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Segregation in the Falicov–Kimball model

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Abstract. The ground state of the one-dimensional Falicov–Kimball model is considered for large values of the interaction strength U. If the ion density $\rho_i = p/q$ (p and q relatively prime) is rational and equals the electron density ρ_e we prove that for $U > U_c^{\text{hom}}(q)$ the ion configuration is the most homogeneous one. If $0 < \rho_e < \rho_i$ and $U > U_c^{\text{seg}}(\rho_e/\rho_i)$ we prove that all the ions condense into one large cluster. This last result proves a recent conjecture known as the segregation principle.

1. Introduction

The Falicov–Kimball model has a long history. Together with the Hubbard model and the periodic Anderson model it is one of the mostly studied models to describe correlation effects in interacting fermion systems. It was originally introduced to study metal–insulator transition in transition-metal oxides [1]. In this context it is a lattice model describing the interaction between mobile d electrons and localized f electrons. The interaction is on-site. The Hamiltonian of the model is then

$$H = -\sum_{x,y\in\Lambda} t_{xy} a_x^+ a_y - U \sum_{x\in\Lambda} W(x) a_x^+ a_x.$$

$\Lambda \subset \mathbb{Z}^\nu$ is usually taken to be a square lattice and $t_{xy} = 1$ if x and y are nearest neighbours and zero otherwise. a_x^+ and a_x are fermion creation and annihilation operators. $W(x)$ is 1 or 0 according to whether the site is occupied by an f electron or empty. The FK model has other physical interpretations. It can be seen as a modification of the Hubbard model (sometimes called the static model [2]) in which one assumes that, for instance, the ↑-spin electrons are infinitely massive. Thus they have no kinetic energy and can be considered as classical particles. Another interpretation is to consider the FK model as a model for crystallization. In this case we think of the classical particles as ions. This is the point of view adopted in this paper. We shall denote a specific ion configuration by s.

Several interesting rigorous results have already been obtained (see [2–10]). In the half-filled band case it was shown that the model exhibits antiferromagnetic long-range order at low temperature, while at high temperature the correlation functions decay exponentially [2, 3]. The ground-state phase diagram in the plane of chemical potentials (grand canonical ensemble) has been investigated analytically in [3–6]. In this paper, we shall focus on the ground state of the one-dimensional model. The simplicity of the model then allows us to work in the canonical ensemble, that is to

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fix the number of electrons N_e and ions N_i rather than the corresponding chemical potentials. In a recent paper [11] Freericks and Falicov investigated the ground-state phase diagram of this model by computing the density of states of a restricted set of ion configurations. Their set contains a finite number (= 10) of periodic configurations as well as the segregated configuration $s_{seg}(N_i)$ in which the N_i ions stick together to form one large box of size N_i. They present two conjectures. The first one claims that, for small U, the ground state satisfies some uniform distribution property. Indeed, we shall prove such a property for large (but finite) U when $N_e = N_i$. To be more specific, we shall make precise the meaning of the following statement: configuration s_1 is more homogeneous than configuration s_2. Then, in section 3 we shall show that the ground state is the most homogeneous configuration $s_{hom}(N_i)$ provided $U > U_c^{hom}(\rho_i)$.

The second conjecture asserts that the segregated phase is the ground state for large U except for $\rho_e = \rho_i$. In agreement with this, we shall prove in section 4 that, for $0 < \rho_e < \rho_i$, there exists a domain in the plane (U, ρ_e), where the segregated configuration $s_{seg}(N_i)$ is the ground state. Both theorems are established in the frame of a rigorous perturbation theory for large $|U|$. These results are summarized in figure 1.

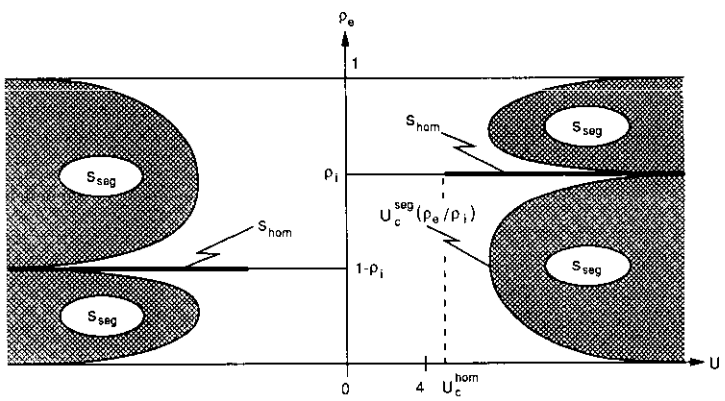

Figure 1. Schematic phase diagram for the ground-state configurations of the 1D FK model.

2. The one-dimensional model

In this section we define the model and fix the notations. For later reference we shall also recall some general properties of the FK model. The model is defined on a segment $\Lambda \subset \mathbb{Z}$ with periodic boundary conditions. The FK Hamiltonian is

$$H(s) = -\sum_{\substack{x,y\in\Lambda \\ |x-y|=1}} a_x^+ a_y - U \sum_{x\in\Lambda} W(x) a_x^+ a_x \tag{1}$$

where $W(x) = 0$ or 1. U may be choosen positive or negative. The argument s in $H(s)$ is the ion configuration in Λ: $s \in \{0,1\}^{|\Lambda|}$. We denote by $\mathrm{supp} s = \{x \in \Lambda | W(x) = 1\}$ the set of occupied sites in s. We say that s' is a *translation* of s if $\mathrm{supp}\, s' = \{x \in \Lambda | W(x-a) = 1\}$ for some $a \in \mathbb{Z}$. For an interval $I \subset \Lambda$ we

denote by $s|_I \in \{0,1\}^{|I|}$ the restriction of s to I, $|I|$ being the number of points in I. $N_e = \sum_{x\in\Lambda} a_x^+ a_x$ and $N_i(s) = \sum_{x\in\Lambda} W(x)$ denote the electron and ion numbers, and $\rho_e = N_e/|\Lambda|$ and $\rho_i = N_i/|\Lambda|$ are the corresponding densities. $N_i = 0$ and $N_i = |\Lambda|$ correspond respectively to the empty and full configurations. The Hamiltonian (1) can be expressed with a single-particle operator $h(s)$,

$$H(s) = \sum_{x,y\in\Lambda} h_{xy}(s) a_x^+ a_y$$

$$h(s) = T - UW. \tag{2}$$

T has matrix elements $-t_{xy}$ where $t_{xy} = 1$ if $|x-y| = 1$ and zero otherwise. W is the diagonal matrix with elements $W(x)$. For fixed N_e and s, $H(s)$ has a ground-state energy $E(N_e, s)$. If $\lambda_j(s)$, $j = 1, \ldots, |\Lambda|$, are the eigenvalues of $h(s)$ in ascending order we have

$$E(N_e, s) = \sum_{j=1}^{N_e} \lambda_j(s). \tag{3}$$

In [2] it was shown that the following operator inequality holds when $|U| > 4$:

$$\frac{|U|}{2} + 2 \geq \left| h(s) + \frac{U}{2} \right| \geq \frac{|U|}{2} - 2 \tag{4}$$

which means that the spectrum of $h(s)$ has a gap if $|U| > 4$. The Hamiltonian $H(s)$ has two important symmetry properties [11]. The first one relates the ground states for s and for its conjugate s^* (corresponding to $W^*(x) = 1 - W(x)$):

$$E(U, N_e, s^*) = E(-U, N_e, s) - UN_e. \tag{5}$$

The second one relates the ground states for N_e electrons and for $|\Lambda| - N_e$ electrons (N_e holes), s being fixed:

$$E(U, |\Lambda| - N_e, s) = E(-U, N_e, s) - UN_i. \tag{6}$$

This last equality follows from the standard unitary transformation $a_x^+ \to (-1)^x a_x$. The properties (5) and (6) allow us to take $U > 0$ (corresponding to the physical case of an attraction between electrons and ions) and $N_e \leq N_i$ without losing any generality. The question we want to address is the following: which configuration s minimizes $E(N_e, s)$ for given N_e, N_i and U? When $N_e = N_i$ we say that the system is *neutral*; this situation is considered in section 3. The case $N_e < N_i$ is considered in section 4. As we shall see, the behaviour of the model is quite different in both cases.

3. The neutral case

Before we state the main result of this section we need to give a few definitions. Let us consider an arbitrary configuration s of N_i ions with periodic boundary conditions.

We denote by d_j the distances between two successively occupied sites x_j and x_{j+1}, i.e. $d_j = |x_{j+1} - x_j|$. We say that s is *homogeneous* if

$$d_j \in \{d, d+1\} \qquad \text{for some } d, \qquad j = 1, \ldots, N_\mathrm{i}.$$

This notion of homogeneity is different from the uniform distribution property considered by Freericks and Falicov in [11]; they consider the size of the islands of occupied sites. For given N_i and Λ, there are in general many (but at least one) homogeneous configurations. Now, we would like to compare two such homogeneous configurations and to be able to decide which of them is the most homogeneous. To do this, we first associate a configuration $s' \in \{0,1\}^{N_\mathrm{i}}$ to each homogeneous configuration s with N_i ions in the following way:

$$W'(j) = \begin{cases} 1 & \text{if } d_j = d \\ 0 & \text{if } d_j = d+1 \end{cases} \qquad j = 1, \ldots, N_\mathrm{i}. \tag{7}$$

If all $d_j = d$, we set $s' = s_{\mathrm{empty}}$. Such an s is said to be *regular*. In other words, we associate an occupied/empty site in s' with each 'short'/'long' couple of occupied sites in s. We say that s' is the *derivative* of s. For a given d the derivative is an invertible application, that is we can 'integrate' an s' to get s (up to a translation). The successive derivatives $s^{(n)}$ are naturally defined by $s^{(n)} = (s^{(n-1)})'$. Now, given two homogeneous configurations s_1 and s_2 on Λ, with the same number of ions, we say that s_2 *is more homogeneous than* s_1 if, for some n, $s_2^{(n)}$ is homogeneous but $s_1^{(n)}$ is not. Figure 2 gives an example.

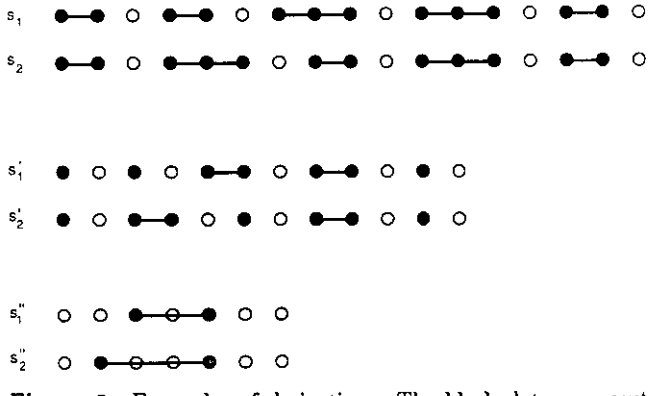

Figure 2. Examples of derivatives. The black dots represent occupied sites. A segment connects each 'short' couple of occupied sites in a given configuration. s_2 is more homogeneous than s_1 because s_2'' is homogeneous whereas s_1'' is not.

We say that two configurations s_1 and s_2 are *equivalent* if s_2 is a translation of s_1. In fact, from now on and to the end of the paper we shall always use the word configuration to speak of one equivalence class. If we fix Λ and N_i, we have then the following.

Lemma 1. There is a unique configuration $s_{\mathrm{hom}}(N_\mathrm{i})$ for which $s_{\mathrm{hom}}^{(n)}(N_\mathrm{i})$ is homogeneous for all $n \geq 0$.

Proof. If s is an homogeneous configuration, then obviously $N_i(s') < N_i(s)$. Therefore, if all $s^{(n)}$ exist, then for some m, $s^{(m)}$ is regular, and $s^{(m+1)}$ is empty. Moreover, if $N_i(s_1) = N_i(s_2)$ then $N_i(s_1^{(n)}) = N_i(s_2^{(n)})$ for all n and in particular for $n = m$. Now, obviously $s_1^{(m)} = s_2^{(m)}$, which implies $s_1 = s_2$. The existence of $s_{\text{hom}}(N_i)$ will be proven at the beginning of the proof of theorem 1.

Clearly the configuration $s_{\text{hom}}(N_i)$ is more homogeneous than any other, and it deserves the name of *most homogeneous configuration*. Notice that if $\rho_i = p/q$ then necessarily $|\Lambda|$ must be an integer multiple of q. Thus we may always construct $s_{\text{hom}}(N_i)$ by repeating periodically the most homogeneous configuration in the minimal volume $|\Lambda| = q$. This remark in particular shows that $s_{\text{hom}}(N_i)$ has period q.

Now, we can state the main result of this section.

Theorem 1. For finite volumes Λ, $N_e = N_i$ and $N_i/|\lambda| = p/q$ (p and q relatively prime) there exists an $U_c^{\text{hom}}(q) < C\,4^q$, with $C > 0$ and independent of Λ, p, q, N_e, such that for $U > U_c^{\text{hom}}(q)$, $E(N_e, s)$ takes its unique minimum at $s = s_{\text{hom}}(N_i)$.

From a physical point of view, this result is rather intuitive. Three effects are in competition: the kinetic energy which tends to delocalize the electrons, the interaction which tends to localize them on the ions and finally the exclusion principle which prevents the electron wavefunctions from overlapping too much. When $N_e = N_i$ and U is large, we can imagine that each electron forms an atom with each ion. The exclusion principle pushes each atom away from the other and the configuration is as homogeneous as possible.

Before we prove theorem 1, we shall first derive a graphical representation for the perturbation series of $h(s)$ in terms of closed paths on the lattice Λ. Changing the normalization of (2), we define

$$\tilde{h}(\kappa; s) = \frac{h(s)}{U} = -W + \kappa T \qquad \kappa = \frac{1}{U} \tag{8}$$

where κ is the perturbation parameter. For $s \neq s_{\text{full}}$ and $s \neq s_{\text{empty}}$, $-W$ has eigenvalues 0 and -1. The degeneracy of -1 is equal to $N_i(s)$. If $N_e = N_i(s)$, the N_e lowest eigenvalues $\tilde{\lambda}_j(\kappa; s)$ of $\tilde{h}(\kappa; s)$ are precisely those for which $\tilde{\lambda}_j(0; s) = -1$. Therefore it is not necessary to resort to degenerate pertubation theory [12]; we can directly consider the perturbation series for the sum of these N_e eigenvalues, which we denote by $\hat{\lambda}(\kappa; s)$:

$$\frac{E(N_e; s)}{U} = \sum_{j=1}^{N_e} \tilde{\lambda}_j(\kappa; s) = \hat{\lambda}(\kappa; s) = -N_e + \sum_{n \geq 2} \hat{\lambda}^{(n)}(s) \kappa^n \tag{9}$$

where

$$\hat{\lambda}^{(n)}(s) = \frac{1}{n} \sum_{k_1 + \ldots + k_n = n-1} \operatorname{Tr} T S^{(k_1)} \times \ldots \times T S^{(k_n)} \tag{10}$$

$$S^{(0)} = -W \qquad S^{(k)} = S = 1 - W \qquad \text{when } k \geq 1. \tag{11}$$

We see that all odd terms vanish in (9). S is the so-called reduced resolvant. The last equality is most easily obtained if we note that W is a projection and that S must satisfy [12]

$$SW = WS = 0 \qquad (1-W)S = S(1-W) = 1-W. \tag{12}$$

W and S are respectively the projectors on occupied and empty sites in Λ. The radius of convergence of (9) is larger than

$$r_0 = \frac{\delta}{2\|T\|} \geq \frac{1}{4} \tag{13}$$

where $\delta = 1$ is the isolation distance of the eigenvalue -1 of $-W$, and $\|T\| \leq 2$. $\kappa < r_0$ implies $U > 4$, which is precisely the condition to have a gap in the spectrum of $h(s)$ (see (4)).

Because $T = (-t_{xy})$ connects only nearest neighbours and the $S^{(k)}$ are diagonal, we can write each trace in (10) as a sum over closed paths γ of length $|\gamma| = n$ ($\gamma = (\gamma_1, \ldots, \gamma_n) \in \mathbb{Z}^n, |\gamma_{j+1} - \gamma_j| = 1, \gamma_{n+1} = \gamma_1, \underline{\gamma} = \bigcup_{i=1}^n \{\gamma_i\}$ is the support of γ):

$$\operatorname{Tr} TS^{(k_1)} \times \ldots \times TS^{(k_n)} = \sum_{\substack{\underline{\gamma} \subset \Lambda \\ \partial\gamma = \varnothing \\ |\gamma| = n}} C^{k_1 \ldots k_n}(s;\gamma) \tag{14}$$

where $\partial\gamma = \varnothing$ means that the path is closed,

$$C^{k_1 \ldots k_n}(s;\gamma) = \begin{cases} (-1)^{m(s;\gamma)} & \text{if } W(\gamma_j) = 1 - \operatorname{sgn}(k_j) \text{ for } j = 1, \ldots, n \\ 0 & \text{otherwise} \end{cases}$$

and $m(s;\gamma) = \sum_{j=1}^n W(\gamma_j)$ is the number of occupied sites visited by γ. Collecting all terms with the same number m of indices $k_j = 0$ in (10), we get a combinatorial factor

$$\frac{(n-2)!}{(n-m-1)!(m-1)!} = \binom{n-2}{n-m-1}$$

equal to the number of partitions of the integer $n-1$ into $n-m$ non-zero integers. (10) can then be rewritten as

$$\hat{\lambda}^{(n)}(s) = \frac{1}{n} \sum_{m=1}^{n-1} \binom{n-2}{n-m-1} \sum_{\substack{\underline{\gamma} \subset \Lambda \\ \partial\gamma = \varnothing \\ |\gamma| = n \\ m(s;\gamma) = m}} (-1)^{m(s;\gamma)}. \tag{15}$$

At last (9) becomes

$$\hat{\lambda}(\kappa;s) + N_e = {\sum_{\substack{\underline{\gamma} \subset \Lambda \\ \partial\gamma = \varnothing}}}' (-1)^{m(s;\gamma)} \frac{\kappa^{|\gamma|}}{|\gamma|} \binom{|\gamma|-2}{|\gamma| - m(s;\gamma) - 1} \tag{16}$$

where $\sum'$ means that the sum is restricted to the paths which visit at least one occupied and one empty site. The representation (16) for the perturbation series for large U is the basic ingredient for the proof of theorem 1. The factor $(-1)^{m(s;\gamma)}$ will play a central role in the proof, and we shall see that it is not as terrible as it looks.

Proof of theorem 1. We must show that for any $s \neq s_{\text{hom}}(N_i)$, with $N_i(s) = N_i$, we have

$$E(N_i, s) > E(N_i, s_{\text{hom}}(N_i)) \qquad \text{when } U > U_c^{\text{hom}}. \tag{17}$$

Let us fix a configuration s. The idea is to construct a sequence $(s_j)_{j=1}^K$ of configurations which interpolates between $s = s_1$ and $s_{\text{hom}}(N_i) = s_K$, and for which it is possible to show that the energy decreases at each step $j \to j+1$, namely

$$E(N_e, s_{j+1}) < E(N_e, s_j) \qquad j = 1, \ldots, K-1 \quad \text{for } U > U_c^{\text{hom}}. \tag{18}$$

Let us first give one more definition. Suppose s_a is an arbitrary configuration (not necessarily homogeneous) for which the minimal distance between two successively occupied sites is d. Let $n_d(s_a)$ be the number of such short couples in s_a. We say that s_b is obtained from s_a by an *elementary move* if, for some interval $I \subset \Lambda$,

1. $s_b|_I = s_a|_I$,
2. $\text{supp}\,(s_b|_{\Lambda \setminus I})$ is a translation of $\text{supp}\,(s_a|_{\Lambda \setminus I})$,
3. $n_d(s_b) = n_d(s_a) - 1$.

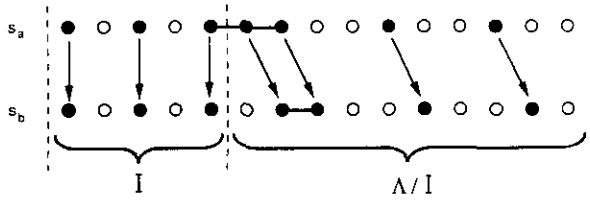

Figure 3. s_b is obtained from s_a by an elementary move. Black dots represent occupied sites. In this example $d = 1$, $n_d(s_a) = 2$ and $n_d(s_b) = 1$.

Figure 3 gives an example of an elementary move.

Now we construct our sequence $(s_j)_{j=1}^K$ as follows. Starting with $s_1 = s$ we look for the smallest $n \geq 0$ such that $s_1^{(n)}$ is not homogeneous. Performing a succession of elementary moves, we can transform $s_1^{(n)}$ into a homogeneous configuration $s_k^{(n)}$. The corresponding configuration $s_1, \ldots, s_k$, obtained by integration, are the k first configurations of our sequence. We go on by iteration, now starting with s_k instead of s, and so on, until we reach a configuration s_K which is infinitely differentiable. This last configuration is then the most homogeneous configuration s_{hom}. Figure 4 shows such a sequence.

Thus, we must show that (18) is true when s_j and s_{j+1} are such that, for some n, $s_{j+1}^{(n)}$ is obtained from $s_j^{(n)}$ by an elementary move. We use (16) to estimate $E(s_{j+1}) - E(s_j)$. This allows us to make systematic cancellations between the paths contributing to $E(s_{j+1})$ and $E(s_j)$. Obviously the dominant (in $\kappa = 1/U$) terms in $E(s_{j+1}) - E(s_j)$ arise from the shortest paths which do not cancel in this difference. Because of their technical nature, a number of combinatorial results are proven in the appendix. Figure 5 summarizes these results and shows the general situation for s_j and s_{j+1}. I_1, I_2 and I_3 denote intervals on which the corresponding restricted configurations are the same. They are also identical on the interval depicted as a wave. The interval I_1 may be empty. It is shown in the appendix that any path which contributes to the

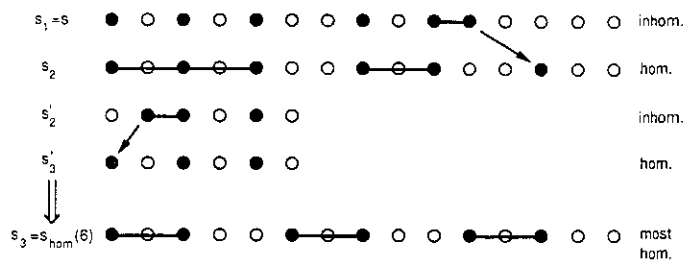

Figure 4. Example of a sequence $(s_j)_{j=1}^{K}$. Here, $|\Lambda| = 15$ and $N_\uparrow = 6$. The sequence contains $K = 3$ configurations $s_1 = s, s_2$ and $s_3 = s_{\mathrm{hom}}(6)$. The arrows represent the two elementary moves.

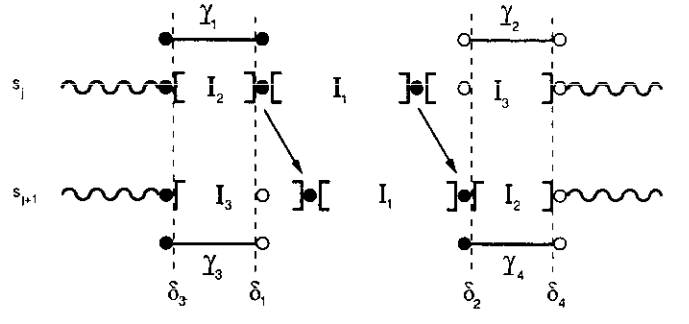

Figure 5. General situation for one step $s_j \to s_{j+1}$.

difference $E(s_{j+1}) - E(s_j)$ necessarily crosses at least one of the four vertical lines δ_k. The segments $\underline{\gamma}_1, \underline{\gamma}_2, \underline{\gamma}_3, \underline{\gamma}_4$ are the supports of the shortest paths contributing to the difference.

Consider for example the shortest paths having the support $\underline{\gamma}_1$. There are $n = |\gamma|$ such paths (this factor and the factor $1/|\gamma|$ in (16) will compensate later). Their length is $|\gamma| = 2(|\underline{\gamma}_1| - 1)$. All points in the interval I_2 (see figure 5) are visited twice by any such path. The two remaining points (the extremities of $\underline{\gamma}_1$) are visited only once. The same considerations apply to $\underline{\gamma}_2$, $\underline{\gamma}_3$ and $\underline{\gamma}_4$. For those γ we see that $m(s;\gamma)$ in (16) is even if the extremities are either both occupied or both empty; it is odd if only one of them is occupied. So, $\underline{\gamma}_1$ and $\underline{\gamma}_2$ give a non-negative contribution to $E(s_j)$, whereas $\underline{\gamma}_3$ and $\underline{\gamma}_4$ give a negative contribution to $E(s_{j+1})$. From

$$\binom{|\gamma| - 2}{|\gamma| - m(s;\gamma) - 1} \geq 1$$

and (16) we get then the following lower bound:

$$\hat{\lambda}(\kappa; s_j) - \hat{\lambda}(\kappa; s_{j+1}) \geq 2\kappa^n + \varepsilon(\kappa; s) \tag{19}$$

$$\varepsilon(\kappa; s) = O(\kappa^{n+2}).$$

To estimate the remainder $\varepsilon(\kappa; s)$ we must consider all paths which cross at least one of the vertical lines δ_k in figure 5, with length $|\gamma| \geq n + 2$. For this we need an upper bound $m_\Lambda(n)$ on the number of closed paths with a given length n which visit one fixed point in Λ:

$$m_\Lambda(n) \leq \frac{3}{\sqrt{4\pi}} \sqrt{n} 2^n \left(1 + \frac{2n}{|\Lambda|}\right). \tag{20}$$

The term in $1/|\Lambda|$ comes from the paths which go around the circle Λ. The proof is standard. We need also a bound on the binomial coefficient in (16). Using Stirling's formula for the largest coefficient we obtain

$$\binom{|\gamma|-2}{|\gamma|-m(s;\gamma)-1} \leq \frac{3}{4}\frac{1}{\sqrt{2\pi}}\frac{2^{|\gamma|}}{\sqrt{|\gamma|}} \qquad \text{if } |\gamma| \geq 4. \tag{21}$$

Because there are four different vertical lines, we then obtain the following bound from (16):

$$|\varepsilon(\kappa;s)| \leq 4\frac{3}{\sqrt{4\pi}}\frac{3}{4}\frac{1}{\sqrt{2\pi}}\sum_{k\geq n+2}\frac{(4\kappa)^k}{k}\left(1+\frac{2k}{|\Lambda|}\right)$$

$$\leq \frac{1}{\sqrt{2}}\frac{9}{2\pi}\frac{(4\kappa)^{n+2}}{1-4\kappa}\left(1+\frac{2}{|\Lambda|}\right). \tag{22}$$

For (19) to be positive, we must require $2\kappa^n \geq |\varepsilon(\kappa;s)|$. So for $|\Lambda|$ and U sufficiently large we must have

$$4^n\kappa^2 \leq C \tag{23}$$

where C is some numerical constant. Remember that $n = 2|I_2|$ is the length of the shortest paths which do not cancel. But if q is the period of $s_{\text{hom}}(N_i)$ then obviously $|I_2| < q$. This shows that $U_c^{\text{hom}}(\rho_i)$ grows exponentialy with the period 'q' of the ground-state configuration and concludes the proof of the theorem.

Although theorem 1 has been proven only for large U, we expect the result to hold for any positive U. The numerical study in [11] seems to support this conjecture. We also expect it to hold, in some generalized version, in any dimension. In [6] we studied the Falicov–Kimball model for dimensions $\nu > 2$ in the grand canonical ensemble. For large U and $\nu = 2$ we derived a formal series up to order U^{-3} for the effective interaction $F(s;\mu_e,\mu_i)$ of the ions. In the domain of the (μ_e,μ_i)-plane where $N_e(\mu_e,\mu_i) = N_i(\mu_e,\mu_i)$, we studied the configurations for $\rho_i = \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}$ and 0. The corresponding ionic configurations are shown in figure 6. Looking at figure 6, it seems in fact that ions are as far as possible from each other for the given densities ρ_i.

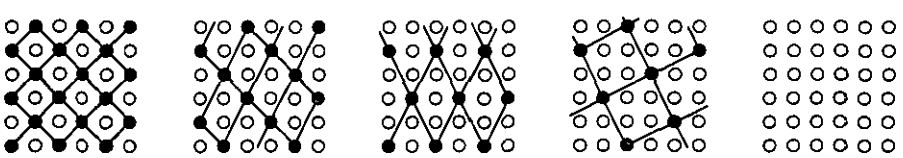

Figure 6. Examples of ground-state configurations for large U in two dimensions.

4. Segregation

In this section, we shall consider the case $\rho_e < \rho_i$ for large U. The segregated configuration $s_{seg}(N_i)$ in which all ions form one unique large cluster of size N_i is our main concern here ($W(x) = 1$ for $x = 1, \ldots, N_i$). We shall show the following.

Theorem 2. If $N_e < N_i$ there exists a function $U_c^{seg}(\rho_e/\rho_i)$ such that for $U > U_c^{seg}(\rho_e/\rho_i)$, $E(N_e, s)$ takes its unique minimum at $s = s_{seg}(N_i)$.

This situation must be contrasted with that of theorem 1. Intuitively the situation is clear: when U is very large, and there are few electrons, the system tends to lower their kinetic energy by making one large box [11]. Indeed, we shall see that the first-order term (in κ) in $E(N_e, s)/U$ is the kinetic energy. Note that this term was absent in (9) because $\mathrm{Tr}\, T = 0$. This is the reason why the behaviour of the system is very different in both cases. The challenge is to prove that this picture remains true when we include the higher order terms.

In contrast with the neutral case, not all eigenstates corresponding to $\tilde{\lambda}_j(0; s) = -1$ are occupied. This makes life a bit more difficult because now we must consider explicitly the degenerate perturbation theory. We start with the usual reduction process [12], defining

$$T(\kappa; s) = \frac{1}{\kappa}(\tilde{h}(\kappa; s) + 1)P(\kappa; s)$$

$$= P(s)TP(s) + \kappa T^{(1)}(\kappa; s) \tag{24}$$

where $P(\kappa; s)$ is the total projection for the group of eigenvalues associated with $\tilde{\lambda}_j(0; s) = -1$; it is holomorphic at $\kappa = 0$. $P(s) = P(0; s) = W$ and $T^{(1)}(\kappa; s)$ given by

$$T^{(1)}(\kappa; s) = \sum_{n \geq 0} \kappa^n T^{(n+1)}(s) \tag{25}$$

$$T^{(n)}(s) = \frac{(-1)^n}{2\pi \mathrm{i}} \oint_\Gamma (R(z)T)^{n+1} R(z)(z+1)\, \mathrm{d}z \tag{26}$$

$$= (-1)^n \sum_{k_1 + \ldots + k_{n+2} = n} S^{(k_1)} T \times \ldots \times S^{(k_{n+1})} T S^{(k_{n+2})}. \tag{27}$$

$R(z) = -(W + z)^{-1}$ is the resolvant of the unperturbed operator $-W$ in (8). Γ is a circle in the complex plane of radius $\frac{1}{2}$ centred at the eigenvalue -1. The operators $S^{(k)}$ have been defined in (11). In the subspace generated by $P(\kappa; s)$, the respective eigenvalues $\eta_j(\kappa; s)$ and $\tilde{\lambda}_j(\kappa; s)$ of $T(\kappa; s)$ and $\tilde{h}(\kappa; s)$ are related through

$$\tilde{\lambda}_j(\kappa; s) = -1 + \kappa \eta_j(\kappa; s) \qquad j = 1, \ldots, N_i. \tag{28}$$

From (28) and the first equality of (9) we also have that

$$E(N_e; s) = \sum_{j=1}^{N_e} \eta_j(\kappa; s) - N_e U. \tag{29}$$

For later reference we give also the formulae analogous to (26) and (27) for the projector $P(\kappa; s) = P(s) + \kappa P^{(1)}(\kappa; s)$:

$$P^{(1)}(\kappa; s) = \sum_{n \geq 0} \kappa^n P^{(n+1)}(s) \tag{30}$$

$$P^{(n)}(s) = -\frac{(-1)^n}{2\pi \mathrm{i}} \oint_\Gamma (R(z)T)^n R(z)\, \mathrm{d}z \tag{31}$$

$$= -(-1)^n \sum_{k_1 + \ldots + k_{n+1} = n} S^{(k_1)} T \times \ldots \times S^{(k_n)} T S^{(k_{n+1})}. \tag{32}$$

For $\kappa = 0$, (24) reduces to

$$T(s) = P(s) T P(s) \tag{33}$$

which is the restriction of the kinetic energy T to the occupied sites of s. Let $\eta_j(s)$ be its eigenvalues. For $U = \infty$ the electrons are trapped into boxes corresponding to supp s. Treating each $\tilde{\lambda}_j(\kappa; s)$ separately leads to problems in the thermodynamic limit, when we want to estimate the convergence radius of the series. So, we try again to consider directly the sum $\sum_{j=1}^{N_e} \eta_j(\kappa; s)$. This is done by simply noting that this sum is nothing but the lowest eigenvalue of the many-body operator corresponding to (a slight modification of) $T(\kappa; s)$.

Proof of theorem 2. We proceed in three steps.

(i) First we take $\kappa = 0$ and show that $\sum_{j=1}^{N_e} \eta_j(s)$ takes its unique minimum at $s = s_{\mathrm{seg}}$ if $N_e < N_i$. For any single-particle operator A, we introduce its N_e fermion version $A_{N_e} = \sum_{j=1}^{N_e} A^{(j)}$ where $A^{(j)}$ acts on the jth electron, and A_{N_e} is restricted to the antisymmetric part $\mathcal{E}$ of $(\mathbb{C}^{|\Lambda|})^{\otimes N_e}$. Let $\mathcal{E}(s)$ be the subspace of antisymmetric wavefunctions Ψ whose support is supp s ($\mathcal{E}(s)\Psi(x_1, \ldots, x_{N_e}) = 0$ if at least one $x_j \notin$ supp s). $\dim \mathcal{E}(s) = \binom{N_e}{N_i} > 1$ if $N_e < N_i$. The variational principle then gives

$$\sum_{j=1}^{N_e} \eta_j(s) = \inf_{\substack{\|\Psi\|=1 \\ \Psi \in \mathcal{E}(s)}} \langle \Psi | T_{N_e} | \Psi \rangle. \tag{34}$$

We introduce the sector $D(s) \subset \Lambda^{N_e}$ defined by

$$D(s) = \{(x_j)_{j=1}^{N_e} | x_1 < x_2 < \ldots < x_{N_e}, \text{all } x_j \in \text{supp } s\}. \tag{35}$$

An example for $N_e = 2$ is given in figure 7.

Because of the antisymmetry of the wavefunctions in $\mathcal{E}(s)$ we need only to consider their restriction to the sector $D(s)$. If $\Psi \in \mathcal{E}(s)$ and $(x_1 \ldots x_{N_e}) = y \in D(s)$ we define $\psi_y = \sqrt{N_e!}\Psi(x_1, \ldots, x_{N_e})$. If $\|\Psi\| = 1$ then ψ_y is normalized as a function on $D(s)$. If $\Psi \in \mathcal{E}(s)$ we have

$$\begin{aligned} \langle \Psi | T_{N_e} | \Psi \rangle &= -\sum_{x_1 \ldots x_{N_e}} \sum_{j=1}^{N_e} \Psi^*(x_1 \ldots x_{N_e})[\Psi(x_1 \ldots x_j + 1 \ldots x_{N_e}) \\ &\quad + \Psi(x_1 \ldots x_j - 1 \ldots x_{N_e})] \\ &= -\sum_{(yy') \subset D(s)} \psi_y^* \psi_{y'} \end{aligned} \tag{36}$$

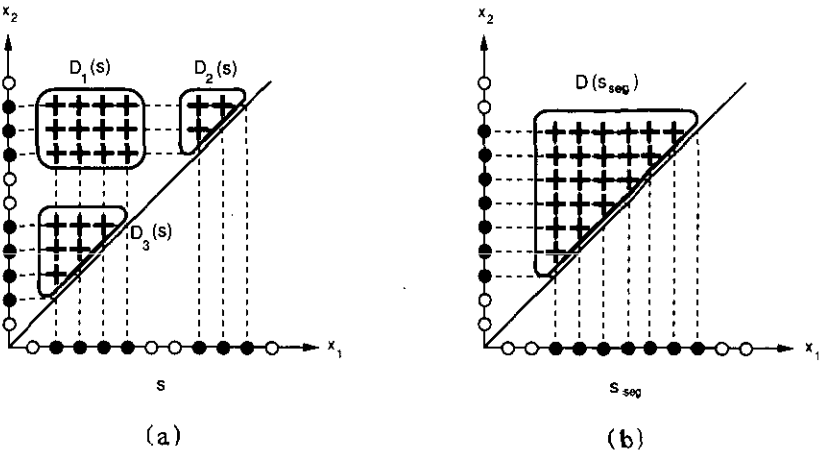

Figure 7. (*a*) The dots on the axes represent the configuration s. The crosses are the points of $D(s)$. (*b*) $D(s_{\mathrm{seg}})$ is connected.

where the last sum is over nearest neighbours in $D(s)$. Then (34) becomes

$$\sum_{j=1}^{N_e} \eta_j(s) = - \sup_{\|\psi\|=1} \sum_{\{yy'\}\subset D(s)} \psi_y^* \psi_{y'}. \tag{37}$$

Let $\psi(s)$ be a function realizing the supremum in (37). The Perron–Frobenius theorem [2] tells us that we can choose $\psi_y(s) \geq 0$ for all $y \in D(s)$. Moreover, if $D(s)$ is connected the inequality is strict and $\psi(s)$ is unique. If $N_e < N_i$ and $s \neq s_{\mathrm{seg}}$, $D(s)$ contains more than one connected component: $D(s) = \bigcup_k D_k(s)$. We can always consider $D(s_{\mathrm{seg}})$ as the union of some translations $D'_k(s) = \tau_k D_k(s)$ of these $D_k(s)$ (see figure 7). Starting from $\psi(s)$, we construct a new function $\psi'(s)$ by sticking together the different parts of $\psi(s)$, namely

$$\psi'_{\tau_k(y)}(s) = \psi_y(s) \qquad \text{if } y \in D_k(s).$$

Thus we get the following inequalities:

$$\sum_{j=1}^{N_e} \eta_j(s) = - \sum_{\{yy'\}\subset D(s)} \psi_y(s)\psi_{y'}(s) \tag{38}$$

$$\geq - \sum_{\{yy'\}\subset D(s_{\mathrm{seg}})} \psi'_y(s)\psi'_{y'}(s) \tag{39}$$

$$\geq - \sup_{\|\psi\|=1} \sum_{\{yy'\}\subset D(s_{\mathrm{seg}})} \psi_y \psi_{y'} \tag{40}$$

$$= \sum_{j=1}^{N_e} \eta_j(s_{\mathrm{seg}}) \tag{41}$$

where (39) follows from $\psi_y(s) \geq 0$. The overall inequality can be made strict. Indeed, if $\psi'(s) = \psi(s_{\text{seg}})$ (39) is strict because $D(s_{\text{seg}})$ contains more nearest neighbours than $D(s)$. In the opposite case, (40) is strict because the vector $\psi(s_{\text{seg}})$ realizing the supremum in (40) is unique.

(ii) Next, we keep $\kappa = 0$ and we derive an estimate for the energy gap $\Delta(s, s_{\text{seg}}) = E(N_e, s) - E(N_e, s_{\text{seg}})$ between a configuration s and s_{seg}. More precisely, we show that

$$\Delta(s, s_{\text{seg}}) \geq (|\partial s| - 2) f\left(\frac{\rho_e}{\rho_i}\right) > 0 \tag{42}$$

where $|\partial s|$ is the number of interfaces between occupied and empty sites in s. In other words, $\frac{1}{2}|\partial s|$ is the number of square wells in the potential W associated with s. We shall prove (42) by induction over $|\partial s|$. We start with $|\partial s| = 4$. For s_{seg} we have a unique well of width $l = N_i$. The eigenvalues $\eta_j(s_{\text{seg}})$ are simply

$$\eta_j(s_{\text{seg}}) = -2\cos\frac{j\pi}{l+1} \qquad j = 1, \ldots, l.$$

The energy of n electrons in one single well is

$$E(n, l) = \sum_{j=1}^{n} \eta_j(s_{\text{seg}}) = 1 - \cos\pi\frac{n}{l+1} - \frac{\sin\pi[n/(l+1)]}{\tan\pi[\frac{1}{2}/(l+1)]}. \tag{43}$$

Take an s for which $|\partial s| = 4$ and $N_i(s) = l$, i.e. we have two square wells of lengths l_1 and l_2, $l_1 + l_2 = l$. The energy of n electrons in these two wells is

$$\sum_{j=1}^{n} \eta_j(s) = E(n_1, l_1) + E(n_2, l_2) \tag{44}$$

for some n_1 and n_2 which depend on l_1 and l_2. From (i) we already know that

$$\Delta(n, l_1, l_2) = \sum_{j=1}^{n} [\eta_j(s) - \eta_j(s_{\text{seg}})] = E(n_1, l_1) + E(n_2, l_2) - E(n, l) > 0. \tag{45}$$

By the way, we note that this last equality is rather hard to derive by direct computation, starting from (43). We now want to verify that moreover

$$\Delta(n, l_1, l_2) \geq h\left(\frac{\rho_e}{\rho_i}\right) > 0. \tag{46}$$

Knowing (45), we can prove (46) by excluding the possibility that $\Delta(n, l_1, l_2)$ vanishes when $l \to \infty$. We first need a good estimate for n_1 and n_2. After a little thought, we see that

$$\frac{n_1 + \nu_1}{l_1 + 1} = \frac{n_2 + \nu_2}{l_2 + 1} = \frac{n}{l+1} \qquad \text{with } |\nu_i| < 1. \tag{47}$$

The constraints $n_1 + n_2 = n$ and $l_1 + l_2 = l$ moreover lead to

$$\nu_1 + \nu_2 = \frac{n}{l+1} < 1. \tag{48}$$

Let us denote $\rho = n/(l+1)$, then from (43), (47) and (48) we obtain

$$\begin{aligned}\Delta(n,l_1,l_2) &= 1-\cos\pi\frac{n}{l+1}\\ &\quad -\frac{2}{\pi}\left[(l_1+1)\left(\sin\pi\frac{n}{l+1}-\frac{\pi\nu_1}{l_1+1}\cos\pi\frac{n}{l+1}\right)+O(l_1^{-1})\right.\\ &\quad +(l_2+1)\left(\sin\pi\frac{n}{l+1}-\frac{\pi\nu_2}{l_2+1}\cos\pi\frac{n}{l+1}\right)+O(l_2^{-1})\\ &\quad \left.-(l+1)\sin\pi\frac{n}{l+1}+O(l^{-1})\right]\\ &= 1-\cos\pi\rho-\frac{2}{\pi}\sin\pi\rho+2\rho\cos\pi\rho+\varepsilon(\rho,l_1)+\varepsilon(\rho,l_2)+\delta(\rho,l)\\ &= g(\rho)+\varepsilon(\rho,l_1,l_2)>0 \qquad (49)\end{aligned}$$

where

$$|\varepsilon(\rho,l_i)|<\frac{a(\rho)}{l_i} \qquad |\delta(\rho,l)|<\frac{b(\rho)}{l} \qquad (50)$$

and

$$g(\rho)>0 \qquad \text{for } 0<\rho<1. \qquad (51)$$

Note that $\delta(\rho,l)<0$ is an increasing function of l. This and the bounds (50) imply that either $\varepsilon(\rho,l_1,l_2)>0$ or

$$\inf_{\substack{l_1\geq 1\\ l_2\geq 1}}\varepsilon(\rho,l_1,l_2)=\varepsilon(\rho,l_1^*,l_2^*) \qquad \text{for some } l_i^*(\rho)<\infty.$$

Therefore (49) shows that $\Delta(n,l_1,l_2)\geq g(\rho)+\varepsilon(\rho,l_1^*,l_2^*)>0$, from which (46) immediately follows. We see that $g(1)=0$, which means that the gap disappears when N_e approaches N_i, as we already know from section 3.

Now we prove (42) in the general case. We start with an arbitrary configuration s_1 with r wells. Suppose n_α, $\alpha=1,\ldots,r$, are the numbers of occupied states in each well when the system is in the ground state ($\kappa=0$). We construct a new configuration $\bar{s}_1$ by changing the order of the wells such that for the first two wells of $\bar{s}_1$ we have

$$\rho_-=\min\left(\frac{\rho_e}{\rho_i},\frac{1}{2}\right)\leq\frac{\bar{n}_1+\bar{n}_2}{\bar{l}_1+\bar{l}_2}\leq\max\left(\frac{\rho_e}{\rho_i},\frac{1}{2}\right)=\rho_+.$$

Suppose s_2 is obtained from $\bar{s}_1$ by sticking together the first two wells of $\bar{s}_1$. Then (46) readily implies

$$E(N_e;\bar{s}_1)-E(N_e;s_2)\geq\inf_{\rho_-\leq x\leq\rho_+}h(x)=2f\left(\frac{\rho_e}{\rho_i}\right). \qquad (52)$$

Iterating the above procedure until $s = s_{\text{seg}}$ yields (42).

(iii) Finally, we take $\kappa \neq 0$ and give an estimate on the error $\varepsilon(\kappa; s)$ defined by

$$\varepsilon(\kappa; s) = \sum_{j=1}^{N_e} [\eta_j(\kappa; s) - \eta_j(s)] \,. \tag{53}$$

Namely, we show there exists a κ_0 such that if $\kappa < \kappa_0$ then

$$|\varepsilon(\kappa; s)| \leq C\kappa|\partial s| \tag{54}$$

where C is a numerical constant. If we want s_{seg} to be the ground state, we must require that the error $|\varepsilon|$ be sufficiently small with respect to the gap Δ:

$$2|\varepsilon(\kappa; s)| < \Delta(s, s_{\text{seg}})$$

or, from (42) and (54),

$$2C|\partial s|\kappa < f\left(\frac{\rho_e}{\rho_i}\right)(|\partial s| - 2) \qquad \text{when } |\partial s| \geq 4$$

from which theorem 2 then immediately follows. To show (54) we shall use the following consequence of the minimax principle ($\lambda_1(A)$ denotes the lowest eigenvalue of an operator A).

Lemma 2. If A and B are two symmetric operators, then $|\lambda_1(A + B) - \lambda_1(A)| \leq \|B\|$.

At first sight, we could be tempted to take $A = T_{N_e}$ and $B = \kappa T^{(1)}_{N_e}(\kappa; s)$, but this does not work because we should remember that $\dim(\ker T(\kappa; s)) = |\Lambda| - N_i > 0$ and thus the $\eta_j(\kappa; s)$, $j = 1, \ldots, N_e$, are not the N_e smallest eigenvalues of $T(\kappa; s)$ (in the case where some of these $\eta_j(\kappa; s)$ are positive). In other words, $\sum_{j=1}^{N_e} \eta_j(\kappa; s) \neq \lambda_1(T_{N_e}(\kappa; s))$. To avoid this problem, we consider the new shifted operator $\bar{h}(\kappa; s) = \tilde{h}(\kappa; s) - 2\kappa$. The reduction process for $\bar{h}$ then goes as follows:

$$\begin{aligned}
\bar{T}(\kappa; s) &= \frac{1}{\kappa}(\bar{h}(\kappa; s) + 1)P(\kappa; s) \\
&= \frac{1}{\kappa}(\tilde{h}(\kappa; s) - 2\kappa + 1)P(\kappa; s) \\
&= P(s)TP(s) + \kappa T^{(1)}(\kappa; s) - 2P(\kappa; s) \\
&= P(s)(T - 2)P(s) + \kappa(T^{(1)}(\kappa; s) - 2P^{(1)}(\kappa; s)) \\
&= \bar{T}(s) + \kappa\bar{T}^{(1)}(\kappa; s)
\end{aligned} \tag{55}$$

where the last equality defines the new unperturbed operator $\bar{T}(s)$ and its perturbation $\bar{T}^{(1)}(\kappa; s)$. But now (4) implies $\bar{T}(\kappa; s) \leq 0$ and thus $\sum_{j=1}^{N_e} \bar{\eta}_j(\kappa; s) = \lambda_1(\bar{T}_{N_e}(\kappa; s))$

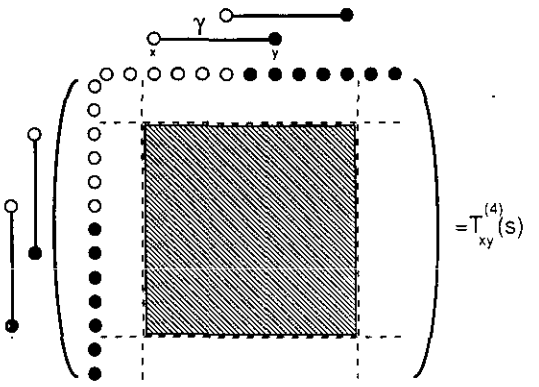

Figure 8. Evaluation of the rank of $T^{(4)}(s)$. A part of the configuration s is shown on the top and on the left of the matrix. Outside the hatched zone, the matrix elements of $T^{(4)}(s)$ vanish.

where $\bar{\eta}_j(\kappa;s) = \eta_j(\kappa;s) - 2$. We therefore take $A = \bar{T}_{N_e}(s)$ and $B = \kappa\bar{T}^{(1)}_{N_e}(\kappa;s)$. From (53), (55), lemma 2, and using the operator norms $\|\ \|_{\mathcal{E}}$ on $\mathcal{E}$, we have

$$\begin{aligned}|\varepsilon(\kappa;s)| &= \left|\lambda_1(\bar{T}_{N_e}(\kappa;s)) - \lambda_1(\bar{T}_{N_e}(s))\right| \\ &\le |\kappa|\ \left\|\bar{T}^{(1)}_{N_e}(\kappa;s)\right\|_{\mathcal{E}} \\ &\le |\kappa|\left(\left\|T^{(1)}_{N_e}(\kappa;s)\right\|_{\mathcal{E}} + 2\left\|P^{(1)}_{N_e}(\kappa;s)\right\|_{\mathcal{E}}\right). \end{aligned} \tag{56}$$

To have good bounds on the norms in (56) we first derive an estimate on the rank of the corresponding single-particle operators. Indeed, for any single-particle operator A, we always have the following relation:

$$\|A_{N_e}\|_{\mathcal{E}} \le (\mathrm{rank}A)\|A\| \qquad \forall N_e. \tag{57}$$

Formulae (27) and (32) are well suited for a calculation of the rank of $T^{(n)}(s)$ and $P^{(n)}(s)$. Following the same lines as in section 3 we rewrite the matrix elements $T^{(n)}_{xy}(s)$ and $P^{(n)}_{xy}(s)$ as sums over paths connecting x and y (we note $\partial\gamma = (x_1, x_{n+1})$ if $\gamma = (x_1, \ldots, x_{n+1})$, $|\gamma| = n$):

$$T^{(n)}_{xy}(s) = \sum_{\substack{\underline{\gamma}\subset\Lambda \\ \partial\gamma=(x,y) \\ |\gamma|=n+1}}{}'' C(\gamma;s) \tag{58}$$

$$P^{(n)}_{xy}(s) = -\sum_{\substack{\underline{\gamma}\subset\Lambda \\ \partial\gamma=(x,y) \\ |\gamma|=n}}{}' C(\gamma;s). \tag{59}$$

The explicit expression for $C(\gamma;s)$ is unimportant here. In both sums the paths must visit at least one empty site. In (58) they must furthermore visit two occupied sites, and in (59) one occupied site. To have an upper bound on the rank of $T^{(n)}(s)$ or $P^{(n)}$, we look for the most distant couple of points (x,y) connected by a path of given length in (58) or (59). Figure 8 shows an example. It may happen that the hatched zones corresponding to different interfaces overlap.

But in any case we have the following bounds:

$$\operatorname{rank} T^{(n)}(s) \leq (2n+1)|\partial s| \tag{60}$$

$$\operatorname{rank} P^{(n)}(s) \leq 2n|\partial s|. \tag{61}$$

To evaluate the norm $\|T^{(n)}(s)\|$ we use (26). We have

$$\|T^{(n)}(s)\| \leq \frac{1}{2\pi}\ell(\Gamma)(\sup_{z\in\Gamma}\|R(z)\|)^{n+2}\|T\|^{n+1}\frac{1}{2} \leq 2 \times 4^n. \tag{62}$$

We have used that $\|R(z)\| = 2$ when $z \in \Gamma$ and the length $\ell(\Gamma)$ is $2\pi\frac{1}{2}$. Similarly, from (31) we have

$$\|P^{(n)}(s)\| \leq 4^n. \tag{63}$$

The upper bound on $\left\|\bar{T}^{(1)}_{N_e}(\kappa;s)\right\|_{\mathcal{E}}$ in (56) follows then from (57) and (60)–(63):

$$\begin{aligned}
\left\|\bar{T}^{(1)}_{N_e}(\kappa;s)\right\|_{\mathcal{E}} &\leq \left\|T^{(1)}_{N_e}(\kappa;s)\right\|_{\mathcal{E}} + 2\left\|P^{(1)}_{N_e}(\kappa;s)\right\|_{\mathcal{E}} \\
&\leq \sum_{n\geq 0}|\kappa|^n\left(\left\|T^{(n+1)}_{N_e}(\kappa;s)\right\|_{\mathcal{E}} + 2\left\|P^{(n+1)}_{N_e}(\kappa;s)\right\|_{\mathcal{E}}\right) \\
&\leq |\partial s|\sum_{n\geq 0}|\kappa|^n[(2n+3)\times 2\times 4^{n+1} \\
&\quad + 2(2n+2)\times 4^{n+1}] \\
&= |\partial s|\left(\frac{32}{(1-4\kappa)^2} + \frac{8}{1-4\kappa}\right).
\end{aligned} \tag{64}$$

The bound (54) follows from (56) and (64); take for example $\kappa < \kappa_0 = \frac{1}{8}$ and $C = 144$.

To make the connection with [11] we mention that in the thermodynamic limit we have indeed the following relation between the densities of state $n(\varepsilon; s)$:

$$n(\varepsilon; s_{\text{seg}}) = \rho_i n(\varepsilon; s_{\text{full}}) + (1-\rho_i)n(\varepsilon; s_{\text{empty}}).$$

As in the neutral case, we think that this segregation takes place in any dimension. One open question is to see what really happens when $\rho_e \to 0$ where our theorem tells us that $U_c^{\text{seg}} \to \infty$. In fact the case for one electron has been studied in [2] where it is shown that s_{seg} is the unique ground state for any U. But, on the other hand, in this situation the Pauli principle plays no role.

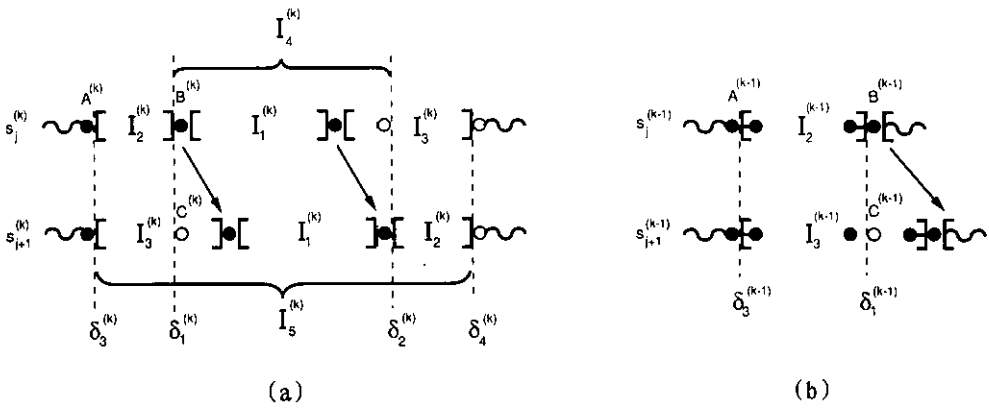

Figure 9. Situation for one induction step $k \to k-1$.

Appendix

In this appendix we give a proof of the results announced in figure 5. We proceed by induction. Suppose indeed that we have the situation depicted in figure 9(a) for $s_j^{(k)}$ and $s_{j+1}^{(k)}$ for some k.

For $k = n$, the intervals $I_2^{(n)}, I_3^{(n)}$ are empty and figure 9(a) represents an elementary move. Looking at figure 9(b), we see that the induction step is almost obvious if we remember that each occupied (resp empty) site in $s_j^{(k)}$ gives two occupied sites in $s_j^{(k-1)}$ with distance $d^{(k-1)}$ (resp $d^{(k-1)}+1$). The left occupied site coming from $A^{(k)}$ is just $A^{(k-1)}$. That $C^{(k-1)}$ is empty follows from the fact that $s_j^{(k-1)}$ and $s_{j+1}^{(k-1)}$ are identical on the interval between the lines $\delta_1^{(k-1)}$ and $\delta_3^{(k-1)}$, and because $C^{(k)}$ is empty. For $k = 0$ we have the situation of figure 5.

Now, using the above construction, we can make systematic cancellations of the contributions to $E(s_j)$ and $E(s_{j+1})$. Consider first the case when $I_1 = \varnothing$. The contributions of paths having their support in I_4 cancel by left–right symmetry. The same is true for those which have their support in $\Lambda \backslash I_4$. Therefore all contributions necessarily come from paths which cross at least one of the lines δ_1 or δ_2. Among those, we can still throw away all paths which have their support in I_5 because they cancel by (left–right) symmetry. The only remaining paths are those who cross either (δ_1 and δ_4) or (δ_1 and δ_3) or (δ_2 and δ_3) or (δ_2 and δ_4). The shortest paths are precisely those depicted in figure 5. When $I_1 \neq \varnothing$, the paths having their support in I_1 cancel. The same is true for those which have their support in $\Lambda \backslash I_4$. Therefore, all contributions come from paths whose support is not completely contained in one of these two intervals. The shortest path starting from B which does not cancel by any symmetry connects B and A. Its support is denoted γ_1 in figure 5. Similar reasoning applies for γ_2, γ_3 and γ_4.

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