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Mean Field Magnetic Phase Diagrams for the Two Dimensional $t - t' - U$ Hubbard Model

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We study the ground state phase diagram of the two dimensional $t - t' - U$ Hubbard model concentrating on the competition between antiferro-, ferro-, and paramagnetism. It is known that unrestricted Hartree–Fock- and quantum Monte Carlo calculations for this model predict inhomogeneous states in large regions of the parameter space. Standard mean field theory, i.e., Hartree–Fock theory restricted to homogeneous states, fails to produce such inhomogeneous phases. We show that a generalization of the mean field method to the grand canonical ensemble circumvents this problem and predicts inhomogeneous states, represented by mixtures of homogeneous states, in large regions of the parameter space. We present phase diagrams which differ considerably from previous mean field results but are consistent with, and extend, results obtained with more sophisticated methods.

KEY WORDS: Hubbard model, mean field theory, phase diagrams

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1. INTRODUCTION AND RESULTS

1.1. Background

Hubbard-type models in two dimensions have been frequently studied in the context of high temperature superconductivity (HTSC) and other strongly correlated systems.[1] Despite of considerable efforts and various different theoretical approaches (for reviews see e.g. Refs. 2–5) no complete picture of its properties has been reached. Thus the problem of getting reliable theoretical understanding of 2D Hubbard-type models in the parameter regime of interest for HTSC remains to be a problem of considerable importance.

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Mean field theory, i.e. Hartree–Fock theory restricted to states which are invariant under a subgroup of translations, is one of the simplest techniques which can be used to study interacting fermion systems. It is conceptually and computationally simple, provides exact upper bounds to ground states energies,[6,7] and has been a valuable guide for developing theoretical understanding of phenomena like superconductivity or magnetism. This technique was applied to 2D Hubbard-like models before and around the discovery of HTSC.[8,9] However, the results obtained then were in qualitative disagreement with what was known from more sophisticated methods. For example, for the 2D (one-band repulsive) Hubbard model, these mean field studies predicted one and the same antiferromagnetic phase not only at half-filling, but also in a finite doping regime around half filling (see Fig. 3 in Ref. 8). It is known from unrestricted Hartree–Fock calculations[10–12] and other methods[8] that commensurate antiferromagnetic states cannot exist away from half filling and intermediate coupling values, in contrast with results from mean field theory. Our aim is to advocate a natural generalization of mean field theory to the grand canonical ensemble[13,14] which is designed to overcome these inconsistencies without increasing the computational effort.[15,16] The main new results in the paper are magnetic phase diagrams for 2D Hubbard-like models obtained with that method. These mean field phase diagrams differ qualitatively from the previous mean field results mentioned above but are consistent with results obtained by other methods.

Our main point is that mean field theory is not only capable to determine homogeneous phases, but it can also be used to detect the possibility that there are regions in phase space where the thermodynamically stable phase is not homogeneous. To be more specific, we revisit mean-field theory for the 2D $t - t' - U$ Hubbard model (see (1) below for precise definitions) restricted to anti-ferromagnetic (AF), ferromagnetic (F) and paramagnetic (P) states.[8,9] However, when answering the question "*which of the following Hartree–Fock states has lowest free energy: a homogeneous AF, F or P state?*," we differ from the previous studies mentioned by also allowing the possible answer "*or a phase separated state where two of such homogeneous states are mixed and coexist at the same time?*". By the term "mixed phase" we refer to a solution to the mean field equations where the free energies of the homogeneous solutions are degenerate. Technically, we allow for mixed phases by using the grand canonical ensemble and carefully accounting for the doping constraint.[13–16] We find that, in a large part of parameter space, the mean field phases are indeed mixed, and the phase diagrams we obtain are thus much richer than the ones in Refs. 8, 9.

As will be explained in Sec. 3, our method is similar to the usual Maxwell construction used in the mean-field description of liquid-vapor phase transitions. Moreover, this method is also justified in detail in recent interesting mathematical work on Hartree–Fock theory for Hubbard-like systems[13,14]; see also Refs. 15, 16 for an alternative derivation. However, this method is usually not used in mean field

studies of the Hubbard-like models; one notable exception is Su[17] who applied a similar method to the 2D $t - U - V$ Hubbard model. Our results show that 2D Hubbard-like models are peculiar in that these co-existing phases persist in large regions of phase space, and thus allowing for inhomogeneous phases changes the results dramatically.

It is important to note that our results are exact for a finite system, despite our using numerics to determine our phase diagrams: the mean field diagrams are given by analytical formulas, and we only use numerics to evaluate and plot the functions determined by them. We made sure the system sizes we use are large enough so that finite size effects are irrelevant, as can be clearly seen in Fig. 5.

It is interesting to compare our phase diagrams with recent results on the 2D $t - t' - U$ Hubbard model obtained with quantum Monte Carlo,[18] exact diagonalization,[19] unrestricted Hartree–Fock,[20] and renormalization group methods.[21] One important common conclusion from these studies is that there is a delicate competition between antiferromagnetism and ferromagnetism which depends sensitively on the band structure and doping. Our results confirm these results, shed interesting light on them, and extend them to parameter regimes which previously have not been studied. A more detailed comparison will be given at the end of the paper.

We stress that, while our method does not account for fluctuations or details of states which are not translational invariant, it allows to detect frustration in the sense of incompatibility between homogeneous states and the doping constraint. Such frustration suggests interesting physical behavior to be explored by more sophisticated methods, and mean field theory provides a simple method to find these interesting parameter regions.

The point we make in this paper ("allow for mixed phases . . . ") is rather elementary. The reason why we elaborate it at such length is that there exist mean field theory phase diagrams for 2D Hubbard-like models in the literature which are well established but which were obtained by ignoring this point and thus are qualitatively wrong. It seems that, due to this, there is a widespread belief that mean field theory cannot be trusted for such models. We feel that this has been very unfortunate, and the aim of this paper is to rehabilitate mean field theory as a useful and trustworthy method also for 2D Hubbard-like models.

1.2. Results

We now describe our results in more details. We use the standard mean field equations,[8,9,22] but we extend them by a method allowing us to detect possible instabilities towards phase separation,[16] as explained in more detail in Secs. 2

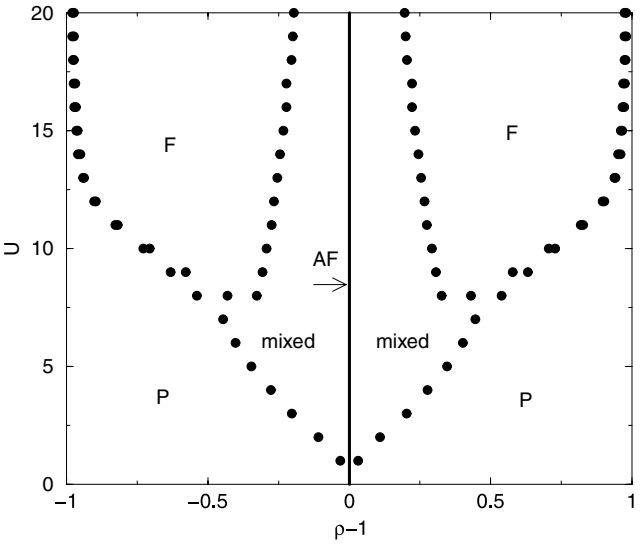

Fig. 1. Phase diagram of the 2D Hubbard model as a function of U and doping $\rho - 1$ for parameters $t = 1$ and $t' = 0$. We use Hartree–Fock theory restricted to ferromagnetic (F), antiferromagnetic (AF) and paramagnetic (P) states, and we find large mixed regimes where neither of these translational invariant states is thermodynamically stable. The results are for $L = 60$ and $\beta = 1000$ which is practically indistinguishable from the thermodynamic limit. (The parameters are defined in the main text.)

and 3. As mentioned, previous mean field phase diagrams for the 2D Hubbard model ($t' = 0$) predict an AF phase in a finite region around half filling.[8] Our corresponding phase mean field diagram is given in Fig. 1. It shows that the AF phase exists only strictly at half filling, and at finite doping close to half filling no simple translation invariant state is thermodynamically stable, in agreement with unrestricted Hartree–Fock theory.[10–12,23] Our discussion in Section 3 gives an intuitive explanation of the seemingly paradoxical fact that, even though the AF phase at half filling is very stable, it cannot persist at any non-zero doping value.

Our main results are the full phase diagrams for 2D $t - t' - U$ Hubbard model for $t' = 0$ and $t' = -0.35t$ in Figs. 1 and 2, respectively. They were obtained for a system size so large that they are practically identical with the thermodynamic limit. The phase diagrams are remarkably rich and very different from corresponding previous results: compare our Fig. 1 with Fig. 3 in Ref. 8 and our Fig. 2 with Fig. 1 in Ref. 9. Our results demonstrate that mixed phases are a typical feature of 2D Hubbard-type models: as one changes doping one never goes directly from one mean field phase to another, but there seems always a finite doping regime with a mixed phase in between. It is also interesting to note that the qualitative features

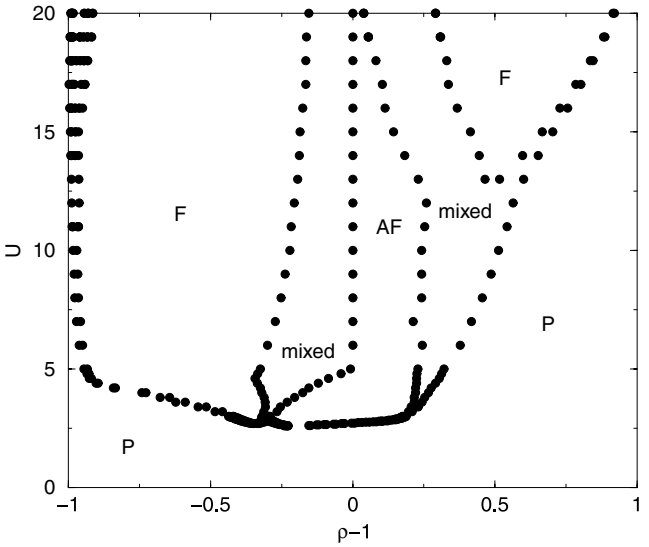

Fig. 2. Phase diagram of the 2D Hubbard model as a function of U and doping $\rho - 1$ for parameters $t = 1$, $t' = -0.35$, $L = 60$ and $\beta = 1000$, computed as Fig. 1. For large U and ρ close to zero it becomes numerically difficult to distinguish between the F and P phase, which is the reason for the fuzzy phase boundaries in this region of the phase diagram.

of the phase diagram are very sensitive to changes in the next-nearest-neighbor (NNN) hopping constant t', as is known from other methods; see e.g. Refs. 18, 20, 21. In particular, while a pure AF phase is possible only at half filling for $t' = 0$, the AF phase can be doped by electrons, but not holes, for $t' < 0$ at larger values of U, in agreement with previous results.[24]

We note that we have not further divided and specified the mixed regions in our phase diagrams since this information can be easily deduced as follows: For example, a point in a mixed region corresponds to a mixture of F and AF if the closest homogeneous phases horizontally are F and AF, etc.

1.3. Plan

The plan of the rest of this paper is as follows. Section 2 summarizes the formalism we use. Section 3 contains a detailed, intuitive discussion of our method to determine the thermodynamically stable mean field phase as a function of parameters, and we also give some computational details there. We conclude with a few remarks in Section 4. Some important technical details are discussed in an appendix.

2. MEAN FIELD THEORY: FORMALISM

In this section we collect the well-known formulas underlying our computations.

We start by fixing our notation. We consider the 2D Hubbard model defined by the Hamiltonian

$$H = -t \sum_{\langle i,j\rangle,\alpha} (c^\dagger_{i,\alpha} c_{j,\alpha} + \text{H.c.}) - t' \sum_{\langle\langle i,j\rangle\rangle,\alpha} (c^\dagger_{i,\alpha} c_{j,\alpha} + \text{H.c.})$$
$$- \mu \sum_{i,\alpha} c^\dagger_{i,\alpha} c_{i,\alpha} + U \sum_i \left(n_{i,\uparrow} - \frac{1}{2}\right)\left(n_{i,\downarrow} - \frac{1}{2}\right) \tag{1}$$

with the on-site repulsion $U > 0$ and the hopping amplitudes $t > 0$ and t' between the nearest neighbor (NN) sites $\langle i, j\rangle$ and next-nearest neighbor (NNN) sites $\langle\langle i, j\rangle\rangle$ on a square lattice with L^2 sites, respectively; the fermion operators $c^{(\dagger)}_{i,\alpha}$ are parametrized by the spin variable $\alpha = \uparrow, \downarrow$ and lattice sites $i = (i_x, i_y)$ where $i_{x,y} = 1, 2, \ldots, L$, $n_{i,\alpha} = c^\dagger_{i,\alpha} c_{i,\alpha}$ are number operators, and μ the chemical potential as usual. The fermion density is

$$\rho = \frac{1}{L^2} \sum_{i,\alpha} \langle n_{i,\alpha}\rangle \tag{2}$$

with $\langle\cdot\rangle$ the ground state expectation value to be specified below. Our conventions are such that particle-hole symmetry is manifest: $\rho - 1 \to 1 - \rho$ corresponds to $\mu \to -\mu$ and $t' \to -t'$ and, in particular, half filling $\rho = 1$ at $t' = 0$ corresponds to $\mu = 0$. Note that this model is defined on a finite dimensional Hilbert space (isomorphic to $\mathbb{C}^{4^{L^2}}$).

We recall that unrestricted Hartree–Fock (HF) theory is formally obtained by introducing

$$q_i = \langle n_i\rangle, \qquad \mathbf{m}_i = \langle \mathbf{s}_i\rangle \tag{3}$$

and replacing the Hubbard interaction by external field terms as follows,

$$n_{i,\uparrow} n_{i,\downarrow} \to \frac{1}{4}\left(\mathbf{m}_i^2 - q_i^2\right) + \frac{1}{2}(q_i n_i - \mathbf{m}_i \cdot \mathbf{s}_i),$$

where $\frac{1}{2} U \mathbf{m}_i$ and $\frac{1}{2} U q_i$ are mean fields coupling to the fermion spin

$$\mathbf{s}_i = \sum_{\alpha,\alpha'} c^\dagger_{i,\alpha} \boldsymbol{\sigma}_{\alpha\alpha'} c_{i,\alpha'}$$

and (local) density

$$n_i = \sum_\alpha c^\dagger_{i,\alpha} c_{i,\alpha},$$

respectively; $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the usual Pauli spin matrices. This replacement leads to a Hamiltonian describing non-interacting fermions in external fields, $H \to H_{HF}$ with

$$H_{HF} = \sum_i \frac{U}{4}\left(\mathbf{m}_i^2 - q_i^2\right) + \sum_{i,j,\alpha,\alpha'} c_{i,\alpha}^\dagger h_{i,\alpha,j,\alpha'} c_{j,\alpha'} \tag{4}$$

where

$$h_{i,\alpha,j,\alpha'} = -t_{ij}\delta_{\alpha\alpha'} + \delta_{ij}\left(\frac{1}{2}U[(q_i - 1)\delta_{\alpha\alpha'} - \mathbf{m}_i \cdot \boldsymbol{\sigma}_{\alpha\alpha'}] - \mu\delta_{\alpha\alpha'}\right) \tag{5}$$

is a self-adjoint $2L^2 \times 2L^2$-matrix which can be interpreted as a one-particle Hamiltonian; t_{ij} here equals t for NN sites, t' for NNN sites, and is zero otherwise. One now interprets $\langle\cdot\rangle$ in (3) as the expectation value in the ground state of H_{HF} in (4) and (5). This yields the Hartree–Fock equations allowing to self-consistently compute q_i and $\mathbf{m}_i$ (see e.g. Section 2 in Ref. 12).

We now observe that these Hartree–Fock equations can also be obtained as saddle point equations $\partial\mathcal{F}/\partial\mathbf{m}_i = \mathbf{0}$, $\partial\mathcal{F}/\partial q_i = 0$ from the free energy function

$$\mathcal{F} = -\frac{1}{\beta L^2}\log\mathcal{Z} \tag{6}$$

where

$$\mathcal{Z} = \mathrm{Tr}\left(\mathrm{e}^{-\beta H_{HF}}\right) \tag{7}$$

is the partition function defined by a trace over the fermion Fock space, and β is the inverse temperature. A straightforward computation yields

$$\mathcal{F} = \frac{U}{4L^2}\sum_i \left(\mathbf{m}_i^2 - (q_i - 1)^2\right) - \frac{1}{\beta L^2}\sum_{\ell=1}^{2L^2} \log\cosh\frac{\beta E_\ell}{2}, \tag{8}$$

with E_ℓ the eigenvalues of the one-particle Hamiltonian $h = (h_{i,\alpha,j,\alpha'})$ in (5).[16]

The physical solution of the Hartree–Fock equations are such that

$$\mathcal{F}_{HF} = \min_{\mathbf{m}_i}\max_{q_i} \mathcal{F}(\mathbf{m}_i, q_i). \tag{9}$$

This somewhat counter intuitive prescription can be shown to actually correspond to minimizing the grand canonical free energy; see the Appendix for details. The corresponding fermion density is obviously given by

$$\rho - 1 = -\frac{\partial\mathcal{F}_{HF}}{\partial\mu}. \tag{10}$$

We stress that the variational principle in (9), while *implying* standard Hartree–Fock theory, is not equivalent to it: the standard Hartree–Fock equations can have several solutions, but (9) provides a simple method to solve Hartree–Fock

equations so as to avoid the unphysical solutions: first maximize $\mathcal{F}$ with respect to the q_i, and then minimize with respect to the $\mathbf{m}_i$. In case we restrict Hartree–Fock theory by making a simplifying ansatz for the mean fields q_i and $\mathbf{m}_i$ as below, it can happen that one finds several Hartree–Fock solutions at a fixed value of μ. In this case one must take the solution minimizing the free energy.

Mean field theory is obtained from Hartree–Fock by restricting to mean fields which are invariant under translations by two sites. In this paper we follow Refs. 8, 9, 22 and restrict ourselves to states describing antiferromagnetism (AF), ferromagnetism (F) and paramagnetism (P). We thus make the following ansätze

$$\begin{aligned} \text{AF}: &\quad q_i = q, \quad \mathbf{m}_i = m_{\text{AF}}(-1)^{i_x+i_y}\mathbf{e}_z \\ \text{F}: &\quad q_i = q, \quad \mathbf{m}_i = m_{\text{F}}\mathbf{e}_z \\ \text{P}: &\quad q_i = q, \quad \mathbf{m}_i = \mathbf{0} \end{aligned} \tag{11}$$

where $\mathbf{e}_z$ is the unit vector in z-direction. With this restrictions it is easy to compute the eigenvalues E_ℓ by Fourier transform. One obtains

$$\begin{aligned} \text{AF}: &\quad E_{\mathbf{k},\pm} = \frac{1}{2}[\epsilon(\mathbf{k}) + \epsilon(\mathbf{k}+\mathbf{Q})] + \frac{U}{2}(q-1) - \mu \\ &\qquad \pm \frac{1}{2}\sqrt{[\epsilon(\mathbf{k}) - \epsilon(\mathbf{k}+\mathbf{Q})]^2 + (Um_{\text{AF}})^2} \\ \text{F}: &\quad E_{\mathbf{k},\pm} = \epsilon(\mathbf{k}) + \frac{U}{2}(q - 1 \pm m_{\text{F}}) - \mu \\ \text{P}: &\quad E_{\mathbf{k},\pm} = \epsilon(\mathbf{k}) + \frac{U}{2}(q-1) - \mu \end{aligned} \tag{12}$$

where the quantum numbers labeling the eigenvalues are $\ell \equiv (\mathbf{k}, \epsilon)$ with $\epsilon = \pm$ a band index and $\mathbf{k} = (k_x, k_y)$ with $k_{x,y} = (2\pi/L)\times$integer momenta restricted to the Brillouin zone $-\pi \le k_{x,y} \le \pi$; $\mathbf{Q} = (\pi, \pi)$ is the AF vector, and

$$\epsilon(\mathbf{k}) = -2t[\cos(k_x) + \cos(k_y)] - 4t' \cos(k_x)\cos(k_y) \tag{13}$$

is the usual tight binding band relation. Thus the mean field free energy becomes

$$\mathcal{F}_X = \frac{U}{4}\left(m_X^2 - (q-1)^2\right) - \frac{1}{\beta L^2}\sum_{\mathbf{k},\varepsilon=\pm} \log\cosh\frac{\beta}{2}E_{\mathbf{k},\varepsilon} \tag{14}$$

for $X =$ AF, F and P ($m_{\text{P}} = 0$), where the $\mathbf{k}$-sum becomes an integral in the thermodynamic limit $L \to \infty$. The standard mean field equations (see e.g. Sec. 2 in Ref. 9) are obtained from this from differentiation, $\partial\mathcal{F}_X/\partial q = \partial\mathcal{F}_X/\partial m_X = 0$. Note that $q = \rho_X$ (fermion density at fixed μ in the X-state) but, as explained in the next section, the relation of ρ_X to the system density ρ is somewhat subtle.

3. MEAN FIELD PHASE DIAGRAMS

We now explain our method to compute phase diagrams, concentrating on the point where we deviate from previous treatments. As a representative example we discuss the computation of the phases by our method for the 2D Hubbard model with $U = 6$, $t = 1$, and $t' = -0.16$; see (1). One reason for this choice is that it shows nicely several qualitative features which can occur in the phase diagram, another that these parameter values are of interest for HTSC compounds.[25]

As discussed, mean field theory for the Hubbard model is obtained by restricting Hartree–Fock theory to translational invariant states describing antiferromagnetism (AF), ferromagnetism (F) and paramagnetism (P). At zero temperature one can start with three variational states which all are Slater determinants[26] built of one-particle wave functions which are eigenstates of a mean field Hamiltonian where the Hubbard interaction is replaced by external field terms,

$$|\text{Slater}\rangle = |X\rangle, \quad X = \text{AF, F or P}. \tag{15}$$

These fields include the the fermions density ρ and the magnetization which is staggered for AF, constant for F, and zero for P, and they are determined by the usual Hartree–Fock equations given in the previous section. It is important to note that the fermion density is fixed in the standard Slater states, but we use a generalization of Slater's variational principle to Gibbs states allowing for finite temperature $1/\beta$ and where the fermion density is varied by changing a chemical potential μ (grand canonical ensemble; see the Appendix for details), but for simplicity we assume $1/\beta = 0$ in the following discussion. We now compute the Hartree–Fock ground state free energy per site, $\mathcal{F}_X$, for each of these states $X =$ AF, F and P, as a function of μ. One thus obtains the formulas given in the previous section. These have to be evaluated numerically which is, however, not very demanding (it can be done with MATLAB and on a PC).

Figure 3 gives the result for our example. At fixed value of μ, the mean field ground state is determined by the minimum,

$$\mathcal{F}_{\min} = \min_{X=\text{AF,F,P}} \mathcal{F}_X. \tag{16}$$

It is now important to recall that the fermion density ρ can be computed as μ-derivative of the free energy as in (10). From Figs. 3 and 4 is is obvious that ρ as a functions of μ is, in general, only piecewise continuous, and it has jumps at the particular values of μ where the minimum free energy curve changes, for example, from the AF to the F curve at the particular value $\mu = \mu_2$. The physical interpretation of this is as follows. We start at $\mu = 0$ where we obviously have the AF ground state and half-filling, $\rho - 1 = 0$. As we decrease μ, $\rho - 1$ remains zero since $\mathcal{F}_{\text{AF}}$ does not change. This is due to the AF gap: as long as μ remains in the gap the fermion density cannot change. For large enough μ values the AF band edge is reached and the slope of $\mathcal{F}_{\text{AF}}$ starts to decrease. However, before this can

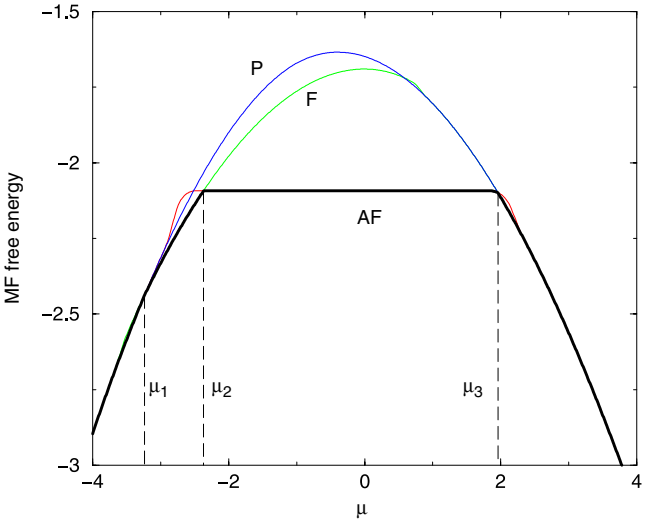

Fig. 3. Mean field free energy $\mathcal{F}_X$ of the 2D Hubbard model with $t = 1$, $t' = -0.16$, $U = 6$, $L = 60$ and $\beta = 1000$ as a function of the chemical potential μ. Shown are the curves for $X =$ AF, F and P (thin lines) and the absolute minimum $\mathcal{F}_{\min}$ (thick line). The dashed lines indicate the particular values μ_i, $i = 1, 2, 3$, of μ where the phases change. At these values the derivative of $\mathcal{F}_{\min}$ has discontinuities, and this leads to doping regimes with mixed phases; see Fig. 4. Color online.

happen the F free energy has become lower and taken over: as one decreases μ the F free energy decreases, and at a value $\mu = \mu_2$ the two curves cross, $\mathcal{F}_{\rm AF} = \mathcal{F}_{\rm F}$ at $\mu = \mu_2$. At this point we go from the AF to the F phase. Since the fermion densities $\rho_X(\mu_2) - 1 = -\partial\mathcal{F}_X/\partial\mu|_{\mu=\mu_2}$ for the states $X =$ AF and $X =$ F are different, it is impossible to get a density value in between with either state. There is, however, a possibility to realize such a fermion density with the following mixed state *exactly at* $\mu = \mu_2$,

$$w|\mathrm{AF}\rangle\langle\mathrm{AF}| + (1-w)|\mathrm{F}\rangle\langle\mathrm{F}|, \tag{17}$$

with the relative weight $0 < w < 1$ determined by the fermion density as follows,

$$\rho = w\rho_{\rm AF}(\mu_2) + (1-w)\rho_{\rm F}(\mu_2), \quad 0 < w < 1. \tag{18}$$

We now discuss the interpretation of this mixed solution. One possibility is that the system has phase separated and split up into AF and F regions.[27] Of course, the spatial structure of the actual state is not available in the mean field description by the mixed state, but it can in principle be calculated using unrestricted Hartree–Fock theory. However, since the bulk free energy dominates over the inter-facial free energies in the thermodynamic limit, the mixed state gives an accurate description of the thermodynamics. We stress that the appearance

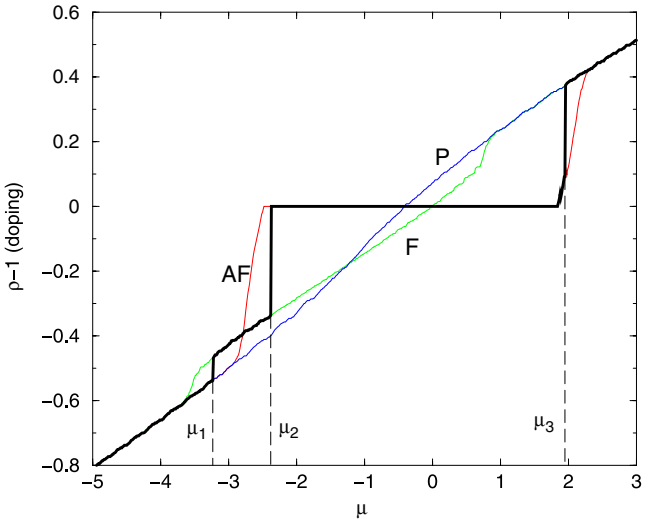

Fig. 4. Doping $\rho - 1$ of the 2D Hubbard model as a function of the chemical potential μ. The parameters are as in Fig. 3 ($t = 1$, $t' = -0.16$, $U = 6$, $L = 60$ and $\beta = 1000$). The curves are the derivatives of the corresponding ones in Fig. 3. The thick line determines the mean-field phase diagram, with the discontinuities at $\mu = \mu_i, i = 1, 2, 3$ determining doping regions where no pure phase F, AF or P is thermodynamically stable. The wiggles of the curves are due to finite size effects which, however, have no effect on the phase boundaries (this is demonstrated in the inset of Fig. 5). Color online.

of such a mixed state does *not* necessarily mean phase separation. The effect of the phase boundaries and other possible states have been excluded in our approximation. To know the actual state in the mixed regions thus is beyond our calculation and can be decided only by doing more work, e.g., using unrestricted Hartree–Fock taking into account more complicated states. Nevertheless, the *occurrence of such a mixed states proves rigorously that no simple translational invariant state of the kind assumed in our mean field ansatz is thermodynamically stable*. The mixed regions of the phase diagram are of particular interest since there the free energy is degenerate and thus the details of the solution can be strongly affected by fluctuations, phase boundaries, or details neglected in the model.

It is important to note that there are two further jumps of ρ and two further corresponding mixed phases: one at $\mu = \mu_1$ with F coexisting with P, and another at $\mu = \mu_3$ with AF and P coexisting. Again these mixed phases persist in finite doping regimes. It is also interesting to note that, while for $t' = 0$ the mean field free energies are invariant under the electron-hole transformation $\mu \to -\mu$, the finite value of $t' = -0.16$ here leads to a qualitative difference between hole doping ($\mu < 0$) and electron doping ($\mu > 0$). As seen in Fig. 3, the F state can

compete with the AF state only for $\mu < 0$, and this implies that it is possible to dope the AF state by electrons but not by holes.

We thus see that, even though we restricted Hartree–Fock theory to simple translation invariant states as in (15), our way of treating the doping constraint has implicitly also included the possibility of having a mixed state as in (17) as ground state, and we find that such a mixed state indeed occurs in a significant part of the doping regime.

We stress that our method to determine the phase boundary does not increase the computational effort of mean field theory, and it is easy to do the computations also for large system sizes. Most of our computations were done for a $L \times L$ lattice with $L = 60$. While at this values of L some finite size effects are still visible in the relation between doping $\rho - 1$ and the chemical potential μ (see Fig. 4), the inset in Fig. 5 demonstrates that resulting phase boundaries are practically identical with the ones in the thermodynamic limit. We also checked that the value $\beta = 1000$ we used for the inverse temperature practically gives the zero temperature phase boundaries.

Figure 5 shows the phases of the 2D Hubbard model as a function of the chemical potential and coupling constant U and for $t'/t = -0.35$. We included

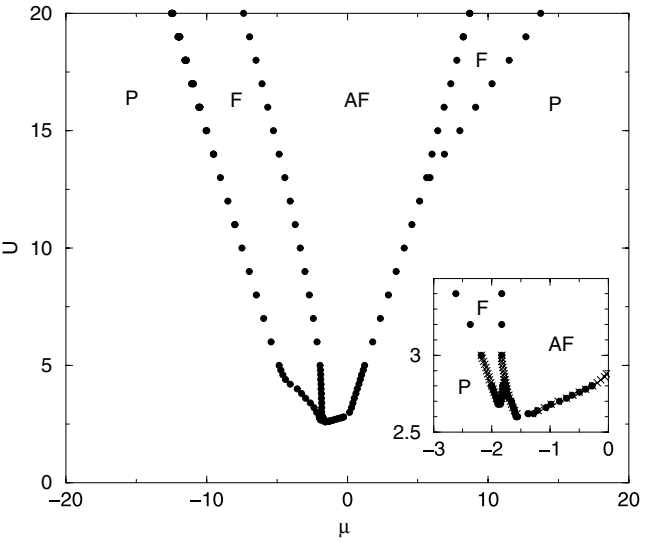

Fig. 5. Phases of the 2D Hubbard model as a function of the chemical potential for the same parameters as in Fig. 2 ($t = 1, t' = -0.35, \beta = 1000, L = 60$). Inset: Blowup of the region around the minimum of the phase lines in the main figure, showing interesting fine structure in the phase diagram. Also shown is the result from a calculation for system size $L = 120$ (crosses). The coincidence between results for two different system sizes demonstrate that $L = 60$ is practically already in the thermodynamic limit.

this also since it is conceivable to have other physical realizations of the model where the particle density is not fixed and the chemical potential can be changed by an external electric field.

4. CONCLUSIONS

In conclusion, we have presented a simple generalization of standard mean field theory, including the possibility of phase separated mean field states. We have presented results for the phase diagram of the 2D $t - t' - U$ Hubbard model, including values of parameters suggested by the HTSC materials. We find that the NNN hopping t' significantly alters the solution, in agreement with what is found by other methods; see e.g. Refs. 18, 20, 21. The resulting rich and nontrivial phase diagrams show significant qualitative differences between electron and hole doping for even small values of t'. Moreover, a finite t' suppresses order in the weak coupling regime, but can have the opposite effect at strong coupling; see Figs. 2 and 5. Our results are much richer than those obtained in previous studies.[8,9] The correctness of our method is justified by mathematical rigorous results.[13,14] The simple theory presented here can be straightforwardly generalized to a number of interesting cases, including more general mean field states like stripes, and to more complicated models with additional interaction terms or more bands, etc.

We stress once more that the method presented here does not necessarily produce accurate solutions to the problem, as is often the case with mean field theory. Nevertheless the method provides a useful starting point for estimating the structure of the phase diagram, providing inexpensive guidance for more accurate but costly calculation methods towards interesting regimes in the phase diagram.

As mentioned, the model we study is generally believed to be relevant for HTSC.[1] In this context is would be important to include the possibility of d-wave superconductivity SC which is believed to occur in this model near the AF phase; see Ref. 4 for review. However, for this more sophisticated methods than Hartree–Fock theory are needed. One example for such a method, which is technically much harder but captures more details, is the renormalized mean-field theory proposed by Zhang *et al.*[28] and further explored in Refs. 29, 30.

It is worth stressing once more that, in case our method predicts a mixed phase, this actually proves rigorously that no homogeneous Hartree–Fock state of the kind taken into account can minimize the Hartree–Fock free energy. However, in case our methods finds a homogeneous phase, it still is possible that the minimizing Hartree–Fock state is inhomogeneous.

Our results show that there is a homogeneous mean field ferromagnetic phase in the 2D Hubbard model at larger coupling values, and at finite coupling this phase is separated from the antiferromagnetic half-filled state by a mixed region. At

increasing coupling this mixed regions shrinks, and our numerical results indicate that it shrinks to zero at infinite coupling, in agreement with Nagaoka's result.[31]

We finally compare in more details our results with two other ones obtained recently by more sophisticated methods. Reference 20 presents the phase diagram for the 2D $t - t' - U$ Hubbard model on a 12×12 lattice obtained by unrestricted Hartree–Fock theory and for the parameter values $t' = 0.3$, $U = 8$ and the doping regime $0 \leq \rho - 1 \leq 0.35$ ($t = 1$). This phase diagram agrees very well with ours in Fig. 2 for $t' = -0.35$ and negative doping values (we recall that the model is invariant under $t' \to -t'$ and $\rho - 1 \to 1 - \rho$): we describe the region where unrestricted Hartree–Fock finds inhomogeneous domain wall- and polaron solutions as mixed AF and F phase, which then is followed by a pure F phase at around the same doping value as given in Ref. 20. We also compare with the Quantum Monte Carlo results on the competition between AF and F in Ref. 18: noting that t' in Ref. 18 corresponds to our $-t'$, they find competition between AF and F in the same parameter region as we, and the increase of the F region with U illustrated by the results for $U = 4$, 2 and 5 in Figs. 6, 8 and 9 in Ref. 18 is consistent with our result in Fig. 5. This clearly demonstrates that mean field theory is a useful method even for 2D Hubbard-like models, contrary to what seems to be generally believed.

Added Note. Jonas de Woul recently extended the results described in the present paper by also including ferrimagnetic and domain wall mean field solutions.[32] His results provide further examples for the importance of mixed phases in restricted Hartree–Fock studies.

APPENDIX: GENERALIZED HARTREE–FOCK THEORY

The derivation of the Hartree–Fock equations in Section 2 is only heuristic, and it does not explain the variational principle in (9) which has central importance for us. In this Appendix we therefore outline a mathematically rigorous derivation of it from first principles[14] (a detailed account appeared recently[32]). An alternative derivation using functional integrals was given in Ref. 16.

A generalization of Hartree–Fock theory for the model defined in (1) to finite temperatures $1/\beta$ and the grand canonical ensemble is obtained by minimizing the grand canonical potential

$$\Omega(q_i, \mathbf{m}_i) = \mathrm{Tr}(HW) + \frac{1}{\beta}\mathrm{Tr}(W \ln W) \tag{19}$$

over the set of all Gibbs states of the form

$$W = \frac{1}{\mathcal{Z}_R} \mathrm{e}^{-\beta H_R}, \quad \mathcal{Z}_R = \mathrm{Tr}\big(\mathrm{e}^{-\beta H_R}\big) \tag{20}$$

where $H_R = H_R(q_i, \mathbf{m}_i)$ is the Hamiltonian

$$H_R = \sum_{i,j,\sigma,\sigma'} c^\dagger_{i,\alpha} h_{i,\alpha,j,\alpha'} c_{j,\alpha'} \tag{21}$$

with the matrix $h_{i,\alpha,j,\alpha'}$ in (5). Note that $\mathbf{m}_i$ and q_i in H_R are regarded as variational parameters, and for $\beta \to \infty$, Ω reduces to the expectation value of the Hubbard Hamiltonian H in the normalized groundstate of the Hamiltonian H_R which is a Slater determinant. Generalized Hartree–Fock theory amounts to the following,

$$\Omega_{HF} = \min_{\mathbf{m}_i, q_i} \Omega(q_i, \mathbf{m}_i). \tag{22}$$

A key result proved in Ref. 14 is that this latter physical variational principle is equivalent to the variational principle in (9) in the sense that they give the same Hartree–Fock states and that $\mathcal{F}_{HF}$ and $\Omega_{HF}/\beta L^2$ are equal, up to an irrelevant additive constant.[14] (We note that in Ref. 14 the variations in (22) are restricted to fields satisfying $|\mathbf{m}_i| \leq 1$, $|q_i - 1| \leq 1$, but this does not change the result since any solution of (22) satisfies the equations in (3) which imply these latter restrictions.)

We have used the functional $\mathcal{F}$ rather than Ω in the main text to follow the tradition in the literature and since the numerics is easier. We have convinced ourselves in a few numerical tests that working with Ω gives the same results.

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REFERENCES

1. M. Imada, A. Fujimori, and Y. Tokura, Metal-insulator transitions. *Rev. Mod. Phys.* **70**:1039 (1998).
2. E. Dagotto, Correlated electrons in high-temperature superconductors. *Rev. Mod. Phys.* **66**:763 (1994).
3. E. Demler, W. Hanke, and S. C. Zhang, SO(5) theory of antiferromagnetism and superconductivity. *Rev. Mod. Phys.* **76**:909 (2004).
4. P. W. Anderson, P. A. Lee, M. Randeria, T. M. Rice, N. Trivedi, and F. C. Zhang, The physics behind high-temperature superconducting cuprates: The 'plain vanilla' version of RVB. *J. Phys.: Condens. Matter* **16**:R755 (2004).
5. P. A. Lee, N. Nagaosa, and X. G. Wen, Doping a Mott insulator: Physics of high-temperature superconductivity. *Rev. Mod. Phys.* **78**:17 (2006).
6. E. H. Lieb, Variational principle for many-fermion systems. *Phys. Rev. Lett.* **46**:457 (1981).
7. V. Bach and J. Poelchau, Accuracy of the Hartree–Fock approximation for the Hubbard model. *J. Math. Phys.* **38**:2072 (1997).

8. J. E. Hirsch, Two-dimensional Hubbard model: Numerical simulation study. *Phys. Rev. B* **31**:4403 (1985).
9. H. Q. Lin and J. E. Hirsch, Two-dimensional Hubbard model with nearest- and next-nearest-neighbor hopping. *Phys. Rev. B* **35**:3359 (1987).
10. D. Poilblanc and T. M. Rice, Charged solitons in the Hartree–Fock approximation to the large-U Hubbard model. *Phys. Rev. B* **39**:9749 (1989).
11. J. Zaanen and O. Gunnarsson, Charged magnetic domain lines and the magnetism of high-Tc oxides. *Phys. Rev. B* **40**:7391 (1989).
12. J. A. Verges, E. Louis, P. S. Lomdahl, F. Guinea, and A. R. Bishop, Holes and magnetic textures in the two-dimensional Hubbard model. *Phys. Rev. B* **43**:6099 (1991).
13. V. Bach, E. Lieb, and J. Solovej, Generalized Hartree–Fock theory and the Hubbard model. *J. Stat. Phys.* **76**:3 (1994).
14. V. Bach and J. Poelchau, Hartree–Fock Gibbs states for the Hubbard model. *Markov Processes Rel. Fields* **2**(1):225 (1996).
15. E. Langmann and M. Wallin, Restricted path integral approach to the doped Hubbard model. *Europhys. Lett.* **37**:219 (1997).
16. E. Langmann and M. Wallin, Mean-field approach to antiferromagnetic domains in the doped Hubbard model. *Phys. Rev. B* **55**:9439 (1997).
17. W. P. Su, Interplay of d-wave superconductivity and antiferromagnetism in cuprate superconductors: Phase separation and pseudogap phase diagram. *Mod. Phys. Lett. B* **19**:1295 (2005).
18. H. Taniguchi, Y. Morita, and Y. Hatsugai, Magnetism in the two-dimensional $t - t'$ Hubbard model: From low- to over-doping. *Phys. Rev. B* **72**:134417 (2005).
19. L. Arrachea, Itinerant ferromagnetism in the two-dimensional $t - t'$ Hubbard model. *Phys. Rev. B* **62**:10033 (2000).
20. B. Valenzuela, M. A. H. Vozmediano, and F. Guinea, Inhomogeneous structures in the $t - t'$ Hubbard model. *Phys. Rev. B* **62**:11312 (2000).
21. C. Honerkamp and M. Salmhofer, Temperature-flow renormalization group and the competition between superconductivity and ferromagnetism. *Phys. Rev. B* **64**:184516 (2001).
22. D. Penn, Stability theory of the magnetic phases for a simple model of the transition metals. *Phys. Rev.* **142**:350 (1966).
23. W. P. Su, Spin polarons in the two-dimensional Hubbard model: A numerical study. *Phys. Rev. B* **37**:9904 (1988).
24. A. Singh and H. Ghosh, Stability of the doped antiferromagnetic state of the $t - t'$ Hubbard model. *Phys. Rev. B* **65**:134414 (2002).
25. M. S. Hybertsen, E. B. Stechel, W. M. C. Foulkes, and M. Schlüter, Model for low-energy electronic states probed by x-ray absorption ins high-T_c cuprates. *Phys. Rev. B* **45**:10032 (1992).
26. J. C. Slater, Note on Hartree's method. *Phys. Rev.* **35**:210 (1930).
27. P. B. Visscher, Phase separation instability in the Hubbard model. *Phys. Rev. B* **10**:943 (1974).
28. F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, A renormalized Hamiltonian approach to a resonant valence bond wave function. *Supercond. Sci. Technol.* **1**:36 (1988).
29. H. X. Huang, Y. Q. Li, and F. C. Zhang, Charge-ordered resonating bond states in doped cuprates. *Phys. Rev. B* **71**:184514 (2005).
30. Q. H. Wang, Z. D. Wang, Y. Chen, and F. C. Zhang, Unrestricted renormalized mean field theory of strongly correlated electron systems. *Phys. Rev. B* **73**:092507 (2006).
31. Y. Nagaoka, Ferromagnetism in a narrow, almost half-filled s band. *Phys. Rev.* **147**:392 (1966).
32. J. de Woul, A restricted Hartree–Fock study of the 2D Hubbard model. Master's thesis, KTH, 2007.