Repulsive particles on a two-dimensional lattice

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Abstract

The problem of finding the minimum-energy configuration of particles on a lattice, subject to a generic short-ranged repulsive interaction, is studied analytically. The study is relevant to charge ordered states of interacting fermions, as described by the spinless Falicov–Kimball model. For a range of particle density including the half-filled case, it is shown that the minimum-energy states coincide with the large–$U$ neutral ground state ionic configurations of the Falicov–Kimball model, thus providing a characterization of the latter as “most homogeneous” ionic arrangements. These obey hierarchical rules, leading to a sequence of phases described by the Farey tree. For lower densities, a new family of minimum-energy configurations is found, having the novel property that they are aperiodic even when the particle density is a rational number. In some cases there occurs local phase separation, resulting in an inherent sensitivity of the ground state to the detailed form of the interaction potential.

1 Introduction

The problem studied in this paper is the search for ground states of a two-dimensional repulsive lattice gas at zero temperature, defined as follows. Suppose a collection of classical particles, which will be called “ions”, is allowed to occupy the sites of an infinite square lattice, such that no two ions occupy the same site. With each spatial arrangement of ions is associated an energy density,

$$\mathcal{E} = N^{-1} \sum_{i<j} V(\mathbf{r}_i - \mathbf{r}_j),$$

(1)
where $\mathbf{r}_i$ is the position of the $i$th ion, $N$ is the number of sites, and $V$ is some repulsive interparticle pair potential. What is the arrangement of ions which minimizes $\mathcal{E}$?

Specific forms of the interaction potential $V$ will be discussed below. Of interest is the case where $V$ is short-ranged, in the sense that it falls off rapidly with distance, so the contribution to the energy from a given ion is dominated by a few near neighbours. Nevertheless, the long-range part of the interaction will be important also, in breaking the degeneracy of configurations with identical short-range correlations.

Our work is motivated by two questions. The first arises in the study of the Falicov–Kimball model (Falicov and Kimball 1969). This is a prototype model of many-body correlations in an interacting fermion system, in which an electron gas of density $\rho_e$ interacts with a collection of heavy classical particles ("ions") of density $\rho_i$ through an on-site interaction of strength $U$. It has several interesting interpretations, including as a model of valence fluctuations in rare earth and transition metal oxides, as a version of the Hubbard model, and as a model of binary alloys (for background discussion, see Kennedy and Lieb 1986, Lieb 1986, Jędrzejewski, Lach and Lyżwa 1989a,b, Kennedy 1994, Watson and Lemański 1995, Gruber et al. 1995, Gruber and Macris 1996). Let us focus on the particular case of the neutral model ($\rho_e = \rho_i$) in the large–$U$ limit, and on the question of determining the ground state ionic configurations, which are those for which the electrons’ energy is a minimum, at fixed density. For the one-dimensional Falicov–Kimball model, this problem has been solved: the ground states for rational densities are the most homogeneous ionic configurations. Lemberger (1992) has provided both a precise definition of this property, and a proof that it is satisfied for the large–$U$ neutral ground states. Here, we investigate the question of whether a similar homogeneity property can be defined which characterizes the large–$U$ neutral ground states for the two-dimensional model. We approach the question via classical energetics, since it is clear that at least some of the model’s properties can be understood as effects of repulsive effective interionic forces (Watson and Lemański 1995).

Thus, our problem captures one aspect of charge ordered states on a two-dimensional lattice: the energetics of static classical interacting particles. Despite the idealized interparticle potential and the neglect of kinetic energy and quantum effects, features emerge which appear to be typical of two-dimensional charge ordering. We find, for example, phases in which charges line up to form slanted stripes, which are also found in the Falicov–Kimball model (Kennedy 1994, Watson and Lemański 1995). Similar charge (and
spin) stripe structures are observed in a family of high-temperature superconductors (Tranquada et al. 1995), in its nickelate (Tranquada et al. 1994) and manganate (Sternlieb et al. 1996) analogues, and in other compounds (Chen and Cheong 1996). In those cases the mechanisms involved are very different from the model considered here, but may also, in some cases, be dominated by static energetics (Emery and Kivelson 1993). Charge stripes are also found, for example, in theories of two-dimensional interacting electrons in a magnetic field (Koulakov, Fogler and Shklovskii 1996, Moessner and Chalker 1996).

The second issue we wish to address is of a more general nature. The problem under study is one in which there is a competition between two length scales. One length scale is the lattice spacing, and the other is the average interparticle distance. The one-dimensional version of the problem has been studied by Hubbard (1978) and others (Pokrovsky and Uimin 1978, Burkov 1983, Aubry 1983a), in the context of a model of quasi-one-dimensional conductors, and in connection with the Frenkel–Kontorova model (Burkov, Pokrovsky and Uimin 1982). In that case, the repulsive forces encourage the ions to spread out evenly with a neighbour distance \(1/\rho\), where \(\rho\) is the ion density, but this distance may be incompatible with the constraint that ions occupy sites of the background lattice. The exact solution obtained by Hubbard for the case of decreasing, convex potentials, has features typical of systems with competing length scales, and in general of systems with modulated phases resulting from frustrated interactions (Bak 1982, Aubry 1983b, Heine 1987, Yeomans 1988, Lovesey, Watson and Westhead 1991). When the ion density is a rational number, the ground state ion configuration is periodic, and may be constructed hierarchically using a simple branching rule displaying the structure of a Farey tree (Aubry 1983a, Levitov 1991, Gruber, Ueltschi and Jędrzejewski 1994). The dependence of ion density on chemical potential is a complete devil’s staircase, a general consequence of the convex form of the potential, which may be understood using a formulation in terms of interacting domain walls (Fisher and Szpilka 1987, Bassler, Sasaki and Griffiths 1991).

The two-dimensional generalization studied here displays a more dramatic kind of lattice mismatch. The natural ionic configuration in the absence of a background lattice is a triangular lattice, with neighbour distance \((2/\sqrt{3}\rho)^{1/2}\). With a square background lattice, the ions are always hindered from adopting their natural arrangement, for any density: the ions would like to form a triangular lattice, but are forced to occupy the sites of a square lattice. Thus, increasing the dimension to two introduces the possibility of a
geometrical mismatch, in addition to the simple length scale mismatch studied for one-dimensional systems. (In three dimensions, the problem is harder still, as then the minimization of repulsive energy is nontrivial even in the absence of a background lattice; see the remarks below concerning the relation with sphere packing, a famous unsolved problem in three-dimensional geometry (Croft, Falconer and Guy 1991, Conway and Sloane 1993)).

The problem of repulsive particles on a two-dimensional lattice is related to other topics of recent interest. As an example, we mention experiments (Baert et al. 1995) investigating flux lines in a superconductor, in the presence of an array of artificial antidots which pin the flux lines to the sites of a square lattice. Although the forces between flux lines are not of the short-ranged type studied here, the kind of lattice mismatch which occurs is the same. In consequence, the pinning force, derived from critical current measurements, shows peaks at certain rational matching fields. (We shall return to this example in Sec. 4.) Hierarchical structures have been found previously in models of flux line lattices (Levitov 1991). Finally, we mention lattice gas models of monolayers of adsorbed atoms on a lattice substrate (Pokrovsky and Uimin 1978, Bak et al. 1979, Villain 1980), and observed in-plane ordering of intercalant layers in graphite (Suzuki and Suematsu 1983, Zabel and Chow 1986).

2 Hierarchical structures in the Falicov–Kimball model

This section presents a short summary of some aspects of the Falicov–Kimball model.

The Hamiltonian of the Falicov–Kimball model, in its usual spinless form, and in the canonical ensemble (fixed \( \rho_e \) and \( \rho_i \)), is

\[
H = - \sum_{\langle ij \rangle} a_i^\dagger a_j - U \sum_i w_i n_i,
\]

where \( a_i^\dagger \) is the creation operator for a spinless “electron” on site \( i \) of a \( d \)-dimensional lattice, and \( w_i \) is a classical variable taking the value 1 if site \( i \) is occupied by an “ion” and 0 otherwise. Hopping is restricted to sites \( i \) and \( j \) which are nearest neighbours, and \( n_i = a_i^\dagger a_i \) is the electron occupation of site \( i \). The Hamiltonian does not contain a kinetic term for the ions, so the ions do not move. However, the ground state is constructed by choosing the particular configuration of ions (i.e. the values of \( w_i \)) for which the total
electronic energy computed from $H$ is a minimum. We take $U > 0$, so the electron–ion interaction is attractive. This is not a restriction, since the attractive and repulsive models are in one-to-one correspondence with each other, via a particle–hole transformation.

The Falicov–Kimball model has been studied using a variety of techniques, for lattices in one dimension and higher, and many interesting features have been found (for a review of exact results, see Gruber and Macris 1996; for numerical studies, see Watson and Lemański 1995, Gajek, Jędrzejewski and Lemański 1996, and references therein). Here we focus on the large–$U$ neutral ground states. It is in the limit of strong electron–ion coupling that the behaviour of the model is simplest. The phase diagram in the grand canonical ensemble contains only segregated phases (phase-separated mixtures of the vacuum and the phase in which every site is occupied) and a family of neutral configurations ($\rho_e = \rho_i$). As mentioned above, the neutral large–$U$ ground states of the one-dimensional model, for rational densities, are fully characterized by the property of being the most homogeneous (Lemberger 1992).

Qualitatively, the homogeneity property means that the ions would like to be as far apart as possible, i.e. that the effective forces between them are repulsive. The physical origin of this effective force may be understood by imagining that each ion traps exactly one electron in a bound state to form an atom, and that the interaction between atoms is repulsive because the Pauli principle inhibits overlap of the electrons’ wavefunctions. Analytical calculations of the effective ion–ion interaction potential have been made (Gruber, Lebowitz and Macris 1993a,b, Gruber, Ueltschi and Jędrzejewski 1994, Watson and Lemański 1995, Micheletti, Harris and Yeomans 1996), in the main for the one-dimensional model. Gruber and co-workers (Gruber, Lebowitz and Macris 1993a,b, Gruber, Ueltschi and Jędrzejewski 1994) showed that in one dimension the total energy is given to leading order in $t/U$ by a sum of two-body potentials for neighbouring ions, and discussed qualitatively three-body and higher potentials. Micheletti, Harris and Yeomans (1996) calculated the general $n$-body interaction to leading order. The crucial feature is that these potentials are exponentially decreasing convex functions of the separation of the outermost ions, and it follows from general arguments (Fisher and Szpilka 1987, Bassler, Sasaki and Griffiths 1991) that the ground state phase diagram exhibits a complete devil’s staircase, in which the ion configurations obey hierarchical branching rules. An alternative, if less rigorous, argument is to imagine that convex repulsive forces exist between all pairs of ions, in which case the work of Hubbard (1978) leads
Figure 1: The first five generations of the Farey tree, according to which periodic large-\(U\) neutral ground states of the Falicov–Kimball model are constructed. The ground state for a given rational density is obtained by concatenating the unit cells of its two parents; for example, density \(3/8\) is obtained by combining \(1/3\) and \(2/5\).

to the same conclusion. Numerical work on the one-dimensional Falicov–Kimball model is in perfect agreement with these ideas, and it is fair to say that a coherent understanding has emerged.

Let us describe the hierarchical construction of the most homogeneous configurations in one dimension. It is based on the Farey tree (Aubry 1983a), part of which is displayed in Fig. 1. The tree extends downwards to infinity, with the rule that each pair of adjacent fractions \(p_1/q_1\) and \(p_2/q_2\) is assigned a descendant \((p_1 + p_2)/(q_1 + q_2)\). Every rational fraction between 0 and 1 occurs somewhere in the tree. The recursive rule for constructing the ion configuration corresponding to a given rational density \(p/q\) is then that it has period \(q\), with a unit cell obtained by concatenating the unit cells of its parent fractions in the Farey tree (the lower density parent on the left). Thus, with the \(\rho = 0\) and \(\rho = 1\) states having unit cells (0) and (1) respectively, \(\rho = 1/2\) corresponds to (01), \(\rho = 1/3\) to (001), \(\rho = 2/5\) to (00101), and so on. The construction given here can be expressed in several equivalent forms: as a recursive criterion for equal spacing of gaps between ions (Lemberger 1992), in terms of the continued fraction expansion of the
density (Burkov 1983), in terms of the solutions of a Diophantine equation
(Hubbard 1978, Freericks and Falicov 1990), and as a “circle sequence”
(Luck 1989). Although the rigorous analysis does not extend to irrational
values of the density, one expects from continuity that the ground states
are given by a similar construction. These are then quasiperiodic, i.e.
one-dimensional quasicrystals. The Fourier spectrum of such a configura
tion has singularities on a dense set of points, namely the frequency module generated
by two noncrystallographic primitive vectors.

Let us now turn to the two-dimensional model, whose behaviour is less
well understood. Published work to date include several preliminary studies
(Jędrejewski, Lach and Łyżwa 1989a,b, Gruber et al. 1990), a collection
of general analytical properties (Gruber, Jędrejewski and Lemberger 1992),
exact analyses of large–U neutral equilibrium states for certain densities, on
square and triangular lattices, in the presence of a magnetic field, and at
zero and nonzero temperature (Gruber, Jędrejewski and Lemberger 1992,
Kennedy 1994, Gruber et al. 1995, Messager and Miracle-Sole 1996), and
a numerical calculation (Watson and Lemański 1995) of restricted phase
diagrams in the grand canonical ensemble. The phase diagrams in two
dimensions are more complex than in one dimension, but there are some
common features, especially for large U where the neutral phases dominate.
Kennedy (1994), in a rigorous perturbative analysis for large U, proved that
the neutral ground states for densities ρ = 1/3, 1/4 and 1/5 are those given
in Fig. 2, and provided a partial characterization of the ground states for
the range 1/4 < ρ < 1/2. Each ground state in this range consists of (not
necessarily equally spaced) stripes of occupied sites, slanted at an angle
which is a piecewise constant function of the density. For ρ = 1/2, the
ground state is the “checkerboard” configuration (Kennedy and Lieb 1986,
Lieb 1986) given in the figure. Watson and Lemański (1995), on the basis of
numerical calculations, suggested that such slanted stripe phases occur over
a wider density range, and that the structure perpendicular to the stripes
obeys hierarchical rules based on the Farey tree.

Thus, these conjectured ground states follow a hierarchical construction
identical to that for the one-dimensional model. However, as pointed out
by Kennedy (1994), such configurations do not appear to be the most ho-
mogeneous, even though the effective interactions are entirely repulsive for
large U (Watson and Lemański 1995). One purpose of the present work
is to show that, at least for a range of densities, these ground states are
in fact the most homogeneous configurations, according to a very reason-
able criterion: they minimize the repulsive energy, \( E \), with \( V \) representing a
Figure 2: Neutral ground state ionic configurations of the two-dimensional large–U Falicov–Kimball model, for densities 1/2, 1/3, 1/4 and 1/5. Large dots: occupied sites; small dots: vacant sites. These are also ground states of the repulsive ion problem, with respect to the “greedy potential” (see Sec. 4).

“generic” short-ranged repulsion. Thus, as in one dimension, the physics is dominated by the tendency for ions to spread as far apart as possible, and the results are not sensitive to the precise form of the effective repulsion. Having demonstrated that \( E \) has the same ground states as the Falicov–Kimball model for the density range \( 1/4 \leq \rho \leq 1/2 \), in which exact results and reliable numerics are available, we can use \( E \) to explore the possibilities for other densities.

3 The interparticle potential

In the notation using site occupation variables \( w_i \), the energy density is

\[
E = \frac{1}{2N} \sum_{ij} V_{i-j} w_i w_j = \frac{1}{2} \sum_j V_j g_j, \tag{3}
\]

where the second equality writes it in terms of the pair correlation function,

\[
g_i = \frac{1}{N} \sum_j w_j w_{i+j}. \tag{4}
\]

We note that \( E \) satisfies a duality property: under a particle–hole transformation, \( w'_j = 1 - w_j \), the pair correlation function becomes

\[
g'_i = 1 - 2\rho + g_i. \tag{5}
\]

Working in the canonical ensemble, where the density is constant, the pair correlation functions of dual configurations differ by a constant, and hence
so do the energies. The conclusion is that the ground states for densities \( \rho \) and \( 1 - \rho \) are duals of one another. Consequently, only densities less than \( 1/2 \) need be considered.

Qualitative features of the effective interionic potential for the two-dimensional Falicov–Kimball model have been discussed previously (Watson and Lemański 1995) and are similar to the one-dimensional case (Gruber, Lebowitz and Macris 1993a,b, Gruber, Ueltschi and Jędrzejewski 1994, Micheletti, Harris and Yeomans 1996). The effective potential has a two-body part, whose long-range asymptotic form for large \( U \) (Watson 1995) is proportional to \( CR\exp(-R/\lambda) \), where \( \lambda \) is a \( U \)-dependent “atomic” length, \( R \) is the “Manhattan distance”, \( R = m + n \), between ions at sites \((0,0)\) and \((m,n)\), and \( C \) is the combinatorial factor \((m+n)!/m!n!\), giving the number of walks from one site to the other. There are also multi-body potentials, evident, for example, in calculated large-\( U \) effective Hamiltonians (Gruber, Jędrzejewski and Lemberger 1992, Kennedy 1994, Gruber et al. 1995, Messager and Miracle-Sole 1996) which include only short-range terms.

Here we are interested in properties which do not depend on any specific numerical form of the interaction potential. Let us then neglect three-body and higher order forces, and attempt to abstract the idea of a short-ranged two-body potential to the extreme of pure combinatorics. We introduce our “greedy potential” as follows. Rather than assigning a numerical value to the energy of a configuration, the greedy potential is a rule for deciding which of two configurations is energetically preferred. The rule is to compare the number of ions per unit area which have neighbours at distance \( r = 1 \), the lower number being preferred. If the \( r = 1 \) correlations of the two configurations are the same, one compares the density of neighbours at \( r = \sqrt{2} \). If this does not break the tie, one continues to distances \( 2, \sqrt{5}, \sqrt{8} \), and so on. In other words, with the greedy potential the configurations are ordered hierarchically with respect to radial correlations. It follows from (5) that the greedy potential obeys the duality property, so that ground states at densities \( \rho \) and \( 1 - \rho \) are related by a particle–hole transformation.

We emphasize that there is no rigorous basis for using the greedy potential in the context of the Falicov–Kimball model. The greedy potential depends only on radial distance, whereas the correct pair potential is a strong function of the Manhattan distance, in the sense that the potential at distance \( R + 1 \) is weaker than that at distance \( R \) by a power of \( U \). Furthermore, the true effective Hamiltonian includes multi-body interactions entering at lower powers of \( 1/U \) than the longer range parts of the two-body term. Nevertheless, as follows from the work of Lemberger (1992), for the
one-dimensional Falicov–Kimball model the neutral large-$U$ ground states coincide precisely with the ground states of the greedy potential. Thus, in one dimension, the pair potential overwhelms other contributions, and an interesting question is whether this occurs also in two dimensions.

4 Ground states

In the following sections we solve completely the problem of finding the ground state ion configurations with the greedy potential, for the density ranges $1/6 \leq \rho \leq 1/5$ and $1/4 \leq \rho \leq 1/2$, and we provide a fairly complete characterization of the ground states for $1/5 < \rho < 1/4$. To begin, we show that for a few special values of the density which best match the background lattice, the ground states may be deduced immediately from elementary considerations.

For any configuration, define $r_{\text{min}}$ as the shortest distance between any pair of ions. Consider the set of ion configurations which have $r_{\text{min}} \geq \sqrt{2}$, i.e. which do not contain any pairs of ions at nearest neighbour distance, $r = 1$. We ask, what is the maximum ion density for a configuration in this set? Since the density is the inverse of the average area of the Voronoi cells of the configuration, one may try to minimize the Voronoi cell area of a single ion, subject to the constraint that all other ions are further than $r = 1$ away from the central ion and from each other. The optimum configuration is clearly that pictured in Fig. 3(a), which has a Voronoi cell area of 2. It happens that there exists a configuration in the infinite square lattice for which every ion has a local arrangement like this, namely the checkerboard configuration in Fig. 2. We conclude that if $r_{\text{min}} \geq \sqrt{2}$ then $\rho \leq 1/2$, and that this minimum is achieved only for the checkerboard configuration. An equivalent statement is that if $\rho = 1/2$ then $r_{\text{min}} \leq 1$ for any configuration except the checkerboard. It follows that the checkerboard is the ground state for density $1/2$.

A similar argument can be applied to configurations with the constraint $r_{\text{min}} \geq 2$. The smallest Voronoi cell area is 4, and up to rotations and reflections there are three local configurations achieving the minimum, illustrated in Fig. 3(b), (c) and (d). The argument must now be extended to take account of the multiplicity of $r = 2$ correlations, but the logic is essentially the same as above and leads to the conclusion that the density $1/4$ ground state configuration is identical to that shown in Fig. 2.

Continuing the same argument to lower densities is straightforward, ex-
cept that it becomes increasingly difficult to prove rigorously that a particular set of local configurations have the minimum Voronoi cell area. Using elementary inequalities (Watson 1995), this task can be reduced to the laborious checking of a finite set of possibilities, which can then be carried out by hand or by computer. The results are as follows: for density $1/5$, the ground state is the configuration pictured in Fig. 2, while for densities $1/8$, $1/9$, $1/10$, $1/13$, $1/15$ and $1/18$, the ground state configurations are those shown in Fig. 4. We have carried this analysis through for densities as low as $1/90$ (corresponding to $r_{\text{min}} \geq 10$); the optimum configurations have the appearance of distorted triangular lattices. The only case found not to be amenable to this analysis is $r_{\text{min}} \geq \sqrt{20}$, for which the minimum area Voronoi cell is a pentagon (area $\approx 19.97$) which fails to tile the plane. The smallest Voronoi cell which tiles the plane has area 20, so it appears likely that the highest packing density with $r_{\text{min}} \geq \sqrt{20}$ on an infinite lattice is $1/20$, but this has not been proved.

The crucial step in the above argument is the maximizing of the density subject to a constraint relating to the distance of closest approach of two ions. It is interesting that the repulsive ion problem is, in this respect, closely related to disc packing (Croft, Falconer and Guy 1991, Conway and Sloane 1993).

The densities for which this simple disc packing argument yields a rigorous determination of the ground state are the magic values $1/2$, $1/4$, $1/5$, $1/8$, and so on. These may be regarded as densities of best fit for which

\[ r_{\text{min}} \geq \sqrt{2}; \ (b)-(d) \ r_{\text{min}} \geq 2. \]
Figure 4: Ion configurations shown to be ground states with respect to the “greedy potential”, for special matching densities $\rho$. 
repulsive particles are “most comfortable” on a square lattice. We note, in passing, that best fit configurations on a square lattice have been considered previously by Baert et al. (1995), who argued that these determine the positions of anomalous peaks in the pinning force measured in experiments on flux lines in a superconductor with a periodic array of pinning centres. However, the authors stated that the matching configurations are tilted square lattices, which appears questionable, assuming that the dominant factor is the mutual repulsion of flux lines. Indeed, it is hard to imagine the tilted square lattices for $\rho = 1/4$ or $1/8$ being lower in energy than those in Figs. 2 and 4 for any reasonable repulsive potential. We would rather suggest that that the flux line configurations corresponding to the rational matching peaks are those in Figs. 2 and 4. On the other hand, our suggestion is not consistent with the claim that a peak is found at $\rho = 1/16$. Neither suggestion explains the absence of peaks at $1/9$, $1/10$ and $1/13$ in the experimental data.

4.1 Density $1/4 \leq \rho \leq 1/2$

We now determine rigorously the ground states of the repulsive ion problem (with the greedy potential) for a range of densities. The technique used is one previously applied to the Falicov–Kimball model (Gruber, Jędrzejewski and Lemberger 1992, Kennedy 1994, Gruber et al. 1995), based on decomposing a Hamiltonian into contributions from $3 \times 3$ blocks. In each case, the property of minimizing the Hamiltonian does not fix a unique state, but reduces the search for the ground state to a subset of possible configurations. Then additional reasoning is used to determine the ground state uniquely.

First, we require an appropriate Hamiltonian. Let us introduce

$$H_r = (1/N) \sum_{(ij)=r} w_i w_j,$$

where the sum is over all bonds of length $r$. Thus, $H_r$ counts the density of pairs of ions at distance $r$. Consider the density range $1/3 \leq \rho \leq 1/2$. It follows from the argument of the previous section that $r_{\text{min}} \geq \sqrt{2}$, and the bound $r_{\text{min}} \leq (2/\sqrt{3}\rho)^{1/2}$ therefore implies $r_{\text{min}} = \sqrt{2}$. Hence, by construction, each ground state for the greedy potential in $1/3 \leq \rho \leq 1/2$ minimizes $H_{\sqrt{2}}$. However, this condition is not sufficient to determine the ground states uniquely, as may be seen from the examples given in Fig. 5. The configurations pictured both have density $2/5$, and they also have identical $r = \sqrt{2}$ correlations. It is necessary to go to $d = 2$ to reveal that (a) is preferred.
Figure 5: Two configurations with density 2/5, having identical correlations up range \( r = \sqrt{2} \). Configuration (a) is preferred when \( r = 2 \) correlations are taken into account.

Thus, we introduce a total Hamiltonian

\[
H = 4H_{\sqrt{2}} + 6\epsilon H_2,
\]

which includes an \( r = 2 \) term weighted by a small coefficient \( \epsilon \), to break the tie between configurations degenerate at \( r = \sqrt{2} \). (The coefficients 4 and 6 are included for later convenience.) We shall use this Hamiltonian to determine the ground state in the density range \( 1/4 \leq \rho \leq 1/2 \).

Let us now define a set of local functions, referring only to sites within a \( 3 \times 3 \) block. Labelling the sites within a block by local coordinates \((i,j)\) with \( 0 \leq i, j \leq 2 \), we write

\[
h_1 = w_{(1,1)}
\]
\[
h_2 = w_{(0,0)} + w_{(2,0)} + w_{(2,2)} + w_{(0,2)}
\]
\[
h_3 = w_{(0,1)} + w_{(1,0)} + w_{(2,1)} + w_{(1,2)}
\]
\[
h_4 = w_{(0,1)}w_{(1,0)} + w_{(1,0)}w_{(2,1)} + w_{(1,2)}w_{(1,1)} + w_{(1,2)}w_{(0,1)}
\]
\[
h_5 = w_{(0,0)}w_{(1,1)} + w_{(2,0)}w_{(1,1)} + w_{(2,1)}w_{(1,1)} + w_{(0,2)}w_{(1,1)}
\]
\[
h_6 = w_{(0,0)}w_{(2,0)} + w_{(0,1)}w_{(2,1)} + w_{(0,2)}w_{(2,2)} + w_{(0,0)}w_{(0,2)} + w_{(1,0)}w_{(1,2)} + w_{(2,0)}w_{(2,2)}
\]

These satisfy

\[
4 \sum_B h_1 = \sum_B h_2 = \sum_B h_3 = 4N\rho \tag{14}
\]
\[
\sum_B h_4 = \sum_B h_5 = 2NH_{\sqrt{2}} \tag{15}
\]
\[
\sum_B h_6 = 3NH_2, \tag{16}
\]
where \(\sum_B\) denotes the sum over all blocks.

The approach is now as follows. One constructs a block Hamiltonian \(h\) which is a linear combination of \(h_1\) to \(h_6\), in such a way that \(N^{-1}\sum_B h\) differs from \(H\) only by a term proportional to the density. Since we are working in the canonical ensemble, the difference is a constant, and minimizing \(N^{-1}\sum_B h\) is equivalent to minimizing \(H\). One then writes out all possible configurations of ions in a single \(3 \times 3\) block: there are 20 possibilities, up to rotations and reflections, listed by Kennedy (1994). One determines a subset of block configurations such that \(h\) is minimized on that subset, for all sufficiently small \(\epsilon\). Then, provided there exists at least one configuration of the required density on the infinite lattice which is made up entirely of blocks in that subset, it follows that the ground state for the greedy potential is made up entirely of blocks in the subset.

Clearly, the trick is to find a suitable block Hamiltonian. Here we shall just state a choice that works. For \(1/3 \leq \rho \leq 1/2\), let

\[
h = -(4 + 4\epsilon)h_1 - (1 + 4\epsilon)h_2 - (2 + 4\epsilon)h_3 + h_4 + h_5 + 2\epsilon h_6, \tag{17}
\]

and for \(1/4 \leq \rho \leq 1/3\), let

\[
h = -(4 - 6\epsilon)h_1 - (1 - \epsilon)h_2 - (2 - 2\epsilon)h_3 + (1 + \epsilon)h_4 + (1 - \epsilon)h_5 + 2\epsilon h_6. \tag{18}
\]

The remaining analysis is identical to that used by Kennedy (1994) for the Falicov–Kimball model: in his notation, the former \(h\) is found to be minimized for block configurations 12, 13, 17, 19 and 20, while the latter is found to be minimized for configurations 2, 5, 6, 11, 12 and 13. These are precisely the same block configurations which determine the ground states of the Falicov–Kimball model in the same density ranges, and the same conclusion follows immediately (Kennedy 1994). For \(1/3 \leq \rho \leq 1/2\), the ground states consist of fully occupied stripes of slope 1 separated by unoccupied sites, i.e. the ground states are invariant under translations by \((1,1)\) or \((0,-1)\). (Examples of such configurations are the first two configurations in Fig. 2, and Fig. 5(a).) For \(1/4 \leq \rho \leq 1/3\), the ground states consist of stripes of slope \(1/2\), i.e. are invariant under translation by one of the vectors \((2,1), (1,2), (2,-1)\) or \((-1,2)\).

The stripe property does not determine the configuration uniquely. However, it does reduce the problem to a one-dimensional one, since the only
remaining freedom is the arrangement of stripes in the perpendicular direction. When restricted to the set of configurations satisfying the stripe property, the greedy potential leads to a purely repulsive interaction between stripes. In fact, this interaction is described by the one-dimensional form of the greedy potential, and it follows from Hubbard’s (1978) result that the stripe arrangement is the “most homogeneous” one, constructed according to the Farey tree as described in Sec. 2. We have therefore arrived at a complete description of the ground states, in this density range, of the repulsive ion problem with the greedy potential. A recursive construction of the ground states for rational densities can be made, as follows. The \( \rho = 1/2 \) state has primitive vectors \( A \) and \( C \), where \( A = (-1, 1) \) and \( C = (1, 1) \). It is convenient to think of it as being constructed by placing a stripe generated by \( C \), then a second identical stripe separated from the first by \( A \), a third stripe separated from the second by \( A \), and so on. The structure transverse to the stripes is then \( \ldots AAA\ldots \), denoted \( (A) \). Similarly, the \( \rho = 1/3 \) state is \( (B) \), where \( B = (-2, 1) \). Their descendant, the \( \rho = 2/5 \) state, is then \( (AB) \), which is the configuration in Fig. 5(a). The \( \rho = 3/7 \) ground state is \( (ABB) \), and so on. The ground states in \( 1/4 \leq \rho \leq 1/3 \) are generated in the same manner by \( A = (-1, 1) \), \( B = (0, 2) \) and \( C = (2, 1) \).

The ground states of our repulsive ion problem and the neutral large–U ground states of the Falicov–Kimball model have the same stripe structure in this density range. This is not sufficient to deduce that the two sets of ground states are identical. However, the numerical evidence that the Farey tree rules are obeyed for the ground states of the Falicov–Kimball model is most persuasive (Watson and Lemański 1995). It seems reasonable, therefore, to conjecture that the repulsive ion problem does in fact have the same ground states as the Falicov–Kimball model, i.e. that the greedy potential captures the dominant physics in the neutral large–U limit, for this range of densities. This result suggests that there is a well-defined sense in which the large–U neutral ground states of the Falicov–Kimball model could be regarded as the “most homogeneous” configurations.

As Kennedy (1994) has noted, the stripe structure does not accord with plausible intuitive ideas about what homogeneity might mean in two dimensions. As an example, he imagines forming a configuration with density slightly less than 1/2 by starting with the checkerboard and removing ions in such a way that these vacancies are as far apart as possible; the configuration in Fig. 5(b) is of this type. This example raises an interesting point. If a finite number of vacancies is introduced into the checkerboard configuration they cannot destroy the long-range order, and it is clear that they
will repel each other, in order to maximize the number of neighbouring ions whose repulsive energy is reduced. If the number of vacancies is increased beyond a certain point, presumably of order $N^{1/2}$, the vacancies suddenly come together to form a domain wall, and the full long-range order of the checkerboard is destroyed.

4.2 Density $1/5 \leq \rho \leq 1/4$: General structure

For densities less than 1/4, we have $r_{\text{min}} \geq 2$, i.e. no two ions may be closer than $r = 2$. This implies that the nine of the twenty $3 \times 3$ block configurations do not occur in the ground state. Defining the block Hamiltonian

$$h = -3h_1 - h_2 - 2h_3 + h_6,$$

(19)

we find that the block configurations 2, 5, 8 and 11 (in Kennedy’s notation) minimize $h$, amongst the remaining eleven possible blocks. Since $N^{-1} \sum_B h$ is a multiple of $H_2$, apart from a term proportional to the density, and since the ground state lies in the set of configurations which minimize $H_2$, it follows that the ground state is composed entirely of blocks of type 2, 5, 8 and 11. The same property was shown by Kennedy to hold for the Falicov–Kimball model. It is not sufficient to determine the ground state uniquely, but it does place strong constraints on it.

Each block centred on an occupied site is of type 2. The block one site to the right of a type 2 block must be type 5, type 8 (in one of two orientations) or type 11. Considering all possibilities for adjacent blocks, one finds as in Fig. 6 that the ions to the right of any given ion (circled) must be arranged as in (a), (b) (with two possible orientations) or (c).

Therefore, we may join ions by lines in such a way that each ion is a vertex of a quadrilateral lying to its right. That quadrilateral is either a “diamond” in one of two orientations, as in (a) or (c), or a square in one of two orientations, as in (b). The same applies to the three other orthogonal directions from any central ion. Hence each ion is the common vertex of four such quadrilaterals. The ion configuration has a square lattice “skeleton”, in the sense that the lattice formed by the ions, with edges drawn to form quadrilaterals as described, is topologically equivalent to a square lattice. Equivalently, the configuration could be described as a tiling of the plane by two kinds of tiles, the diamond and the square. Configurations made up only of blocks of type 2, 5, 8 and 11 are in one-to-one correspondence with such tilings.
Figure 6: Possible configurations of ions to the immediate right of any given ion (circled), for a ground state configuration in the density range $1/5 \leq \rho \leq 1/4$.

Next, we consider the structure of the tilings. One can construct a tiling by beginning with a tiling of squares only, and then introducing one or more “kinks”, where a kink is a line of diamonds, running along one of the two possible orthogonal directions. Two orthogonal kinks may intersect, as illustrated in Fig. 7(a). Clearly, any arrangement of kinks is a valid tiling, and conversely, it can be shown that any tiling corresponds to an arrangement of kinks. For any tile configuration, the ion density does not depend on the arrangement of kinks, but only on the kink densities $\alpha$ and $\beta$ in the two directions: $\rho = 1/(5 - \alpha - \beta + 2\alpha\beta)$. The problem is to find the best kink configuration, subject to the constraint of constant density.

The definition of a kink is such that a transformation which turns a kink into an antikink (the absence of a kink) leaves all configurations invariant, up to rotation. Since this transforms the kink densities as $\alpha \rightarrow 1 - \alpha$ and $\beta \rightarrow 1 - \beta$, we need consider only $\alpha \leq 1/2$.

The argument so far depends only on the information as to which $3 \times 3$ block configurations may occur in the ground state, and applies equally in the case of the Falicov–Kimball model. To take further the analysis for the greedy potential, we include longer range correlations by considering possible configurations of four tiles meeting at a vertex. There are four cases, illustrated in Fig. 8, A–D. If a configuration is such that a fraction $\lambda_A$ of its ions correspond to type A vertices, a fraction $\lambda_B$ to type B vertices, and so on, with $\sum \lambda_i = 1$, then its density is

$$\rho = (5\lambda_A + 9\lambda_B/2 + 9\lambda_C/2 + 4\lambda_D)^{-1}. \quad (20)$$

The weights of correlations at particular distances, or, equivalently, values
Figure 7: (a) An ion configuration corresponding to a plane tiling in which two orthogonal kinks intersect. (b) A configuration with density 2/9, constructed from a tiling in which the kink density is 1/2 in both directions. The lines are a guide to the eye, showing the corresponding tile arrangement.

of the radial distribution function $g(r)$, are related to the fractions $\lambda_i$ of the four types of vertex. We find

$$g(2) = (\lambda_B + \lambda_C)/2 + \lambda_D = 5 - 1/\rho$$  \hspace{1cm} (21)

$$g(\sqrt{5}) = 2$$  \hspace{1cm} (22)

$$g(\sqrt{8}) = g(3) = 0$$  \hspace{1cm} (23)

$$g(\sqrt{10}) = 2\lambda_A + \lambda_B + \lambda_C = 2(1/\rho - 4)$$  \hspace{1cm} (24)

$$g(\sqrt{13}) = \lambda_C/2 + \lambda_D = 5 - 1/\rho - \lambda_B/2.$$  \hspace{1cm} (25)

All except the last of these is independent of the $\lambda$ coefficients. Hence, it is necessary to go at least to $r = \sqrt{13}$ correlations to break the degeneracy of tile configurations. From (25), the ground state belongs to the set of configurations for which $\lambda_B$, the fraction of type B vertices, is maximum.

Type B sites occur only where kink-antikink neighbour pairs intersect pairs running in the orthogonal direction. Their density is maximized for kink densities less than 1/2 by requiring all kinks to be isolated, and for kink densities greater than 1/2 by requiring all antikinks to be isolated. If $\alpha$ and $\beta$ are both less than or equal to 1/2, this gives a B site density $\lambda_B = 4\alpha\beta$, which must now be minimized subject to the constraint of fixed density. The optimum is easily shown to be

$$\alpha = \beta = [1 - (9 - 2/\rho)^{1/2}]/2,$$  \hspace{1cm} (26)
so the kink densities are the same in both directions. This case corresponds to $\rho \leq 2/9$. If $\alpha \leq 1/2$ and $\beta \geq 1/2$, we have $\lambda_B = \alpha(1 - \beta)$, and the optimum now has the density of kinks in the $\alpha$ direction equal to the density of antikinks in the $\beta$ direction, i.e. $\beta = 1 - \alpha$. The two cases may be written as

$$\rho = \frac{2}{9} \pm \left(1 - 2\alpha\right)^2,$$  \hspace{1cm} (27)

where the sign is plus for $\rho < 2/9$ and minus for $\rho > 2/9$.

Special cases of interest are $\alpha = 0$ and $\alpha = 1/2$. The former yields the $\rho = 1/4$ and $\rho = 1/5$ ground states of Fig. 2, which correspond to diamond and square tilings, respectively. The latter gives a $\rho = 2/9$ ground state with alternating kinks and antikinks, which is the configuration shown in Fig. 7(b).

We have shown that the ground state consists of a distribution of isolated kinks or antikinks in a tilted square lattice background, and we have determined the kink densities. The precise arrangements of the kinks will be considered in the next subsection. First, let us note one interesting consequence of the relationship (27) between kink density and ion density. If the ground state ion configuration is periodic, then the kink configuration is periodic and the kink density must be a rational number. It follows that the ion density is of the form $\rho = 2/[9 \pm (p/q)^2]$, with $p$ and $q$ integers such that $0 \leq p/q \leq 1$. For all ion densities other than this set of special values, the ground state configuration is certainly not periodic, because the kink density is an irrational number. The ion densities for which an aperiodic ground state is found includes “most” rational values. This is a somewhat

Figure 8: The four possible types of vertex which can occur in a configuration corresponding to a tiling of the plane by diamonds and squares.
surprising result: in previous investigations of related models, it has been found that the ground state is periodic whenever it is possible for it to be periodic, i.e. whenever the density is a rational number.

4.3 Density $1/5 \leq \rho \leq 1/4$: Kink configurations

Having determined the kink densities, it is necessary to study the kink–kink interaction to find the arrangement of kinks in the ground state. We already know that the interactions are such as to rule out nearest-neighbour kinks or antikinks, i.e. they are repulsive at the shortest range.

It is possible to study the kink interactions systematically beginning with short range terms. For example, given a configuration containing the segment 000101, where 1 denotes a kink and 0 denotes an antikink, one may examine the change in energy on moving the kink by one step to 001001. Such a move involves shifting a single row of ions by (-1,1), or a vector equivalent under rotation. The energy change depends on the arrangement of kinks in the perpendicular direction. In this case, however, it can be shown that, regardless of the perpendicular structure, the energy is always lowered by an amount of magnitude at least $V(\sqrt{34})$. Since a move of the form 10010001 to 10001001 always gives an energy change at a range greater than $\sqrt{34}$, it follows that no ground state contains both 101 and 10001 segments. Hence, for kink densities $1/3 \leq \alpha \leq 1/2$, the configuration is made up entirely of kinks spaced 2 or 3 units apart, while for $\alpha \leq 1/2$, the ground state does not contain any kinks spaced 2 units apart. In other words, kinks are purely repulsive at range 2, implying that the ground states for $1/3 \leq \alpha \leq 1/2$ have homogeneous kink configurations, in the terminology of Lemberger (1992). However, the kink configurations may or may not be the most homogeneous, depending on longer range interactions.

If kink interactions were purely repulsive in all cases, the ground states would indeed be those with the most homogeneous kink arrangements. That this is not true can be seen in the example of Fig. 9. Here we see a kink configuration 0001010 along an axis (2,1). If kink interactions were repulsive at range 3, the energy could be lowered by moving the central kink one unit to the left, yielding the configuration 001010001. This move corresponds to shifting a row of ions by (-1,1), to the sites shown in the figure as open circles. The resulting changes in radial correlations all cancel out to range $\sqrt{58}$. The lowest order change in energy comes at range $\sqrt{61}$, from the pair of sites joined by an arrow in the figure, and is positive. Hence the range 3 kink interaction is attractive, and this conclusion holds for any kink
structure in the perpendicular direction with $0 < \alpha \leq 1/3$.

The consequence of such an attractive kink force is dramatic. Since, with the greedy potential, a correlation at range $\sqrt{61}$ can never be outweighed by longer range correlations, no matter how large their weight, it is always energetically favourable for two kinks to come together to a distance of 3 units. The result is phase separation: for $\alpha < 1/3$, all the kinks will clump together in a region in which all neighbouring kinks are 3 units apart, and the rest of the lattice will be free of kinks. This occurs in both directions, so the result is four distinct regions: one with density 1/5 (kink free), two regions of density 3/14 (kink free in one direction but not the other), and one region of density 9/41 (intersecting kinks with spacing 3 in both directions).

We have argued above that the greedy potential provides a sensible definition of most homogeneous configurations in two dimensions. The appearance of phase separation in the ground state kink configurations reveals one of the limitations of this idea. It would be perverse to regard configurations with macroscopic phase separation as the most homogeneous. Nevertheless, the occurrence of attractive kink interactions is an informative result. Here, phase separation is a consequence of the singular nature of the greedy potential, coming from the fact that $V(r_1)$ is considered infinitely larger than
$V(r_2)$ if $r_2 > r_1$. For a real interaction potential, where $V(r_2)$ is a finite, though perhaps small, fraction of $V(r_1)$, long-range forces would prevent macroscopic phase separation. Instead, the result would be local phase separation, yielding a state which appears inhomogeneous (phase separated) on short length scales but is macroscopically homogeneous. This is an example of frustrated phase separation (Emery and Kivelson 1993). The magnitude of the intermediate length scale is sensitively dependent on the relative magnitude of long-range and short-range components of the potential. No matter how small the long-range part, it will eventually be magnified to a macroscopic scale as the system tends toward phase separation.

Thus, the occurrence of phase separation in our model with the greedy potential suggests that in two dimensions, and in this density range, the ground state is inherently sensitive to the details of the interaction potential. It also suggests that a useful and rigorous definition of a unique “most homogeneous” configuration in two dimensions is likely to be elusive.

The exact kink structure of the ground state is the outcome of the competition between long-range forces and the tendency towards phase separation. In addition, there is the complicating factor that there are two arrays of kinks intersecting one another, with kink interactions in one direction coupled to the kink positions in the other. The problem of finding the ground states for a given model potential appears difficult, and of limited value. Let us merely note a few qualitative properties. The appearance of attractive kink interactions leads to an incomplete devil’s staircase, with a tendency to ‘lock in’ to a rational kink density, such as 1/3 in the example described above. For nearby densities, there is local phase separation, stabilized by a repulsive interaction on an intermediate length scale. On this scale, there are domains of kink-rich and kink-free structure. One may then look at the effective forces between domains, and apply the same reasoning to them as for the kinks: if domain interactions are attractive at some range, there is a tendency to phase separation and longer-range interactions come into play.

It may be that for some density range the kinks (or domains) are purely repulsive, independently of the kink arrangement in the orthogonal direction. In that case, we may conclude that they adopt a “most homogeneous” configuration in each direction separately, and that in a restricted interval the devil’s staircase is complete. The kink arrangement is periodic if the kink (or domain) density is a rational number, and quasiperiodic if it is irrational. In the latter case, the ground state is a two-dimensional quasicrystal.
4.4 Density $1/6 \leq \rho \leq 1/5$

The analysis for lower densities is very similar to the preceding cases. For $\rho \leq 1/5$, we have $r_{\text{min}} \geq \sqrt{5}$, and we may eliminate from consideration all block configurations except types 1, 2, 3, 4, 8 and 9 (using the labelling of Kennedy 1994). We define a new block function,

$$h_7 = w_{0,0}w_{1,2} + w_{0,0}w_{2,1} + w_{2,0}w_{0,1} + w_{2,0}w_{1,2}$$

$$+ w_{0,2}w_{1,0} + w_{0,2}w_{2,1} + w_{2,2}w_{0,1} + w_{2,2}w_{1,0},$$

which counts $r = \sqrt{5}$ correlations, and a block Hamiltonian

$$h = -2h_1 - h_2 - 2h_3 + h_7,$$

for which $N^{-1} \sum_B h$ equals $2H\sqrt{5}$ plus a term proportional to the density. Since $h$ is minimized for block types 2, 3, 8 and 9, the ground state is composed entirely of those block configurations.

By considering the possible blocks in the immediate neighbourhood of a given ion, one may show that the local environment of an ion reduces to just a few possibilities. The conclusion is similar to the case in the previous section: the ground state configuration has a square lattice “skeleton”, and by drawing appropriate bonds between neighbours can be constructed from a tiling of the plane by polygons. The tiles in this case are a square, a parallelogram and a “kite”, shown in Fig. 10.

Amongst all possible tilings, we must now select the ground state by considering correlations at $r > \sqrt{5}$. It is easy to see that correlations up to $r = \sqrt{13}$ are the same for all tilings for a given ion density, but that $g(4)$ equals the density of kite tiles and is therefore minimized by choosing this density to be zero. Thus, the ground state corresponds to a tiling of the plane by squares and parallelograms only. In such a tiling, the arrangement

![Figure 10: The square, parallelogram and kite tiles, from which the ground state ion configurations in the density range $1/6 \leq \rho \leq 1/5$ are constructed.](image)
Figure 11: The four possible types of vertices at which four tiles meet, in a tiling of the plane by squares and parallelograms.

of tiles at an ion, corresponding to a vertex at which four tiles meet, is limited to the four types shown in Fig. 11. Once again, we rely on longer range correlations to reduce the number of possibilities: for all tilings of fixed density, correlations are equal for \( r < \sqrt{18} \), and \( g(\sqrt{18}) \) is nonzero only when vertices of type D are present. The ground state tiling is made up only of type A, B and C vertices.

We now have sufficient information to specify the ground state uniquely. A tiling using only these three types of vertex corresponds to a *slanted stripe* configuration, of a similar kind to those found in Sec. 4.1 to be ground states for \( 1/4 \leq \rho \leq 1/2 \). In this case the slope of the stripes is 1/2. The structure of the ground state configurations perpendicular to the stripes is obtained, as before, by considering the stripe interaction, which turns out once again to be purely repulsive. From Hubbard’s (1978) result for one-dimensional systems, the conclusion is that the spacing of the stripes follows the “most homogeneous” arrangement, constructed using the hierarchical rules described previously. In the notation of Sec. 4.1, the primitive vectors of the ground states are \( A = (-1, 2), B = (-2, 2) \) and \( C = (2, 1) \).

We note, in passing, that the ground state configuration for ion density 1/6 (which is a tiling using only parallelograms in configuration C), does not coincide with the configuration conjectured by Watson and Lemański (1995) to be the \( \rho = 1/6 \) neutral large–\( U \) ground state of the Falicov–Kimball model. The latter is a tiling using parallelograms in configuration D, and is therefore higher in energy according to the greedy potential.

The analysis could readily be continued to lower densities. However, for \( \rho < 1/6 \), the ground states involve block configuration 1 (the empty block), and it is necessary to go to \( 4 \times 4 \) blocks to obtain useful information using
the block Hamiltonian approach. We shall stop here.

5 Discussion

In the previous section we have succeeded in determining rigorously the ground states of our repulsive lattice gas model in the density ranges $1/6 \leq \rho \leq 1/5$ and $1/4 \leq \rho \leq 1/2$. In the range $1/5 < \rho < 1/4$ we have found a characterization of the ground states in terms of maximally intersecting kink configurations, and have discussed qualitatively the consequences of kink interactions. (By particle–hole duality, the results apply also to the range $1/2 \leq \rho \leq 5/6$.)

The results are not rigorously applicable to the Falicov–Kimball model. As described in Sec. 3, our “greedy potential” has been chosen to mimic qualitative aspects of the effective interionic potential in the large–$U$ limit of the neutral Falicov–Kimball model, but the two potentials differ in their details. Their two-body components do not have the same dependence on the separation of the ions, and the greedy potential does not include three-body and higher order forces.

Nevertheless, we have observed that the ground states of the two models are the same in all cases ($\rho = 1/2, 1/3, 1/4, 1/5$) where both are known, and that the repulsive lattice gas ground states are consistent with all known properties of the Falicov–Kimball model ground states. These are, namely, that the ground states for $1/4 \leq \rho \leq 1/2$ satisfy the stripe property (Kennedy 1994; see Sec. 4.1). They are also consistent with numerical results (Watson and Lemański 1995) suggesting that the arrangement of the stripes follows a hierarchical pattern, according to the Farey tree. The properties of the ground states found here for $1/5 < \rho < 1/4$ are not consistent with the configurations conjectured by Watson and Lemański (1995) to be ground states of the Falicov–Kimball model in the same range, but this could be due to the limited set of trial configurations used in their numerical work.

The agreement between the ground states of the two models provides a characterization of the large–$U$ neutral ground states of the Falicov–Kimball model. For a limited range of densities, it is possible to define homogeneity in a natural way, such that the Falicov–Kimball model ground states are the most homogeneous ion configurations on the square lattice. Potentially, this provides a generalization of a result known rigorously to hold for all densities in the one-dimensional Falicov–Kimball model.

Of equal importance is the finding that the repulsive ion model does
not provide a useful definition of the most homogeneous configuration for the density range $1/5 < \rho < 1/4$, because of the tendency for phase separation. It shows that the ground state configuration is inherently sensitive to the precise form of the forces between the ions. This suggests that it is unlikely to be possible to characterize the corresponding large-$U$ neutral ground states of the Falicov–Kimball model as unique “most homogeneous” configurations. Instead, there is a whole class of configurations which could be described as homogeneous, a qualitative discussion of which has been given in Sec. 4.3.

Thus, although there is not a full correspondence between ground states found here and those in the Falicov–Kimball model, our approach is of value in exploring the possibilities. As we have seen, the possibilities are rather interesting. The stripe property, which is satisfied for the greedy potential ground states for densities $1/4 \leq \rho \leq 1/2$, breaks down for densities less than 1/4 (although stripe phases re-enter below $\rho = 1/5$). In the range $1/5 < \rho < 1/4$, the ground states do not have this essentially one-dimensional structure; instead, they consist of arrays of maximally intersecting kinks, or domain walls. Amongst the interesting properties of this novel phase is the fact that for almost all densities, including rational numbers, the ground state is not periodic. The only possible exceptions are densities that can be written $2/[9 \pm (p/q)^2]$ for integer $p$ and $q$.

The repulsive lattice gas studied here is one of a family of models, involving two competing length scales, that has been investigated extensively in one dimension. The ground states of the one-dimensional model have properties which are characteristic of a wide range of related systems: they are periodic for rational densities and follow a construction according to hierarchical rules. Our results suggest that a similar generality is possessed by the two-dimensional model. All the ground states we have found can be described as arrays of linear domain walls in an otherwise periodic configuration of ions. In some cases these domain walls align parallel with one another, and stripe phases result, which are periodic when the density is rational. In other cases, it happens that an intersection of domain walls has negative energy, in which case the ground state is a maximally intersecting pattern of domain walls. Here, the densities for which it is possible for the ground state configuration to be periodic are a rational function of the square of a rational number.

This picture is analogous to the situation in one dimension, where the ground states can also be represented as configurations of (zero-dimensional) domain boundaries. The crucial feature of two dimensions is that two do-
main walls may intersect, and the intersection energy may be positive or negative, leading to two distinct kinds of ground states. It would be interesting to investigate the obvious extension of this idea to three dimensions.

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