Stripe Phases in the Two-Dimensional Falicov-Kimball Model

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The observation of charge stripe order in the doped nickelate and cuprate materials has motivated much theoretical effort to understand the underlying mechanism of the stripe phase. Numerical studies of the Hubbard model show two possibilities: (i) stripe order arises from a tendency toward phase separation and its competition with the long-range Coulomb interaction or (ii) stripe order inherently arises as a compromise between itinerancy and magnetic interactions. Here we determine the restricted phase diagram of the two-dimensional Falicov-Kimball model and see that it displays rich behavior illustrating both possibilities in different regions.

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The discovery of charge stripes in the nickelate [1] and cuprate [2] materials has encouraged much theoretical work to explain the underlying physical principles behind the stripe order and to examine whether the stripes are related to the mechanism for high-temperature superconductivity. There are two schools of thought for the physics that drives stripe formation: (i) Kivelson, Emery, and coworkers [3] propose that strongly correlated systems have a natural tendency toward phase separation and the inhomogeneous spatial charge ordering arises from a competition between this tendency to phase separate and the long-range Coulomb interaction which does not allow the electron density to stray too far from its average; and (ii) White and Scalapino [4] propose that the stripe order arises from a competition between kinetic and exchange energies in a doped antiferromagnet which does not require long-range Coulomb forces to stabilize the stripes. Despite a large amount of numerical work ranging from high-temperature expansions [5], to Monte Carlo simulations [6], to exact diagonalization [7], to semiclassical Hartree-Fock theory [8], no consensus has been reached about the region of stability for the phase-separated states or the microscopic mechanism for stripe formation.

Here we take an alternate point of view. Rather than try to prove phase separation in the Hubbard or t-J models, we choose an even simpler model—the spinless Falicov-Kimball (FK) model [9], which can be analyzed exactly. The relation of the FK model to the Hubbard model is analogous to the relation between the Ising and the Heisenberg models of magnetism (the FK model can be viewed as a Hubbard model where the downspin electrons are frozen and do not hop). The Hamiltonian is

$$H = -t \sum_{\langle x,y \rangle} c_x^\dagger c_y + U \sum_x c_x^\dagger c_x w_x, \qquad (1)$$

with $c_x^\dagger$ (c_x) the creation (annihilation) operator for a spinless electron at site x, and w_x is a classical variable that denotes the presence (absence) of an ion at site x when it is equal to 1 (0), respectively. The hopping occurs between nearest neighbors on a square lattice (all energies are measured in units of t) and the interaction strength is denoted by U. For any given configuration of ions $\{w_x\}$ the ground state for N_e electrons is determined by diagonalizing a one-body operator given by the above Hamiltonian and filling in the lowest N_e states. We typically are interested in the ground-state configuration of the ions for a given number of electrons $N_e = \sum_x \langle c_x^\dagger c_x \rangle$ and a given number of ions $N_i = \sum_x w_x$ (or their densities $\rho_e = N_e/N$ and $\rho_i = N_i/N$, respectively, with N the number of lattice sites).

The possibility of phase separation when $U \to \infty$ was proposed in 1990 [10] and is called the segregation principle. It was proved in the one-dimensional case [11], in the infinite-dimensional case [12], and recently in the general case [13]. This phase separation is a special type of phase separation, often referred to as the segregated phase, where the electrons and ions avoid each other and reside in separate domains. It is the analog of the ferromagnetic state in the Hubbard model. At half filling for the electrons and the ions, the ground state is known to be the chessboard phase [14,15]. This state is the analog of the antiferromagnetic state in the Hubbard model.

Of fundamental interest for the FK model is the question of how the many-body system evolves from a phase-separated state into an ordered chessboard phase, which are two states about as different as can be. In order to make contact with the Hubbard model, we examine this question when the number of electrons is equal to the number of ions and vary the concentration ($0 \leq \rho_e = \rho_i \leq 1/2$). This problem is then the analog of doping the $S_z = 0$ phase of the Hubbard model away from half filling.

It is well known that the ground-state phase diagram of the FK model typically includes a large number of different phases as functions of the particle concentrations and the interaction strength. As such, it seems unlikely that

one can rigorously analyze ground-state phases in the general case, although a number of interesting results exist for special cases [16] (usually for large U). Instead, we work with the restricted phase diagram technique, where we consider all possible periodic phases for which the number of sites per unit cell N_0 is less than or equal to $N_c = 16$. The technique first identifies all nonequivalent periodic phases, which number 23 755 in our case. Then for each periodic phase in our trial set, we calculate the total energy at a given value of U. Since, unlike the 1D case (see [17]), there are no exact formulas known for the density of states of general periodic phases in 2D, we have performed a numerical solution of the corresponding eigenvalue problem to determine the band structure (see Ref. [18] for the details). This involves finding the eigenvalues of an N_0-dimensional matrix for each value of k in a two-dimensional grid covering the Brillouin zone. Our calculations were performed with a k-space grid of 110×110 points for each phase. Then the grand-canonical phase diagram is constructed as a function of the electron and ion chemical potentials, and finally the grand-canonical phase diagram is translated to the canonical phase diagram for arbitrary ρ_i and ρ_e. This procedure assures thermodynamical stability of all phases (both periodic and their mixtures) present in the resulting canonical phase diagram. The stability problem is discussed extensively in Ref. [19], where the canonical phase diagrams of the 1D FK model were studied. Finally, we make the restriction $\rho_i = \rho_e$ in the canonical phase diagram to analyze the problem at hand.

The ground-state phase diagram is quite complex. We find many different stable phases occur. These phases fall into a number of different categories: (i) *the empty lattice* ($\rho_i = 0$ and $\rho_e \neq 0$) denoted E; (ii) *the full lattice* ($\rho_i = 1$ and $\rho_e = 0$) denoted F; (iii) *the chessboard phase* ($\rho_i = \rho_e = 1/2$ and ions occupy the A sublattice only) denoted Ch and shown in Fig. 1(a); (iv) *diagonal neutral* ($\rho_i = 1 - \rho_e$) *stripe phases* (the ions are arranged as diagonal chessboard phases separated by fully occupied striped regions with a slope of 1, or equivalently, Ch phases separated by diagonal antiphase boundaries) denoted DNS and illustrated in Fig. 1(b); (v) *diagonal non-neutral* ($\rho_i \neq 1 - \rho_e$) *stripe phases* (the ions are arranged as diagonal chessboard phases but separated by empty striped regions with a slope of 1) denoted DS and illustrated in Fig. 1(c) for $\rho_i = \rho_e = 7/15$; (vi) *axial non-neutral stripes* ($\rho_i \neq 1 - \rho_e$ and ions arranged in stripes parallel to the y axis and translationally invariant along the axis) denoted AS and shown in Fig. 1(d); (vii) *axial non-neutral chessboard stripes* ($\rho_i \neq 1 - \rho_e$ and ions arranged in stripes of the chessboard phase oriented parallel to the y axis) denoted AChS and illustrated in Fig. 1(e); (viii) *other neutral phases* ($\rho_i = 1 - \rho_e$ but the arrangement is not in any simple stripelike phase) denoted N and shown in Fig. 1(f) [note that many N phases can be described as stripe phases with slope different from 0, 1, or ∞ as the slope $1/2$ shown here, but we prefer to think of them as nonstripe phases]; (ix) non-neutral *four-molecule phases* (where $\rho_i \neq 1 - \rho_e$ and empty sites are arranged out of "bound" four-molecule empty-site squares tiled inside an occupied latticework) denoted 4M and shown in Fig. 1(g); and (x) truly two-dimensional non-neutral arrangements of ions (where $\rho_i \neq 1 - \rho_e$ and the ions are arranged in a fashion that is not stripelike, but rather requires a two-dimensional unit cell to describe it) denoted 2D and illustrated in Fig. 1(h) for nonstripelike arrangements and Fig. 1(i) for a phase that could be a slope 2/3 "stripe." Generically, the phase diagram includes mixtures of two or three of the periodic phases (iii)–(x), or of one or two periodic phases and the empty lattice (i). The empty lattice is usually needed in the phase mixtures to ensure that the average electron and ion fillings are equal for the mixtures. When the filling is sufficiently far from half filling, the system is in the segregated phase, which is a mixture of E and F.

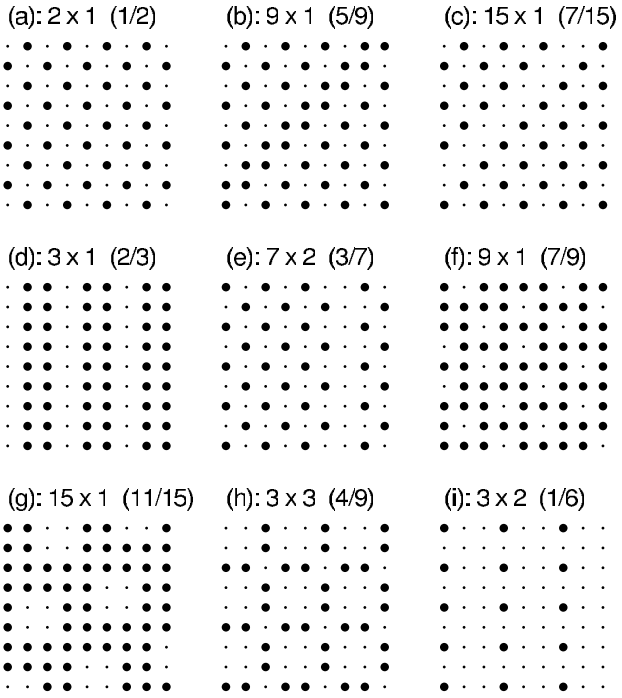

FIG. 1. Representative configurations of stable phase categories displayed in the phase diagram: (a) Ch, (b) DNS, (c) DS, (d) AS, (e) AChS, (f) N, (g) 4M, (h) 2D, and (i) another 2D. The large dots correspond to ion-occupied sites and the small dots correspond to ion-vacant sites. The numbers written above each configuration indicate the dimensions of the unit cell; the corresponding ion densities are given in parentheses.

The number of phases stable or appearing in mixtures tends to grow as U is decreased in magnitude. For $U = 8$ there are 25 phases: E (1); F (1); Ch (1); DNS (6); and N (16). For $U = 6$ there are 30 phases: E (1); F (1); Ch (1); AS (20); N (6); and 2D (1). For $U = 4$ there are 42 phases: E (1); F (1); Ch (1); AS (35); N (1); and 2D (3). For $U = 2$ there are 38 phases: E (1); F (1); Ch (1); AS (14); DNS (4); 4M (2); and 2D (15). For $U = 1$ there are 50 phases: E (1);

F (1); Ch (1); DS (1); AS (9); AChS (6); 4M (3); and 2D (28).

The empty lattice, the full lattice, and the chessboard phase are present in the phase diagram for all U; the diagonal neutral stripes generally for large U ($U > 7$) (occasionally they can appear for moderate U as well—as occurs for $U = 2$); the axial stripes for moderate and small U ($U < 7$); the axial chessboard stripes for small U ($U < 3$); the other neutral phases for large U ($U > 4$); the four-molecule phases for small U ($U < 3$); and the two-dimensional phases for moderate and small U ($U < 7$) (growing significantly in number as U decreases). The total number of phases appearing in the phase diagram is too large for us to show all ion configurations here. Instead, we show an illustrative member from each category in Fig. 1. The summary of all of the stable phases will appear in a longer publication [20].

The phase diagram is shown in Fig. 2 and its simplified, schematic version, in Fig. 3. The phase boundary between the segregated phase and mixtures with periodic phases approaches half filling as U gets large, as expected. When $U = 8$, we find the mixtures, when doped just away from half filling, occur between the chessboard phase, the empty lattice, and diagonal neutral stripe phases. This picture is similar to those that propose the phase separation scenario, but *there is no requirement of the long-range Coulomb interaction to generate the stripes*—they also occur as part of the periodic phases that compose the different stable mixtures. As the system is doped further away from half filling, mixtures with other neutral phases occur, before the system fully segregates. This shows that the phase separation scenario for stripe formation does not necessarily require long-range Coulomb interactions.

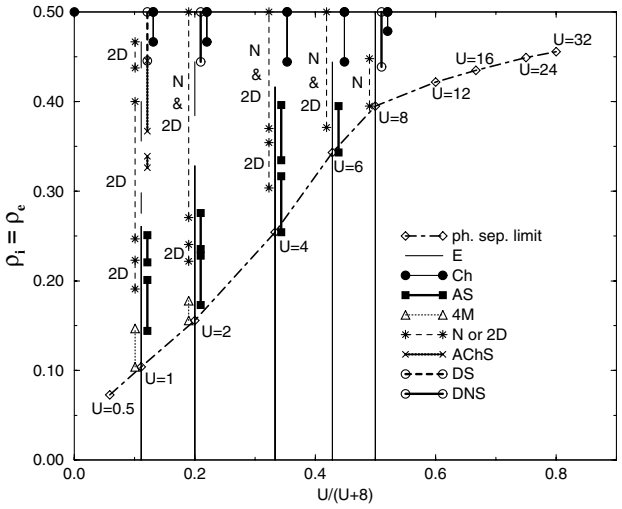

FIG. 2. Phase diagram of the 2D FK model along the $\rho_e = \rho_i$ line for a set of U values. The dot-dashed line separates the segregated phase and mixtures of the E phase with periodic phases. Below this line only the E and F phases coexist (in fact, the F phase is also stable slightly above the line, forming three-component mixtures within narrow intervals of densities). Vertical line segments mark intervals of the densities where the corresponding phases (of a given class) are involved in the formation of stable phases. [All the segments, except for those corresponding to the E phase, are moved slightly right or left of the value of $U/(U + 8)$.] Bold lines correspond to various types of stripe phases. Mixtures of phases in one category occur within each line segment; when segments overlap, mixtures form between phases in the overlapping categories.

As U is reduced, the phase diagram becomes more complicated. Near half filling, the chessboard phase is always one of the phases in the stable mixtures, but we find the empty lattice and diagonal neutral phases disappear and are replaced by other neutral or 2D phases in the mixtures. Then as U is reduced further, the diagonal neutral stripe phases occasionally reenter into the mix, replacing the N or 2D phases, as can be seen for $U = 2$. Finally, for smaller U, the mixtures are between the diagonal non-neutral stripes and the chessboard phase only. Farther away from half filling, the behavior is even more complex, with axial non-neutral stripes first entering near the segregation boundary, and then the 4M phases appearing as U is reduced further. The axial neutral chessboard phases also appear for small U. It is in this moderate-to-small U region where we see many stripe phases form due to a delicate balance between kinetic-energy and potential-energy effects. This is the alternate scenario for stripe formation that does not require phase separation or the long-range Coulomb interaction.

Diagonal stripes occur near half filling because the structure factor for those phases are nonzero along the diagonal and peaked near $(0, 0)$ and (π, π) corresponding to the stable chessboard phase at half filling. Axial stripes occur near the phase-segregation boundary, because the structure factor is nonzero along the zone edge and peaked near $(0, 0)$, corresponding to the nearby segregated phase. As the segregation becomes too strong, the axial stripes disappear. The transition between diagonal and axial stripes is not direct, but passes through

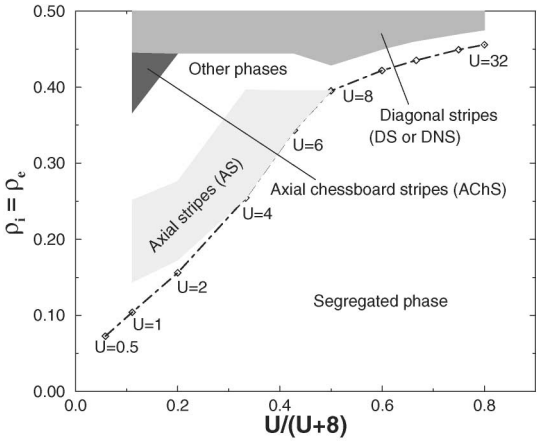

FIG. 3. Schematic phase diagram with highlighted regions of stability of the stripe phases.

other types of phases and mixtures not ordinarily considered in Hubbard model studies (the peaks in the structure factors lie in all directions in the Brillouin zone). *These FK model results indicate that such two-dimensional phases may play a role in the crossover region of the Hubbard model (particularly for weak to moderate U).* We also find the complexity is significantly increased for the weak-coupling region of the phase diagram where the White-Scalapino scenario is correct; the Kivelson-Emery phase separation scenario is much simpler, but requires U larger than the bandwidth (which we can quantitatively estimate with these results). Naturally, we expect the number of stable phases to be reduced in the Hubbard model because the quantum fluctuations from the now mobile "ions" should break some of the static order. For example, we know the ground state far from half filling is paramagnetic in the Hubbard model for U small enough, but is always segregated in the FK model.

In summary, we have calculated the restricted phase diagram of the two-dimensional FK model showing in detail how the chessboard phase evolves to the segregated phase as a function of doping. Our investigation considered approximately 25 000 inequivalent configurations in the energy minimization, but cannot rule out the possibility that phases with larger unit cells may appear in the complete phase diagram. We constrained the system to have the same number of localized and itinerant particles, which is the analog of the $S_z = 0$ state of the Hubbard model. We find that, in addition to the phase separation of the segregated phase, the system generically forms a number of stripe and nonstripe phases. For large U (larger than the bandwidth), we find the stripes to be diagonal and appearing only close to half filling. As U is reduced, we find diagonal stripes evolving into axial chessboard stripes and then axial stripes as the system is doped further away from half filling. In addition, we find a number of truly two-dimensional phases present as well. While we cannot say anything rigorous about what happens in the Hubbard model itself, our results suggest that one should expect a complex phase diagram when stripe phases are present and *see a competition between the stability of the stripes and other, more two-dimensional, structures.* We also predict that the Kivelson-Emery scenario of phase separation does not require the long-range Coulomb interaction to stabilize stripes. We expect that the phase diagram also simplifies for the Hubbard model, since quantum fluctuations between different low-energy "ionic" configurations will destroy some of the static order.

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