16$ (including different bond and spin combinations).

439 The mean-field Hamiltonian can be written as

$$\frac{V}{2} \sum_{i,j} (\bar{\Delta}_i^* M_{ij} \Delta_j + \Delta_i^\dagger M_{ij} \bar{\Delta}_j - \bar{\Delta}_i^* M_{ij} \bar{\Delta}_j) \quad (\text{A.2})$$

440 where $i, j = (\mathbf{r}, \mathbf{r}', \sigma, \sigma')$ and the matrix M_{ij} describes the combinations of the pairing fields
 441 defined on different bonds which appear in the Hartree-Fock decomposition of the ~~intercluster~~
 442 ~~inter-cluster~~ interactions. The matrix M turns out to be an identity matrix for the Fock and

443 pairing fields f and Δ respectively, but the corresponding matrix for the Hartree fields n is
 444 off-diagonal.

445 Defining the eigen-combinations of the pairing fields by

$$E_\alpha = U_{\alpha i} \Delta_i \quad (\text{A.3})$$

446 and the eigenvalues of the matrix M by λ_α , such that

$$M_{ij} = \sum_{\alpha, \beta} U_{\alpha i}^* \lambda_\alpha \delta_{\alpha\beta} U_{\beta j}$$

447 we can rewrite Eq. (A.2), above, as

$$\frac{V}{2} \sum_{\alpha} \lambda_{\alpha} (\bar{E}_{\alpha}^* E_{\alpha} + E_{\alpha}^{\dagger} \bar{E}_{\alpha} - \bar{E}_{\alpha}^* \bar{E}_{\alpha}) \quad (\text{A.4})$$

448 The mean-field values \bar{E}_{α} of the relevant eigen-combinations E_{α} of the pairing operators de-
 449 fined on different nearest-neighbor bonds are obtained self-consistently within the CDMFT
 450 loop, and likewise for the other mean fields that are the appropriate eigen-combinations of
 451 $\bar{n}_{\mathbf{r}\sigma}$ and $\bar{f}_{\mathbf{r}\mathbf{r}'\sigma\sigma'}$.

452 **B CDMFT convergence**

453 The CDMFT procedure is iterative and aims at finding a solution to a set of nonlinear equations
 454 that can be schematically expressed as

$$\mathbf{x} = \mathbf{f}(\mathbf{x}) \quad , \quad (\text{B.1})$$

455 where \mathbf{x} stands for the set of bath and inter-cluster Hartree-Fock parameters and \mathbf{f} is an equally
 456 large set of functions that returns the next set of parameters from the current set, following
 457 a procedure that combines the CDMFT update with the inter-cluster mean-field one. The
 458 canonical way to solve Eqs (B.1) is the fixed-point method: the map $\mathbf{x}_{n+1} = \mathbf{f}(\mathbf{x}_n)$ is iterated
 459 until the difference $\Delta\mathbf{x}_{n+1} = \mathbf{x}_{n+1} - \mathbf{x}_n$ is smaller than some preset accuracy.

460 However, if the purpose is to find a solution to (B.1), there are more efficient and stable
 461 alternatives. Specifically, one could use the classic Broyden method for finding roots of sets
 462 of nonlinear equations, a generalization to many variables of Newton's root-finding method.
 463 Broyden's method relies on a computation of the Jacobian matrix $\mathbf{J} = \partial\mathbf{f}/\partial\mathbf{x}$ that is improved
 464 at each iteration. It typically finds a solution with fewer iterations than the fixed-point method,
 465 and with greater accuracy. In addition, it is "stickier", meaning that upon performing an
 466 external loop over model parameters, it will "stick" to the current solution (or the current
 467 phase), whereas the fixed-point method will be prone to instabilities and will more likely
 468 switch to more stable solutions.

469 This means that the fixed-point method, although less efficient, is more appropriate to
 470 detect phase transitions, whereas the Broyden method is better at keeping the current solution
 471 into its metastable regime. Hence the Broyden method will typically result in wider hysteresis
 472 loops than the fixed-point method when the external parameter is cycled in both directions
 473 (ascending and descending).

474 In practice, we can converge the CDMFT-DHF procedure on the difference $\Delta\mathbf{x}_{n+1}$, but we
 475 can also ask for the convergence of physical quantities, such as the cluster self-energy $\Sigma(\omega)$, or
 476 relevant order parameters. It may happen that physical quantities converge even though bath
 477 parameters do not, because the latter are sometimes subject to discrete "gauge" symmetries

478 that do not affect physical observables. But even though convergence criteria may be based
479 on physical quantities, the iteration $\mathbf{x}_n \rightarrow \mathbf{x}_{n+1}$ is still based on either the fixed point or the
480 Broyden method. In this work, we used the self-energy and relevant order parameters as
481 convergence criteria, with accuracies of the order of 10^{-4} .

482 As an illustration, we compare the behavior of the relevant order parameters for the phases
483 observed at the particle-hole symmetric chemical potential as a function of $U > 0$ for $V = -0.6$
484 in Fig. 15 and as a function of $V < 0$ for $U = 2$ in Fig. 16, using the fixed-point and the
485 Broyden methods for obtaining the optimal set of CDMFT parameters. As expected, the region
486 of hysteresis is found to be much larger when the Broyden method is used, consistent with
487 the tendency of this method to stick to the current solution. Interestingly, we find that the
488 existence of d -wave order does not necessarily coincide with phase separation, and there may
489 be a region with a nontrivial d - order parameter even at half-filling. However, such a region is
490 not easily observed with the fixed-point method and is usually significantly amplified when the
491 Broyden method is used, as illustrated in the lower plot of Fig. 15. We also observe oscillations
492 between the d -wave solutions obtained in the presence and absence of phase separation within
493 the gray hysteresis region, for both the methods. Although the Broyden method converges
494 faster even with a higher accuracy, we obtain more oscillatory solutions in general with this
495 method, which includes oscillations between densities greater than and less than 1 in the
496 phase-separated region for small U , as well as between the normal state and the AF state,
497 close to the transition from d -wave to antiferromagnetism for increasing U . In Fig. 16, we see
498 that d -wave superconducting state persists well into the region of half-filling as V becomes
499 less negative, for both methods. When the Broyden method is used, we find that the system
500 continues in the AF state down to $V = -1.8$ and then undergoes a transition to the normal
501 state, without the appearance of a d -wave order or phase separation. This is an extreme
502 example of the tendency of this method to preserve the existing solution. In contrast, the
503 fixed-point method gives rise to a phase transition towards the d -wave superconducting state,
504 close to $V = -0.9$. Therefore, for most situations, it is more convenient for us to employ the
505 fixed-point method for our computations.

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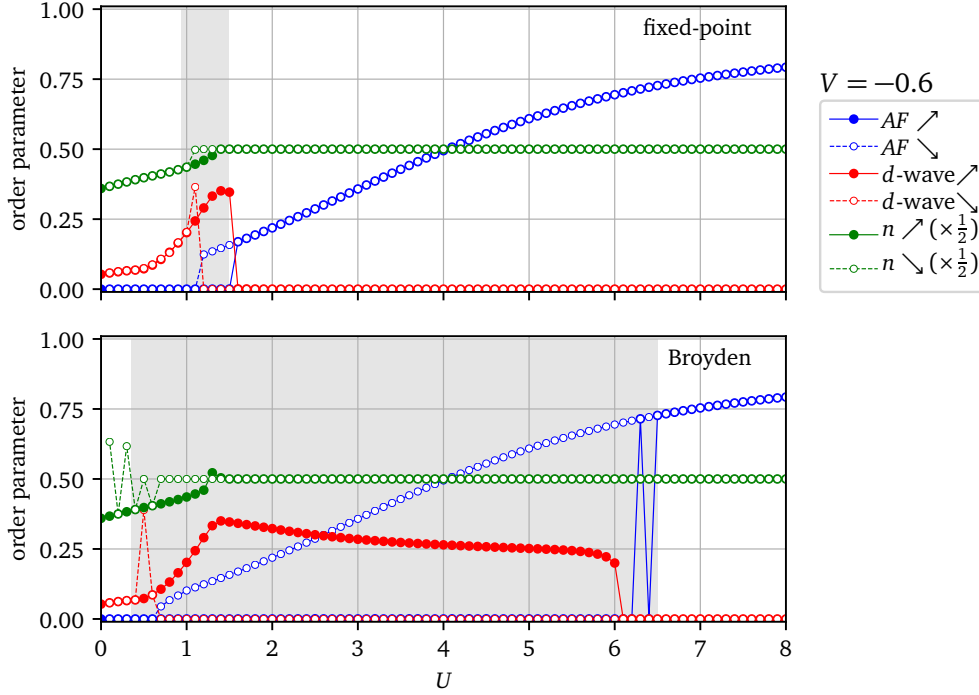


Figure 15: Order parameters for the different phases observed at the particle-hole symmetric chemical potential for $V = -0.6$, as a function of U , using the fixed-point method (above) and the Broyden method (below) for obtaining the optimal set of bath and mean-field parameters. The hysteresis loop obtained for increasing and decreasing U is found to be much larger for the Broyden method, indicating that it has a tendency to stick to the current solution. A prominent region with a nontrivial d -wave superconducting order parameter is observed at half-filling for the Broyden method (indicated by the region with filled red circles in the lower plot). The transition from the phase-separated to the half-filled state is indicated by a shoulder-like feature in the corresponding d -wave order parameter. Oscillations are observed between the d -wave solutions with and without phase separation, within the hysteresis region, for both methods. In the presence of phase separation, the density is found to oscillate between values greater than and less than 1, when the Broyden method is used, and sometimes also with the fixed-point method. Moreover, some oscillations are also observed between the AF and normal states, close to the phase transition towards AF for increasing U (see open blue circles in the lower plot).

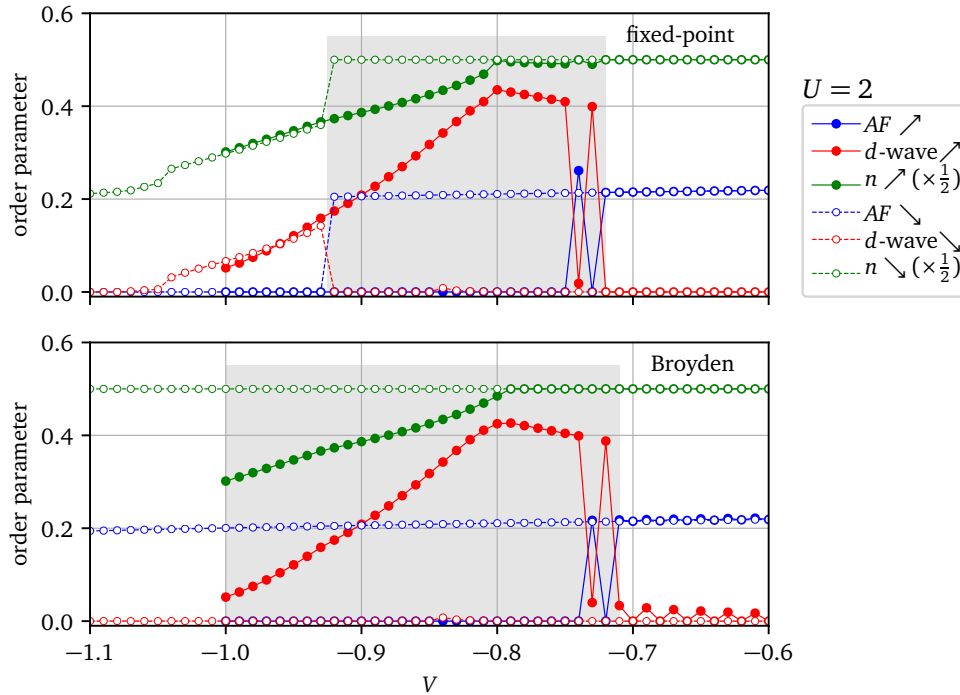


Figure 16: Order parameters corresponding to the different phases observed at the particle-hole symmetric chemical potential for $U = 2$, as a function of V , using the fixed-point method (above) and the Broyden method (below) for obtaining the optimal bath and mean-field parameters. Once again, the hysteresis region between increasing and decreasing negative V is found to be much larger when the Broyden method is employed. Interestingly, the AF region is found to persist all the way to $V = -1.8$ for decreasing (more negative) V with the Broyden method (not shown in the figure), beyond which the system directly undergoes a transition to the normal state, and the intervening d -wave superconducting region is found to be absent (the open blue circles in the lower plot depict the behavior up till $V = -1.1$). For increasing (less negative) V , a part of the d -wave superconducting phase observed is found to be very close to half-filling for both methods (indicated by the filled red circles). Moreover, oscillations are observed between the d -wave and AF phases, which are found to occur more frequently when the Broyden method is used. Note that the results for increasing V have been plotted starting from $V = -1.0$ in both cases for convenience, but may be smoothly extrapolated to more negative values of V .

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