THE FALICOV-KIMBALL MODEL

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1. A BRIEF HISTORY

The "Falicov-Kimball model" was first considered by Hubbard and Gutzwiller in 1963–65 as a simplification of the Hubbard model. Falicov and Kimball introduced in 1969 a model that included a few extra complications, in order to investigate metal-insulator phase transitions in rare-earth materials and transition-metal compounds. Experimental data suggested that this transition is due to the interactions between electrons in two electronic states: non-localized states (itinerant electrons), and states that are localized around the sites corresponding to the metallic ions of the crystal (static electrons).

A tight-binding approximation leads to a model defined on a lattice (the crystal) and two species of particles are considered. The first species consists of spinless quantum fermions (we refer to them as "electrons"), and the second species consists of localized holes or electrons ("classical particles"). Electrons hop between nearest-neighbor sites but classical particles do not. Both species obey Fermi statistics (in particular, the Pauli exclusion principle prevents more than one particle of a given species to occupy the same site). Interactions are on-site and thus involve particles of different species; they can be repulsive or attractive.

The very simplicity of the model allows for a broad range of applications. It was studied in the context of mixed valence systems, binary alloys, and crystal formation. Adding a magnetic field yields the flux phase problem. The Falicov-Kimball model can also be viewed as the simplest model where quantum particles interact with classical fields.

The fifteen years following the introduction of the model saw studies based on approximate methods, such as Green's function techniques, that gave rise to a lot of confusion. A breakthrough occurred in 1986 when Brandt and Schmidt, and Kennedy and Lieb, proposed the first rigorous results. In particular, Kennedy and Lieb showed in their beautiful paper that the electrons create an effective interaction between the classical particles, and that a phase transition takes place for any value of the coupling constant, provided the temperature is low enough.

Many studies by mathematical-physicists followed and several results are presented in this short survey. Recent years have seen an increase of interest by condensed matter physicists. Only a few references are given here, see the "bibliographical notes" below. We encourage interested readers to consult the reviews [6, 7, 9].

2. MATHEMATICAL SETTING

2.1. **Definitions.** Let $\Lambda \subset \mathbb{Z}^d$ denote a finite cubic box. The configuration space for the classical particles is

$$\Omega_\Lambda = \{0, 1\}^\Lambda = \big\{\omega = (\omega_x) : x \in \Lambda, \text{ and } \omega_x = 0, 1\big\},$$

where $\omega_x = 0$ or 1 denotes the absence or presence of a classical particle at the site x. The total number of classical particles is $N_c(\omega) = \sum_{x \in \Lambda} \omega_x$. The Hilbert space for the spinless quantum particles ("electrons") is the usual fermionic Fock space

$$\mathcal{F}_\Lambda = \bigoplus_{N=0}^{|\Lambda|} \mathcal{H}_{\Lambda,N},$$

where $\mathcal{H}_{\Lambda,N}$ is the Hilbert space of square summable, antisymmetric, complex functions $\Psi = \Psi(x_1, \ldots, x_N)$ of N variables $x_i \in \Lambda$. Let $a_x^\dagger$ and a_x denote the standard creation and annihilation operators of an electron at x; recall that they satisfy the anticommutation relations

$$\{a_x, a_y\} = 0, \quad \{a_x^\dagger, a_y^\dagger\} = 0, \quad \{a_x, a_y^\dagger\} = \delta_{xy}.$$

The Hamiltonian for the Falicov-Kimball model is an operator on $\mathcal{F}_\Lambda$ that depends on the configurations of classical particles. Namely, for $\omega \in \Omega_\Lambda$, we define

$$H_\Lambda(\omega) = - \sum_{\substack{x,y \in \Lambda \\ |x-y|=1}} a_x^\dagger a_y - U \sum_{x \in \Lambda} \omega_x a_x^\dagger a_x.$$

The first term represents the kinetic energy of the electrons. The second term represents the on-site attraction ($U > 0$) or repulsion ($U < 0$) between electrons and classical particles.

The Falicov-Kimball Hamiltonian can be written with the help of a one-body Hamiltonian h_Λ, which is an operator on the Hilbert space for a single electron $\ell^2(\Lambda)$. Indeed, we have

$$H_\Lambda(\omega) = \sum_{x,y \in \Lambda} h_{xy}(\omega) a_x^\dagger a_y.$$

The matrix $h_\Lambda(\omega) = (h_{xy}(\omega))$ is the sum of a hopping matrix (adjacency matrix) t_Λ, and of a matrix $v_\Lambda(\omega)$ that represents an external potential due to the classical particles. Namely, we have

$$h_{xy}(\omega) = -t_{xy} - U\omega_x \delta_{xy},$$

where t_{xy} is one if x and y are nearest-neighbors, and is zero otherwise. The spectrum of t_Λ lies in $(-2d, 2d)$, and the eigenvalues of $v_\Lambda(\omega)$ are $-U$ (with degeneracy $N_c(\omega)$) and 0 (with degeneracy $|\Lambda| - N_c(\omega)$). Denoting $\lambda_j(A)$ the eigenvalues of a matrix A, it follows from the minimax principle that:

$$\lambda_j(A) - \|B\| \leqslant \lambda_j(A + B) \leqslant \lambda_j(A) + \|B\|.$$

Let $\lambda_1(\omega) \leqslant \lambda_2(\omega) \leqslant \ldots \leqslant \lambda_{|\Lambda|}(\omega)$ be the eigenvalues of $h_\Lambda(\omega)$. Choosing $A = v_\Lambda(\omega)$ and $B = t_\Lambda$ in the inequality above, we find that for $U > 0$,

$$-U - 2d < \lambda_j(\omega) < -U + 2d \quad \text{for } j = 1, \ldots, N_c(\omega),$$
$$-2d < \lambda_j(\omega) < 2d \qquad \text{for } j = N_c(\omega) + 1, \ldots, |\Lambda|.$$

In particular, for any configuration ω and any Λ,

$$\text{Spec } h_\Lambda(\omega) \subset (-U - 2d, -U + 2d) \cup (-2d, 2d).$$

Thus for $U > 4d$ the spectrum of $h_\Lambda(\omega)$ has the "universal" gap $(-U + 2d, -2d)$. A similar property holds for $U < -4d$.

2.2. **Canonical ensemble.** A fruitful approach towards understanding the behavior of the Falicov-Kimball model is to fix first the configuration of the classical particles and to introduce the ground state energy $E_\Lambda(N_e, \omega)$ as the lowest eigenvalue of $H_\Lambda(\omega)$ in the subspace $\mathcal{H}_{\Lambda, N_e}$:

$$E_\Lambda(N_e, \omega) = \inf_{\Psi \in \mathcal{H}_{\Lambda, N_e}, \|\Psi\|=1} \langle \Psi | \, H_\Lambda(\omega) \, | \Psi \rangle = \sum_{j=1}^{N_e} \lambda_j(\omega).$$

A typical problem is to find the set of ground state configurations, i.e. the set of configurations that minimize $E_\Lambda(N_e, \omega)$ for given N_e and $N_c = N_c(\omega)$.

In the case $U > 4d$ and $N_e = N_c(\omega)$, the ground state energy $E_\Lambda(N_c(\omega), \omega)$ has a convergent expansion in powers of U^{-1}:

$$E_\Lambda(N_c(\omega), \omega) = -U N_c(\omega) + \sum_{k \geqslant 2} \frac{1}{k \, U^{k-1}} \sum_{\substack{x_1, \ldots, x_k \in \Lambda \\ |x_i - x_{i-1}| = 1 \\ 0 < m(\{x_i\}) < k}} (-1)^{m(\{x_i\})} \binom{k-2}{m(\{x_i\}) - 1}, \quad (1)$$

where $m(x_1, \ldots, x_k)$ is the number of sites x_i with $\omega_{x_i} = 0$. The last sum also includes the condition $|x_k - x_1| = 1$. Simple estimates show that the series is less than $\frac{2d}{U-4d} N_c(\omega)$. The lowest order term is a nearest-neighbor interaction,

$$-\frac{1}{U} \sum_{\{x,y\}:|x-y|=1} \delta_{w_x, 1-w_y},$$

that favors pairs with different occupation numbers. Formula (1) is the starting point for most studies of the phase diagram for large U. A similar expansion holds for $U < -4d$ and $N_e = |\Lambda| - N_c(\omega)$.

Phase diagrams are better discussed in the limit of infinite volumes where boundary effects can be discarded. Let Ω^{per} be the set of configurations on $\mathbb{Z}^d$ that are periodic in all d directions, and $\Omega^{\text{per}}(\rho_c) \subset \Omega^{\text{per}}$ be the set of periodic configurations with density ρ_c. For $\omega \in \Omega^{\text{per}}$ and $\rho_e \in [0,1]$, we introduce the energy per site in the infinite volume limit by

$$e(\rho_e, \omega) = \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} E_\Lambda(N_e, \omega). \quad (2)$$

Here, the limit is taken over any sequence of increasing cubes, and $N_e = \lfloor \rho_e |\Lambda| \rfloor$ is the integer part of $\rho_e |\Lambda|$. Existence of this limit follows from standard arguments.

In the case of the empty configuration $\omega_x \equiv 0$, we get the well-known energy per site of free lattice electrons: For $k \in [-\pi, \pi]^d$, let $\varepsilon(k) = -\sum_{\nu=1}^d \cos k_\nu$; then

$$e(\rho_e, \omega \equiv 0) = \frac{1}{(2\pi)^d} \int_{\varepsilon(k) < \varepsilon_F(\rho_e)} \varepsilon(k) \mathrm{d}k,$$

where $\varepsilon_F(\rho_e)$ is the Fermi energy, defined by

$$\rho_e = \frac{1}{(2\pi)^d} \int_{\varepsilon(k) < \varepsilon_F(\rho_e)} \mathrm{d}k.$$

The other simple situation is the full configuration $\omega_x \equiv 1$, whose energy is $e(\rho_e, \omega \equiv 1) = e(\rho_e, \omega \equiv 0) - U \rho_e$.

Let $e(\rho_e, \rho_c)$ denote the absolute ground state energy density, namely,

$$e(\rho_e, \rho_c) = \inf_{\omega \in \Omega^{\text{per}}(\rho_c)} e(\rho_e, \omega).$$

Notice that $e(\rho_e, \omega)$ is convex in ρ_e, and that $e(\rho_e, \rho_c)$ is the convex envelope of $\{e(\rho_e, \omega) : \omega \in \Omega^{\text{per}}(\rho_c)\}$. It may be locally linear around some (ρ_e, ρ_c). This is the case if the

infimum is not realized by a periodic configuration. The non-periodic ground states can be expressed as linear combinations of two or more periodic ground states ("mixtures"). That is, for $1 \leqslant i \leqslant n$ there are $\alpha_i \geqslant 0$ with $\sum_i \alpha_i = 1$, $\omega^{(i)} \in \Omega^{\mathrm{per}}$, and $\rho_{\mathrm{e}}^{(i)}$, such that

$$\rho_{\mathrm{e}} = \sum_i \alpha_i \rho_{\mathrm{e}}^{(i)}, \qquad \rho_{\mathrm{c}} = \sum_i \alpha_i \rho_{\mathrm{c}}(\omega^{(i)}),$$

and

$$e(\rho_{\mathrm{e}}, \rho_{\mathrm{c}}) = \sum_i \alpha_i e(\rho_{\mathrm{e}}^{(i)}, \omega^{(i)}).$$

The simplest mixture is the "segregated state" for densities $\rho_{\mathrm{e}} < \rho_{\mathrm{c}}$: Take $\omega^{(1)}$ to be the empty configuration, $\omega^{(2)}$ to be the full configuration, $\rho_{\mathrm{e}}^{(1)} = 0$, $\rho_{\mathrm{e}}^{(2)} = \frac{\rho_{\mathrm{e}}}{\rho_{\mathrm{c}}}$, and $\alpha_2 = 1 - \alpha_1 = \rho_{\mathrm{c}}$.

If $d \geqslant 2$, a mixture between configurations $\omega^{(i)}$ can be realized as follows. First, partition $\mathbb{Z}^d$ into domains $D_1 \cup \cdots \cup D_n$ such that $\frac{|D_i|}{|\Lambda|} \to \alpha_i$ and $\frac{|\partial D_i|}{|\Lambda|} \to 0$ as $\Lambda \nearrow \mathbb{Z}^d$. Then define a non-periodic configuration ω by setting $\omega_x = \omega_x^{(i)}$ for $x \in D_i$. See the illustration in Fig. 1. The canonical energy can be computed from (2), and it is equal to

$$e(\rho_{\mathrm{e}}, \omega) = \inf_{(\rho_{\mathrm{e}}^{(i)}): \sum_i \alpha_i \rho_{\mathrm{e}}^{(i)} = \rho_{\mathrm{e}}} \sum_{i=1}^n \alpha_i \, e(\rho_{\mathrm{e}}^{(i)}, \omega^{(i)}).$$

Furthermore, the infimum is realized by densities $\rho_{\mathrm{e}}^{(i)}$ such that there exists μ_{e} with $\rho_{\mathrm{e}}(\mu_{\mathrm{e}}, \omega^{(i)}) = \rho_{\mathrm{e}}^{(i)}$ for all i. (See (4) below for the definition of $\rho_{\mathrm{e}}(\mu_{\mathrm{e}}, \omega)$.)

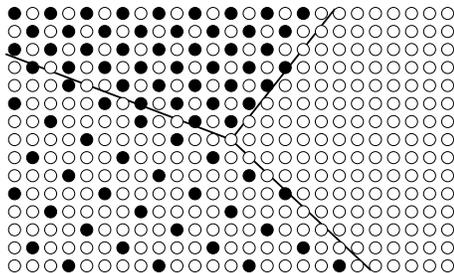FIGURE 1. A two-dimensional mixed configuration formed by periodic configurations of densities 0, $\frac{1}{5}$, and $\frac{1}{2}$.

We define the *canonical ground state phase diagram* as the set of ground states ω (either a periodic configuration or a mixture) that minimize the ground state energy for given densities $\rho_{\mathrm{e}}, \rho_{\mathrm{c}}$:

$$G_{\mathrm{can}}(\rho_{\mathrm{e}}, \rho_{\mathrm{c}}) = \big\{ \omega : e(\rho_{\mathrm{e}}, \omega) = e(\rho_{\mathrm{e}}, \rho_{\mathrm{c}}) \text{ and } \rho_{\mathrm{c}}(\omega) = \rho_{\mathrm{c}} \big\}.$$

2.3. **Grand-canonical ensemble.** Properties of the system at finite temperatures are usually investigated within the grand-canonical formalism. The equilibrium state is characterized by an inverse temperature $\beta = 1/k_{\mathrm{B}}T$, and by chemical potentials $\mu_{\mathrm{e}}, \mu_{\mathrm{c}}$, for the electrons and for the classical particles respectively. In this formalism the thermodynamic properties are derived from the partition functions

$$\begin{aligned} Z_\Lambda(\beta, \mu_{\mathrm{e}}, \omega) &= \mathrm{Tr}_{\mathcal{F}_\Lambda} \, \mathrm{e}^{-\beta[H_\Lambda(\omega) - \mu_{\mathrm{e}} N_\Lambda]}, \\ Z_\Lambda(\beta, \mu_{\mathrm{e}}, \mu_{\mathrm{c}}) &= \sum_{\omega \in \Omega_\Lambda} \mathrm{e}^{\beta \mu_{\mathrm{c}} N_{\mathrm{c}}(\omega)} \, Z_\Lambda(\beta, \mu_{\mathrm{e}}, \omega). \end{aligned} \qquad (3)$$

Here, $N_\Lambda = \sum_{x \in \Lambda} a_x^\dagger a_x$ is the operator for the total number of electrons. We then define the free energy by

$$F_\Lambda(\beta, \mu_e, \mu_c) = -\tfrac{1}{\beta} \log Z_\Lambda(\beta, \mu_e, \mu_c).$$

The first partition function in (3) allows to introduce an effective interaction for the classical particles, mediated by the electrons, by

$$F_\Lambda(\beta, \mu_e, \mu_c, \omega) = -\mu_c N_c(\omega) - \tfrac{1}{\beta} \log Z_\Lambda(\beta, \mu_e, \omega).$$

It depends on the inverse temperature β. Taking the limit of zero temperature gives the corresponding ground state energy of the electrons in the classical configuration ω,

$$E_\Lambda(\mu_e, \mu_c, \omega) = \lim_{\beta \to \infty} F_\Lambda(\beta, \mu_e, \mu_c, \omega) = -\mu_c N_c(\omega) + \sum_{j : \lambda_j(\omega) < \mu_e} (\lambda_j(\omega) - \mu_e).$$

Notice that F_Λ and E_Λ are strictly decreasing and concave in μ_e, μ_c (E_Λ is actually linear in μ_c). We also define the energy density in the infinite volume limit by considering a sequence of increasing cubes. For $\omega \in \Omega^{\text{per}}$,

$$e(\mu_e, \mu_c, \omega) = \lim_{\Lambda \nearrow \mathbb{Z}^d} \tfrac{1}{|\Lambda|} E_\Lambda(\mu_e, \mu_c, \omega).$$

The corresponding electronic density is

$$\rho_e(\mu_e, \omega) = \lim_{\Lambda \nearrow \mathbb{Z}^d} \tfrac{1}{|\Lambda|} \#\{j : \lambda_j(\omega) < \mu_e\} = -\tfrac{\partial}{\partial \mu_e} e(\mu_e, \mu_c, \omega), \tag{4}$$

and the density of classical particles is $\rho_c(\omega) = \lim_\Lambda N_c(\omega)/|\Lambda|$. One can check that canonical and grand-canonical energies are related by

$$e(\mu_e, \mu_c, \omega) = e(\rho_e(\mu_e, \omega), \omega) - \mu_e \rho_e(\mu_e, \omega) - \mu_c \rho_c(\omega). \tag{5}$$

Given (μ_e, μ_c), the ground state energy density $e(\mu_e, \mu_c)$ is defined by

$$e(\mu_e, \mu_c) = \inf_{\omega \in \Omega^{\text{per}}} e(\mu_e, \mu_c, \omega).$$

The set of periodic ground state configurations for given chemical potentials μ_e, μ_c is the *grand-canonical ground state phase diagram*:

$$G_{\text{gc}}(\mu_e, \mu_c) = \big\{ \omega \in \Omega^{\text{per}} : e(\mu_e, \mu_c, \omega) = e(\mu_e, \mu_c) \big\}.$$

It may happen that no periodic configuration minimizes $e(\mu_e, \mu_c, \omega)$ and that $G_{\text{gc}}(\mu_e, \mu_c) = \emptyset$. Results suggest that $G_{\text{gc}}(\mu_e, \mu_c)$ is nonempty for almost all μ_e, μ_c, however.

The situation simplifies for $U > 4d$ and $\mu_e \in (-U + 2d, -2d)$. Since μ_e belongs to the gap of $h_\Lambda(\omega)$, we have $\rho_e(\mu_e, \omega) = \rho_c(\omega)$, and

$$e(\mu_e, \mu_c, \omega) = e(\rho_c(\omega), \omega) - (\mu_e + \mu_c) \rho_c(\omega).$$

Thus $G_{\text{gc}}(\mu_e, \mu_c)$ is invariant along the line $\mu_e + \mu_c = \text{const}$ (for μ_e in the gap).

2.4. **Symmetries of the model.** The Hamiltonian H_Λ clearly has the symmetries of the lattice (for a box with periodic boundary conditions, there is invariance under translations, rotations by $90°$, and reflections through an axis). More important, it also possesses particle-hole symmetries and these are useful since they allow to restrict investigations to positive U and to certain domains of densities or chemical potentials (see below).

- The classical particle–hole transformation $\omega_x \mapsto \overline{\omega}_x = 1 - \omega_x$ results in

$$H_\Lambda^U(\overline{\omega}) = H_\Lambda^{-U}(\omega) - U N_\Lambda,$$

and $N_c(\overline{\omega}) = |\Lambda| - N_c(\omega)$. It follows that $E_\Lambda^U(N_e, \overline{\omega}) = E_\Lambda^{-U}(N_e, \omega) - UN_e$, and

$$G_{\text{can}}^{-U}(\rho_e, \rho_c) = \{\overline{\omega} : \omega \in G_{\text{can}}^U(\rho_e, 1 - \rho_c)\},$$
$$G_{\text{gc}}^{-U}(\mu_e, \mu_c) = \{\overline{\omega} : \omega \in G_{\text{gc}}^U(\mu_e - U, -\mu_c)\}.$$

- An electron–hole transformation can be defined via the unitary transformation $a_x \mapsto \varepsilon_x a_x^\dagger$ and $a_x^\dagger \mapsto \varepsilon_x a_x$, where ε_x is equal to 1 on a sublattice, and to -1 on the other sublattice. Then

$$H_\Lambda^U(\omega) \mapsto H_\Lambda^{-U}(\omega) - UN_c(\omega),$$

and $N_\Lambda \mapsto |\Lambda| - N_\Lambda$. It follows that $E_\Lambda^U(|\Lambda| - N_e, \omega) = E_\Lambda^{-U}(N_e, \omega) - UN_c(\omega)$, and

$$G_{\text{can}}^{-U}(\rho_e, \rho_c) = G_{\text{can}}^U(1 - \rho_e, \rho_c),$$
$$G_{\text{gc}}^{-U}(\mu_e, \mu_c) = G_{\text{gc}}^U(-\mu_e, \mu_c - U).$$

- Finally, the particle–hole transformation for both the classical particles and the electrons give

$$H_\Lambda^U(\overline{\omega}) \mapsto H_\Lambda^U(\omega) + UN_\Lambda + UN_c(\omega) - U|\Lambda|.$$

It follows that $E_\Lambda^U(|\Lambda| - N_e, \overline{\omega}) = E_\Lambda^U(N_e, \omega) + U(N_e + N_c(\omega) - |\Lambda|)$, and

$$G_{\text{can}}^U(\rho_e, \rho_c) = \{\overline{\omega} : \omega \in G_{\text{can}}^U(1 - \rho_e, 1 - \rho_c)\},$$
$$G_{\text{gc}}^U(\mu_e, \mu_c) = \{\overline{\omega} : \omega \in G_{\text{gc}}^U(-\mu_e - U, -\mu_c - U)\}.$$

Any of the first two symmetries allow to choose the sign of U. We assume from now on that $U \geqslant 0$. The third symmetry indicates that the phase diagrams have a point of central symmetry, given by $\rho_e = \rho_c = \frac{1}{2}$ in the canonical ensemble and $\mu_e = \mu_c = -\frac{U}{2}$ in the grand-canonical ensemble. Consequently, it is enough to study densities satisfying $\rho_e \leqslant \frac{1}{2}$ and chemical potentials satisfying $\mu_e \leqslant -\frac{U}{2}$.

These symmetries have also useful consequences at positive temperatures. In particular, both species of particles have average density $\frac{1}{2}$ at $\mu_e = \mu_c = -\frac{U}{2}$, for all β.

3. THE GROUND STATE — ARBITRARY DIMENSIONS

3.1. **The segregated state.** What follows is best understood in the limit $U \to \infty$ and when $\rho_e < \rho_c$. In this case the electrons become localized in the domain $\mathcal{D}_\Lambda(\omega) = \{x \in \Lambda : w_x = 1\}$ and their energy per site is that of the full configuration, $e(\rho, \omega \equiv 1)$ (see Section 2.2), where $\rho = \rho_e/\rho_c$ is the effective electronic density. The presence of a boundary for $\mathcal{D}_\Lambda(\omega)$ raises the energy and the correction is roughly proportional to

$$B_\Lambda(\omega) = \#\{(x, y) : x \in \mathcal{D}_\Lambda(\omega) \text{ and } y \in \mathbb{Z}^d \setminus \mathcal{D}_\Lambda(\omega)\}.$$

Theorem 1.

(a) *Let $\Lambda \subset \mathbb{Z}^d$ be a finite box, and $U > 4d$. Then for all $\omega \in \Omega_\Lambda$, and all $N_e \leqslant N_c(\omega) = N_c$, we have the following upper and lower bounds:*

$$\frac{1}{2d}|e(\tfrac{N_e}{N_c})|B_\Lambda(\omega) \geqslant E_\Lambda(N_e, \omega) - N_c e(\tfrac{N_e}{N_c}, \omega \equiv 1) \geqslant \left[a(\tfrac{N_e}{N_c}) - \gamma(U)\right]B_\Lambda(\omega).$$

Here, $a(\rho) = a(1 - \rho)$ is strictly positive for $0 < \rho < 1$. $\gamma(U)$ behaves as $\frac{8d^2}{U}$ for large U, in the sense that $U\gamma(U) \to 8d^2$ as $U \to \infty$.

(b) *For any $\rho_e \neq \rho_c$ that differ from zero, the segregated state is the unique ground state if $a(\frac{\rho_e}{\rho_c}) > \gamma(U)$, i.e. if U is large enough.*

The proof of (a) is rather lengthy and we only show here that it implies (b). Let $b(\omega) = \lim_\Lambda \frac{B_\Lambda(\omega)}{|\Lambda|}$, and notice that $b(\omega) = 0$ for the empty, the full, and the segregated configurations; $0 < b(\omega) < d$ for all other periodic configurations or mixtures. Recall that $\rho_c e(\frac{\rho_e}{\rho_c}, \omega \equiv 1)$ is the energy density of the segregated state. For all densities such that $a(\frac{\rho_e}{\rho_c}) > \gamma(U)$, and all configurations such that $\rho_c(\omega) = \rho_c$, we have

$$e(\rho_e, \omega) \geqslant \rho_c\, e(\tfrac{\rho_e}{\rho_c}, \omega \equiv 1),$$

and the inequality is strict for any periodic configuration. This shows that the segregated configuration is the unique ground state.

3.2. **General properties of the grand-canonical phase diagram.** We have already seen that the grand-canonical phase diagram is symmetric with respect to $(-\frac{U}{2}, -\frac{U}{2})$. Other properties follow from concavity of $e(\mu_e, \mu_c)$.

Let $\omega \in G_{gc}(\mu_e, \mu_c) \setminus G_{gc}(\mu'_e, \mu'_c)$ and $\omega' \in G_{gc}(\mu'_e, \mu'_c) \setminus G_{gc}(\mu_e, \mu_c)$. Then

   (i) $\mu_e = \mu'_e$ and $\mu'_c > \mu_c$ imply $\rho_c(\omega') > \rho_c(\omega)$;
   (ii) $\mu_c = \mu'_c$ and $\mu'_e > \mu_e$ imply $\rho_e(\mu'_e, \omega') > \rho_e(\mu_e, \omega)$, and ω cannot be obtained by adding some classical particles to the configuration ω'.

It follows from (ii) that if $\omega \equiv 1 \in G_{gc}(\mu_e, \mu_c)$, then $\omega \equiv 1 \in G_{gc}(\mu'_e, \mu'_c)$ for all $\mu_e \geqslant \mu'_e$, $\mu_c \geqslant \mu'_c$. A similar property holds for the empty configuration. To establish these properties, we can start from

$$e(\mu_e, \mu_c, \omega') - e(\mu_e, \mu_c, \omega) > 0 > e(\mu'_e, \mu'_c, \omega') - e(\mu'_e, \mu'_c, \omega). \tag{6}$$

Since $e(\mu_e, \mu_c, \omega)$ is concave with respect to μ_e and linear with respect to μ_c, we have

$$e(\mu'_e, \mu'_c, \omega) \leqslant e(\mu_e, \mu_c, \omega) + (\mu_e - \mu'_e)\rho_e(\mu_e, \omega) + (\mu_c - \mu'_c)\rho_c(\omega). \tag{7}$$

Using this inequality for both terms of the right side of (6), we obtain the inequality

$$(\mu'_e - \mu_e)\big[\rho_e(\mu'_e, \omega') - \rho_e(\mu_e, \omega)\big] + (\mu'_c - \mu_c)\big[\rho_c(\omega') - \rho_c(\omega)\big] \geqslant 0,$$

which proves (i) and the first part of (ii). The second part of (ii) follows from

$$e(\mu_e, \mu_c, \omega) = -\int_{-\infty}^{\mu_e} \rho_e(\mu, \omega)\mathrm{d}\mu - \mu_c\rho_c(\omega).$$

Indeed, the minimax principle implies that eigenvalues $\lambda_j(\omega)$ are decreasing with respect to ω (if $U \geqslant 0$), so that $\rho_e(\mu_e, \omega)$ is increasing (with respect to ω). Then for any $\omega'' > \omega$ and $\mu'_e > \mu_e$,

$$e(\mu'_e, \mu_c, \omega'') - e(\mu'_e, \mu_c, \omega) > e(\mu_e, \mu_c, \omega'') - e(\mu_e, \mu_c, \omega),$$

and $\omega'' \notin G_{gc}(\mu_e, \mu_c)$ implies $\omega'' \notin G_{gc}(\mu'_e, \mu_c)$.

Next we discuss domains in the plane of chemical potentials where the empty, full, and chessboard configurations have minimum energy. One easily sees that $\omega \equiv 1$ is the unique ground state configuration if $\mu_c > 0$, or if $\mu_e > 2d$ and $\mu_c > -U$. Similarly, $\omega \equiv 0$ is the unique ground state if $\mu_c < -U$, or if $\mu_e < -U - 2d$ and $\mu_c < 0$. For $U > 4d$, it follows from the expansion (1) that the full configuration is also ground state if $-U + 2d < \mu_e < -2d$ and $\mu_e + \mu_c + U > \frac{4d}{U-4d}$. These domains can be rigorously extended using energy estimates that involve correlation functions of classical particles. The results are illustrated in Figs 2 ($U < 4d$) and 3 ($U > 4d$).

Finally, canonical and grand-canonical phase diagrams are related by the following properties:

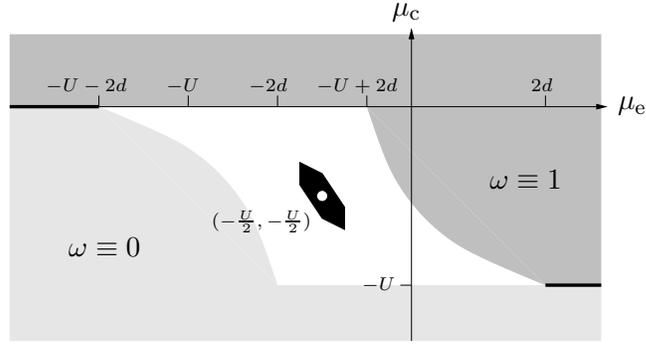   (iii) If $\omega \in G_{gc}(\mu_e, \mu_c)$, then $\omega \in G_{can}(\rho_e(\mu_e, \omega), \rho_c(\omega))$.

FIGURE 2. Grand-canonical ground state phase diagram for $U < 4d$. Domains for the empty, chessboard, and full configurations, are denoted in light gray, black, and dark gray respectively.
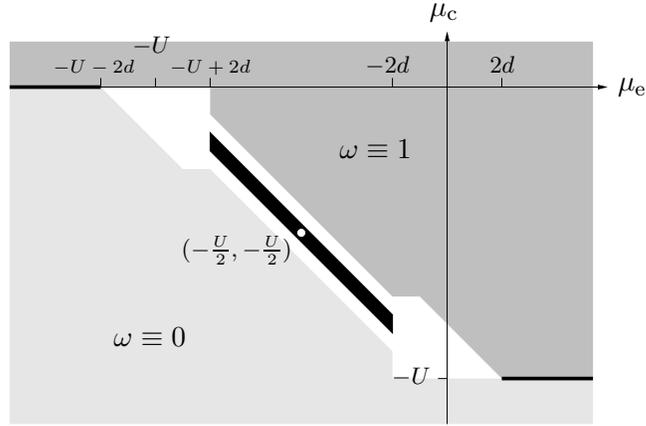

FIGURE 3. Grand-canonical ground state phase diagram for $U > 4d$. Domains for the empty, chessboard, and full configurations, are denoted in light gray, black, and dark gray respectively.

(iv) More generally, suppose that $\omega^{(1)}, \ldots, \omega^{(n)} \in G_{\mathrm{gc}}(\mu_{\mathrm{e}}, \mu_{\mathrm{c}})$, and consider a mixture with coefficients $\alpha_1, \ldots, \alpha_n$. The mixture belongs to $G_{\mathrm{can}}(\rho_{\mathrm{e}}, \rho_{\mathrm{c}})$, with $\rho_{\mathrm{e}} = \sum_i \alpha_i \rho_{\mathrm{e}}(\mu_{\mathrm{e}}, \omega^{(i)})$ and $\rho_{\mathrm{c}} = \sum_i \alpha_i \rho_{\mathrm{c}}(\omega^{(i)})$.

To establish (iii), observe that any ω' satisfies $e(\mu_{\mathrm{e}}, \mu_{\mathrm{c}}, \omega') \geqslant e(\mu_{\mathrm{e}}, \mu_{\mathrm{c}}, \omega)$ if $\omega \in G_{\mathrm{gc}}(\mu_{\mathrm{e}}, \mu_{\mathrm{c}})$. Let $\rho_{\mathrm{e}} = \rho_{\mathrm{e}}(\mu_{\mathrm{e}}, \omega)$ and $\rho_{\mathrm{c}} = \rho_{\mathrm{c}}(\omega)$, and let μ'_{e} such that $\rho_{\mathrm{e}}(\mu'_{\mathrm{e}}, \omega') = \rho_{\mathrm{e}}$. By Eqs (5) and (7),

$$e(\rho_{\mathrm{e}}(\mu'_{\mathrm{e}}, \omega'), \omega') - \mu_{\mathrm{e}}\rho_{\mathrm{e}}(\mu'_{\mathrm{e}}, \omega') - \mu_{\mathrm{c}}\rho_{\mathrm{c}}(\omega') \geqslant e(\rho_{\mathrm{e}}(\mu_{\mathrm{e}}, \omega), \omega) - \mu_{\mathrm{e}}\rho_{\mathrm{e}}(\mu_{\mathrm{e}}, \omega) - \mu_{\mathrm{c}}\rho_{\mathrm{c}}(\omega).$$

Then $e(\rho_{\mathrm{e}}, \omega') \geqslant e(\rho_{\mathrm{e}}, \omega)$ for any configuration ω' such that $\rho_{\mathrm{c}}(\omega') = \rho_{\mathrm{c}}$. Property (iv) follows from (iii) by a limiting argument, because a mixture can be approximated by a sequence of periodic configurations.

Next we describe further properties of the phase diagrams that are specific to dimensions 1 and 2.

4. GROUND STATE CONFIGURATIONS — DIMENSION ONE

A large number of investigations, either analytical or numerical, have been devoted to the study of the ground state configurations in one dimension. One-dimensional results also serve as guide to higher dimensions. Recall that symmetries allow to restrict to $U \geqslant 0$ and $\rho_{\mathrm{e}} \leqslant \frac{1}{2}$.

Most ground state configurations that appear in the canonical phase diagram seem to be given by an intriguing formula, which we now describe. Let $\rho_e = \frac{p}{q}$ with p relatively prime to q. Then corresponding periodic ground state configurations have period q and density $\rho_c = \frac{r}{q}$ (r is an integer). The occupied sites in the cell $\{0, 1, \ldots, q-1\}$ are given by the solutions $k_0, \ldots, k_{r-1}$ of

$$(pk_j) = j \mod q, \qquad 0 \leqslant j \leqslant r - 1. \tag{8}$$

Note that the first classical particle is located at $k_0 = 0$, and $k_0, \ldots, k_{p-1}$ are *not* in increasing order. In order to discuss the solutions of (8), we introduce $\ell = \lfloor \frac{q}{p} \rfloor$ (the integer part of $\frac{q}{p}$), and we write

$$q = (\ell + 1)p - s, \tag{9}$$

where $1 \leqslant s \leqslant p - 1$, and s is relatively prime to p. Next, let $L(x)$ denote the distance between the particle at x and the one immediately preceding it (to the left).

Let us observe that if $\rho_c = \rho_e$, i.e. if $r = p$, then

(a) $L(k_j) = \ell$ for $0 \leqslant j \leqslant s - 1$ and $k_j - \ell = k_{j+p-s}$.
(b) $L(k_j) = \ell + 1$ for $s \leqslant j \leqslant p - 1$ and $k_j - (\ell + 1) = k_{j-s}$.

Indeed, for $pk_j = j + nq$, Eq. (9) implies

$$p(k_j - \ell) = j + (n-1)q + (p - s) = j + p - s \mod q,$$

and

$$p(k_j - \ell - 1) = j - s \mod q.$$

Therefore $k_j - \ell$ is solution of (8) if $j + p - s \leqslant p - 1$, while $k_j - (\ell + 1)$ is solution of (8) if $j - s \geqslant 0$.

These properties show that the configuration defined by (8) is such that $L(x) \in \{\ell, \ell+1\}$ for all occupied x. A periodic configuration such that all distances between consecutive particles are either ℓ or $\ell+1$ is called *homogeneous*. Let ω be a homogeneous configuration with period q and density $\rho_c = \frac{r}{q}$, and let $x_0 < \cdots < x_{p-1}$ be the occupied sites in $\{0, 1, \ldots, q - 1\}$. We introduce the *derivative* ω' of ω as the periodic configuration with period r defined by (see Fig. 4)

$$\omega_i' = \begin{cases} 1 & \text{if } L(x_i) = \ell, \\ 0 & \text{if } L(x_i) = \ell + 1. \end{cases}$$

A configuration is *most homogeneous* if it can be "differentiated" repeatedly until the empty or the full configuration is obtained.
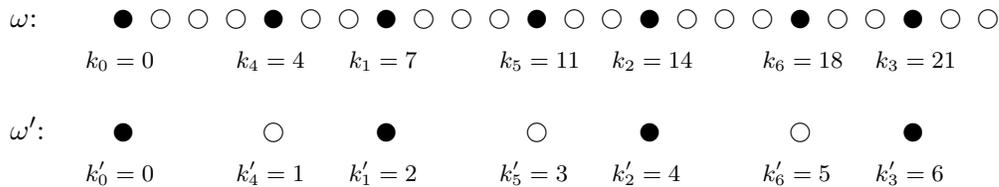

FIGURE 4. The configuration ω given by the formula (8) with $q = 24$ and $p = 7$, and its derivative ω'. Notice that $\ell = 3$ and $s = 4$.

Let ω be the homogeneous configuration from (8) and ω' be its derivative. Using the same arguments as for properties (a) and (b) above, and the fact that s is relatively prime to p, we obtain:

(c) Let $k'_0, \ldots, k'_{p-1}$ be the solutions of

$$(sk'_j) = j \mod p.$$

Then $(k'_0, \ldots, k'_{p-1})$ is a permutation of $(0, 1, \ldots, p-1)$. Further, $k'_j - 1 = k'_{j+p-s}$ for $0 \leqslant j \leqslant s-1$, and $k'_j - 1 = k'_{j-s}$ for $s \leqslant j \leqslant p-1$.

Consider the periodic configuration with period p where sites $k'_0, \ldots, k'_{s-1}$ are occupied and sites $k'_s, \ldots, k'_{p-1}$ are empty. Since $k'_0 = 0$, this configuration is precisely the derivative ω' of ω. Iterating, these properties prove that the solutions of (8) are most homogeneous.

One of the most important result in one dimension is that only most homogeneous configurations are present in the canonical phase diagram, for U large enough and for equal densities $\rho_e = \rho_c$.

Theorem 2. *Suppose that $\rho_e = \rho_c = \frac{p}{q}$. There exists a constant c such that for $U > c4^q$, the only ground state configuration is the most homogeneous configuration, given by (8) (together with translations and reflections).*

This theorem was established using the expansion (1) of $E_\Lambda(N_e, \omega)$ in powers of U^{-1}. It suggests a devil's staircase structure with infinitely many domains. However, the number of domains for *fixed* U could still be finite. Results from Theorem 2 are illustrated in Fig. 5.
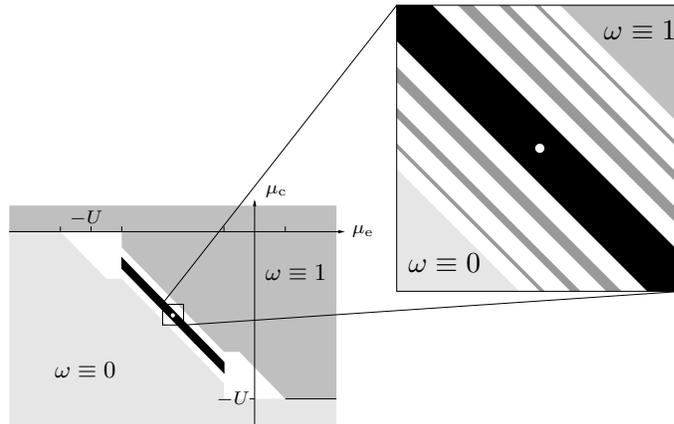

FIGURE 5. Grand-canonical ground state phase diagram in one dimension for $U > 4$ and μ_e in the universal gap. Chessboard configurations occur in the black domain. Dark gray oblique domains correspond to densities $\frac{1}{5}$, $\frac{1}{4}$, $\frac{1}{3}$, $\frac{1}{2}$, $\frac{2}{3}$, $\frac{3}{4}$, $\frac{4}{5}$. Total width of these domains is of order U^{-1}.

For small U, on the other hand, one can use a (non-rigorous) Wigner-Brillouin degenerate perturbation theory (a standard tool in band theory). Let $\rho_e = \frac{p}{q}$ with p relatively prime to q, and ω be a periodic configuration with period nq, $n \in \mathbb{N}$. Then for U small enough ($U \ll \frac{1}{q}$), we obtain the following expansion for the ground state energy

$$e(\rho_e, \omega) = -\frac{2}{\pi} \sin \pi \rho_e - U \rho_e \rho_c(\omega) - \frac{|\widehat{\omega}(\rho_e)|^2}{4\pi \sin \pi \rho_e} U^2 |\log U| + O(U^2), \tag{10}$$

where $\widehat{\omega}(\rho_e)$ is the "structure factor" of the periodic configuration ω, namely

$$\widehat{\omega}(\rho_e) = \frac{1}{nq} \sum_{j=0}^{nq-1} e^{-2\pi i \rho_e j} w_j.$$

This expansion suggests that the ground state configuration can be found by maximizing the structure factor. The following theorem holds independently of U.

Theorem 3. *Let $\rho_{\mathrm{e}} = \frac{p}{q}$. There exist $r_1 \geqslant \frac{q}{4}$ and $r_2 \leqslant \frac{3q}{4}$ such that the configurations maximizing the structure factor are given as follows:*

(a) *For $\rho_{\mathrm{c}} = \frac{r}{q}$ with $r_1 \leqslant r \leqslant r_2$, use the formula (8).*

(b) *For $\rho_{\mathrm{c}} \in (\frac{r}{q}, \frac{r+1}{q})$ with $r_1 \leqslant r \leqslant r_2 - 1$, the configuration is a mixture of those for $\rho_{\mathrm{c}} = \frac{r}{q}$ and $\rho_{\mathrm{c}} = \frac{r+1}{q}$.*

(c) *For $\rho_{\mathrm{c}} \in (0, \frac{r_1}{q})$, the configurations are mixtures of $\omega \equiv 0$ and that for $\rho_{\mathrm{c}} = \frac{r_1}{q}$. For $\rho_{\mathrm{c}} \in (\frac{r_2}{q}, 1)$, the configurations are mixtures of $\omega \equiv 1$ and that for $\rho_{\mathrm{c}} = \frac{r_2}{q}$.*

Some insight for low densities is provided by computing the energy of just one classical particle and one electron on the infinite line, and to compare it with two consecutive classical particles and two electrons. It turns out that the former is more favorable than the latter for $U > \frac{2}{\sqrt{3}} \approx 1.15$, while "molecules" of two particles are forming when $U < \frac{2}{\sqrt{3}}$. Smaller U shows even bigger molecules for $\rho_{\mathrm{c}} = n\rho_{\mathrm{e}}$, and n-molecules are most homogeneously distributed according to the formula (8). It should be stressed that the canonical ground state cannot be periodic if U is small and $\rho_{\mathrm{c}} \notin [\frac{1}{4}, \frac{3}{4}]$, which is different from the case of large U.

Only numerical results are available for intermediate U. They suggest that configurations occuring in the phase diagram are essentially given by Theorem 3 (together with the segregated configuration). This is sketched in Fig. 6, where bold coexistence lines for $\mu_{\mathrm{e}} > -U - 2$ and $\mu_{\mathrm{e}} < 2$ represent segregated states.
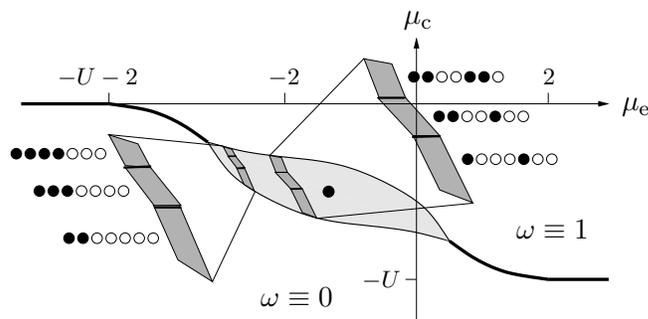

FIGURE 6. Grand-canonical ground state phase diagram for $U \approx 0.4$. Enlarged are domains for $\rho_{\mathrm{e}} = \frac{1}{7}$ and $\frac{2}{7}$, with the same densities $\rho_{\mathrm{c}} = \frac{2}{7}, \frac{3}{7}, \frac{4}{7}$.

5. GROUND STATE CONFIGURATIONS — DIMENSION TWO

We discuss the canonical ensemble only, but many results extend to the grand-canonical ensemble. Recall that $G_{\mathrm{can}}(\frac{1}{2}, \frac{1}{2})$ consists of the two chessboard configurations for any $U > 0$, and that segregation takes place when $\rho_e \neq \rho_{\mathrm{c}}$, providing U is large enough (Theorem 1). Other results deal with the case of equal densities, and for U large enough.

Theorem 4. *Let $\rho_{\mathrm{e}} = \rho_{\mathrm{c}} \equiv \rho \leqslant \frac{1}{2}$.*

(a) *If $\rho \in \{\frac{1}{2}, \frac{2}{5}, \frac{1}{3}, \frac{1}{4}, \frac{2}{9}, \frac{1}{5}, \frac{2}{11}, \frac{1}{6}\}$, then for U large enough, the ground state configurations are those displayed in Fig. 7. If $\rho = \frac{1}{n^2+(n+1)^2}$ with integer n, then for U large enough (depending on ρ), the ground state configurations are periodic.*

(b) *If ρ is a rational number between $\frac{1}{3}$ and $\frac{2}{5}$, then for U large enough (depending on the denominator of ρ), the ground state configurations are periodic. Further, the restriction to any horizontal line is a one-dimensional periodic configuration given by (8), and the configuration is constant in either the direction $\left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right)$ or $\left(\begin{smallmatrix} 1 \\ -1 \end{smallmatrix}\right)$.*

(c) *Suppose that U is large enough. If $\rho \in (\frac{1}{6}, \frac{2}{11})$, the ground state configurations are mixtures of the configurations $\rho = \frac{1}{6}$ and $\rho = \frac{2}{11}$ of Fig. 7. If $\rho \in (\frac{1}{5}, \frac{2}{9})$, the ground state configurations are mixtures of the configurations $\rho = \frac{1}{5}$ and $\rho = \frac{2}{9}$. If $\rho \in (\frac{2}{9}, \frac{1}{4})$, the ground state configurations are mixtures of the configurations $\rho = \frac{2}{9}$ and $\rho = \frac{1}{4}$.*

The canonical phase diagram for $\rho_e = \rho_c$ is presented in Fig. 8.

$\rho = \frac{1}{2}$ $\rho = \frac{2}{5}$ $\rho = \frac{1}{3}$ $\rho = \frac{1}{4}$

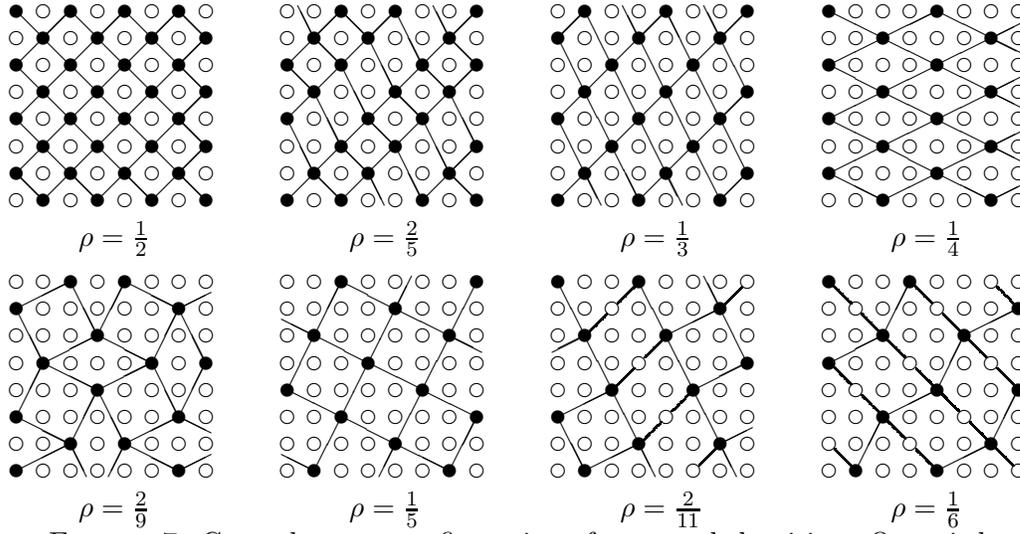$\rho = \frac{2}{9}$ $\rho = \frac{1}{5}$ $\rho = \frac{2}{11}$ $\rho = \frac{1}{6}$

FIGURE 7. Ground states configurations for several densities. Occupied sites are denoted by black circles, empty sites by white circles. Lines are present only to clarify the patterns.

The situation for densities $\rho \leqslant \frac{1}{2}$ that are not mentioned in Theorem 4 is unknown. All these periodic configurations are present in the grand-canonical phase diagram as well. Item (b) suggests that the two-dimensional situation is similar to the one-dimensional one where a devil's staircase structure may occur. Let us stress that no periodic configurations occur for large U and densities $\rho_e = \rho_c$ in the intervals $(\frac{1}{6}, \frac{2}{11})$, $(\frac{1}{5}, \frac{2}{9})$, and $(\frac{2}{9}, \frac{1}{4})$. This resembles the one-dimensional situation, but for small U.
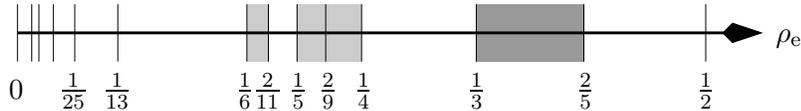

FIGURE 8. Canonical ground state phase diagram in two dimensions for $U > 8$.

BIBLIOGRAPHICAL NOTES

The Falicov-Kimball model was introduced in [3], and the first rigorous results appeared in [1] and [10]. A simple derivation of the expansion (1) using Cauchy formula can be found in [7]. It can be extended to positive temperatures with the help of Lie-Schwinger series [2]. Segregation in arbitrary dimension (Theorem 1) was proposed in [5]. Domains in

the grand-canonical phase diagram for the empty, full, and chessboard configurations, were obtained using lower bounds involving correlation functions of classical particles, see [7] for references. Eq. (10) for the ground state energy for U small was derived using Wigner-Brillouin degenerate perturbation theory in [4]. For the results in two dimensions (Theorem 4), we refer to [8] and references therein. Results on the ground state for μ_e in the universal gap have been extended to positive temperatures [2] using "quantum Pirogov-Sinai theory" (see the review in this Encyclopedia). Further studies and extensions of the Falicov-Kimball model include interfaces, non-bipartite lattices, bosonic particles, continuous fields instead of classical particles, magnetic fields, correlated and extended hoppings. An extensive list of references can be found in the reviews [6, 7, 9].

See also: Equilibrium Statistical Mechanics. Quantum Statistical Mechanics. Fermionic Systems. Hubbard Model. Pirogov-Sinai Theory.

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