# Some Symmetry Remarks on the Ground State Configurations of the Two Dimensional Bosonic Falicov-Kimball Model

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**Abstract**

We show that the ground state configuration of the nuclei in a system composed by itinerant bosons in two dimensions described by the Falicov-Kimball Hamiltonian is composed by symmetric intervals centered on 45°-degree lines on thje cartesian plane. This adds up to the previous result about this problem which asserted symmetry of intervals centered on the coordinate axii. The combination of these facts strongly suggest the convexity of the nuclear distributions.

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# 1 Introduction

The Falicov-Kimball model was introduced in 1969 [1] as a way to describe semiconductor-metal phase transitions in transition-metal oxides. The Hamiltonian which defines the system is given by

$$H = -\sum_{x,y\in\Lambda;|x-y|=1} c_x^\dagger c_y + U\sum_{x\in\Lambda} W(x) c_x^\dagger c_x \tag{1}$$

where, $\Lambda \subset \mathbf{Z}^{\mathrm{d}}$, and, according to the original purposes of the authors, $c_x^\dagger$ and $c_x$ were respectivelly thought to be creation and annihilation operators for mobile electrons in $d-$shells, while the $W(x)$ indicated the positions of localized $f-$electrons assuming the values $W(x) = 1$ if the site is occupied and $W(x) = 0$ otherwise.

The Hamiltonian operator can then be stated as

$$H = T - V.$$

Here, $T$ is the operator given by

$$T = -\Delta - 2d.\mathbf{1}.$$

$\Delta$ is the lattice Laplacean, whose action, in $d$ dimensions is

$$(-\Delta f)(x) = \sum_{i=1}^{d} [2f(x) - f(x+\mathbf{e}_i) - f(x-\mathbf{e}_i)]$$

where $\mathbf{e}_i$ is a unit vector in the $i$-direction. $\mathbf{1}$ represents here the identity operator. The operator $V$ is just a diagonal operator whose elements of the principal diagonal are respectively $U$ or 0 according to the fact that the corresponding site is occupied or empty.

The same Hamiltonian can be interpreted in several other different ways. It could just represent a simplification of the Hubbard model where, say, the spin-down electrons are taken to be infinitely massive. Or, if $U$ is chosen to be positive, the atractive interaction between mobile and fixed particles assumes the form of the interaction between itinerant negative charged electrons and fixed positive nuclei.

Indeed, adopting this last point of view, Kennedy and Lieb [2] showed that, in the half-filled case ($\sum_x c_x^\dagger c_x = \sum_x W(x) = |\Lambda|/2$, where $|\Lambda|$ is the cardinality of the set $\Lambda$), when $\Lambda$ is connected and can be decomposed into two sublattices, $\Lambda_1$ and $\Lambda_2$ such that $\Lambda = \Lambda_1 \cup \Lambda_2$, the ground state of the system is attained when the nuclei arrange themselves in a checkerboard configuration, occupying all sites of one of the sublattices. This result shows that the Falicov-Kimball model can be viewed as a very simple model of matter, leading to the formation of crystals.

However, an interesting remark in [2] is related to the fermionic nature of the mobile particles. It is proved that, when the itinerant particles happen to be bosons, the ground state changes into a configuration where all the nuclei are packed together.

In order to appreciate this result in its total extent, some definitions are necessary.

**Definition 1**: A function $f(x) : [-L, L] \cap \mathbf{Z} \to \mathbf{R}^+$ is said to be *Left Symmetric Decreasing* (LSD) when:

$$f(0) \geq f(-1) \geq f(1) \geq f(-2) \geq ... \geq f(m)$$

where we denote by $m$ the biggest integer contained in $[-L, L]$.

**Definition 2**: A function $f(x) : [-L, L] \cap \mathbf{Z} \to \mathbf{R}^+$ is said to be *Right Symmetric Decreasing* (RSD) when:

$$f(0) \geq f(1) \geq f(-1) \geq f(2) \geq ... \geq f(-m)$$

where by $-m$ we denote the smallest integer in $[-L, L]$.

**Definition 3**: A function $f(x) : [-L, L] \cap \mathbf{Z} \to \mathbf{R}^+$ is said to be *Symmetric Decreasing* (SD) if it is, at the same time, LSD and RSD.

**Definition 4**: A *coordinate line* in the $y_1$ direction is a set $l \subset \mathbf{Z}^d$ of the form

$$l = \{(z, y_2, y_3, ..., y_d) | z \in \mathbf{Z}\}.$$

Given these four definitions, Kennedy and Lieb [2] proved that, due to the bosonic nature of the itinerant particles, the ground state wave function $\psi$ is, on every coordinate line in a given direction, positive definite and RSD (or LSD). It can be also SD, in which case $\psi(x) = \psi(y)$ only if $x$ is the reflection of $y$ through the midpoint of the line. It is also proved the existence of a positive threshold $\psi_0$ such that

$$V(x) = 2U \Leftrightarrow \psi \geq \psi_0 \tag{2}$$

and

$$V(x) = 0 \Leftrightarrow \psi < \psi_0. \tag{3}$$

The crucial difference between the bosonic and the fermionic cases is that, in the case of itinerant fermions, to obtain the ground state it is necessary to calculate the $|\Lambda|/2$ eigenstates corresponding to the $|\Lambda|/2$ lowest eigenvalues and then putting one electron in each of these states. In the bosonic case, it is only necessary to find out the lowest eigenvalue of the Hamiltonian (unique, as a consequence of Perron-Frobenius theorem) so that all particles can be simultanously accomodated in the corresponding eigenstate.

The allowed configurations of nuclei in the ground state, given the above results, would then be composed by intervals over the coordinate lines either symmetric to the $x$ or to the $y$ axis (two dimensional model). Figures like centered squares, rectangles, crosses, and the like are good examples. In this note we are going to extend these results to 45°-lines. Some configurations will then be ruled out, like the rectangle and the cross. However, despite our result is still not sufficient to assert the convexity (in a lattice sense) of the distributions of nuclei, we think that this is a natural conjecture.

We also remark that, although our results are obtained for the two dimensional case, the same techniques used here can be straightforwardly used in higher dimensions.

We obtain our results by exploring the symmetry of the possible configurations of the ground state according to [2] and then by applying rearrangement inequalities to the ground state eigenfunction along the 45°-lines in order to minimize its energy.

# 2 Exploring the Symmetry of the Ground State Eigenfunction

In the two dimensional case, according to [2], only a few different possible configurations of the ground state wave function $\psi$ can exist:

1) $\psi$ could be LSD in the $x$ direction and RSD in the $y$ direction.
2) $\psi$ could be LSD in the $x$ direction and LSD in the $y$ direction.
3) $\psi$ could be LSD in the $x$ direction and SD in the $y$ direction.
4) $\psi$ could be SD in both directions.

And, of course, all cases obtained by replacing LSD by RSD (and vice-versa) above. These are trivially equivalent to the ones presented before.

We now define what is precisely understood as a $45°$-line.

**Definition 5**: A $45°$-*degree line* which contains the point $(x, y)$ and goes from the second to the fourth quadrants is a set of points $\bar{l}^{(2,4)} \subset \mathbf{Z}^2$ of the form

$$\bar{l}^{(2,4)} = \{(x, y) + n(1, -1) | n \in \mathbf{Z}\}.$$

In a similar way one can define a $45°$-degree line that goes from the third to the first quadrants by

$$\bar{l}^{(3,1)} = \{(x, y) + n(1, 1) | n \in \mathbf{Z}\}.$$

We will also be calling the $45°$-lines that contain the origin as *central* and indicating them as $\bar{l}_c^{(2,4)}$ (and, of course $\bar{l}_c^{(3,1)}$).

Let us take, as an example, the ground state wave function $\psi$ corresponding to the first case above. Now, imagine points located over $\bar{l}_c^{(2,4)}$. Since, as a hypothesis, $\psi$ is LSD in the $x$ direction and RSD in the $y$ direction, we have that

$$\psi(0, 0) \geq \psi(-1, 1) \geq \psi(-1, -1) \geq \psi(1, -1) \geq \psi(1, 2) \geq \psi(-2, 2) \geq ...$$

so that

$$\psi(0, 0) \geq \psi(-1, 1) \geq \psi(1, -1) \geq \psi(-2, 2) \geq \psi(2, -2) \geq ...$$

and we have then that the values assumed by $\psi$ over $\bar{l}_c^{(2,4)}$ are also ordered in a symmetric decreasing way. If it is LSD or RSD it depends only on the chosen orientation of the line. Let us call it LSD. It is easy to discover that, for each of the above cases, 1)-4), at least one of the distributions of $\psi$ over central $45°$-lines is ordered in a LSD or RSD way. Both of them can also be ordered, corresponding to the case when the distribution of $\psi$ is SD along one of the coordinate lines. Finally, if the distribution is SD in both directions one is able to find out that both of these central lines are also SD.

# 3 Rearrangement Inequalities

Rearrangement inequalities will be used below in order to minimize the energy of the ground state. The following straightforward inequality (for a proof, see [3]) is a basic Lemma.

**Lemma 1**: For both $f : \mathbf{Z} \to \mathbf{R}^+$ and $g : \mathbf{Z} \to \mathbf{R}^+$ we have that

$$\langle f|g\rangle \leq \langle f^*|g^*\rangle = \langle f^{**}|g^{**}\rangle.$$

where by $f^*$ and $f^{**}$ we respectively indicate the LSD and RSD rearrangements of the function $f$, defined as follows:

**Definition 6**: Given $f : \mathbf{Z} \to \mathbf{R}^+$, it is always possible to arrange the values of $f$ in a strictly decreasing order:

$$f_1 \geq f_2 \geq f_3 \geq ...$$

We then define the *LSD rearrangement of f*, indicated by $f^*$ as $f(0) = f_1$, $f(-1) = f_2$, $f(1) = f_3$, and so on. In a similar way the *RSD rearrangement of f*, indicated by $f^{**}$ can be constructed.

We now introduce the following operator $\Upsilon$:

$$[\Upsilon f](x) = f(x) + f(x+1),$$

whose adjoint is easily verified to be

$$[\Upsilon^\dagger f](x) = f(x-1) + f(x).$$

We then have

**Lemma 2**: Given $f : \mathbf{Z} \to \mathbf{R}^+$, a LSD function, and $g : \mathbf{Z} \to \mathbf{R}^+$, we have that

$$\langle f^*|\Upsilon g\rangle \leq \langle f^*|\Upsilon g^{**}\rangle.$$

**Proof**:

Since $f$ is a LSD function we have that $f^* = f$. Now, since

$$[\Upsilon^\dagger f^*](x) = f^*(x-1) + f^*(x)$$

and

$$[\Upsilon^\dagger f^*](-x) = f^*(-x-1) + f^*(-x)$$

for any $x \in \mathbf{Z}$, we have that $\Upsilon^\dagger f^*$ is a RSD function. This is easy to see, because, since $f^*$ is LSD, we have that

$$f^*(x-1) \geq f^*(-x)$$

and

$$f^*(x) \geq f^*(-x-1).$$

Implying $[\Upsilon^\dagger f^*](x) \geq [\Upsilon^\dagger f^*](-x)$. In a similar fashion one is also able to prove that $[\Upsilon^\dagger f^*](-x) \geq [\Upsilon^\dagger f^*](x+1)$.

So, by using Lemma 1, we have that

$$\langle f^*|\Upsilon g\rangle = \langle \Upsilon^\dagger f^*|g\rangle \leq \langle \Upsilon^\dagger f^*|g^{**}\rangle = \langle f^*|\Upsilon^\dagger g^{**}\rangle.$$

This completes the proof.

# 4 Minimizing the Ground State Energy

Let $\mathcal{F}$ be the functional

$$\mathcal{F} = -\langle\overline{\psi}|V\overline{\psi}\rangle - \langle\overline{\psi}|\widetilde{\Upsilon}_1 Q_1\rangle - \langle\overline{\psi}|\widetilde{\Upsilon}_2 Q_2\rangle \tag{4}$$

so that we are able to define the number

$$E(V, Q_1, Q_2) = \min_{\overline{\psi}}\{\mathcal{F}(\overline{\psi}; V, Q_1, Q_2)|\langle\overline{\psi}|\overline{\psi}\rangle = c\} \tag{5}$$

The notation $\overline{\psi}$ is here being used in order to indicate the fact that these functions have support over $45°$-lines. The operators $\widetilde{\Upsilon}_{1,2}$ are then respectively defined as

$$[\widetilde{\Upsilon}_1\overline{\psi}](x,y) = \overline{\psi}(x+1,y) + \overline{\psi}(x,y\pm 1)$$

and

$$[\widetilde{\Upsilon}_2\overline{\psi}](x,y) = \overline{\psi}(x-1,y) + \overline{\psi}(x,y\mp 1)$$

the upper sign corresponding to the situation where the support of $\psi$ goes from the second to the fourth quadrants, the lower sign when it goes from the third to the first quadrants.

We shall now assume that both (2) and (3) are valid in order to prove the following Lemma.

**Lemma 3**: Given the functional $\mathcal{F}$ defined by (4), we have that, under the assumptions (2) and (3), whenever $\overline{\psi} = \overline{\psi}^*$:

$$E(V, Q_1, Q_2) \geq E(V^*, Q_1^{**}, Q_2^{**}) = E(V^{**}, Q_1^*, Q_2^*).$$

**Proof**:

Follows immediately after Lemma 2 and by noting that, since $\overline{\psi} = \overline{\psi}^*$, the assumptions (2) and (3) imply $V = V^*$ so that

$$\langle \overline{\psi} | V \overline{\psi} \rangle = \langle \overline{\psi}^* | V^* \overline{\psi}^* \rangle = \langle \overline{\psi}^{**} | V^{**} \overline{\psi}^{**} \rangle.$$

Now, in order to simplify the proof of our main result we recall a particular case, namely the one discussed in section 2. This will be done without any loss of generality. The reader will easily find out that a similar version of the theorem below is available for every possible distribution of $\psi$ along the coordinate line directions.

**Theorem**: Let $U < 0$ and take $V$ in order to minimize the ground state energy of the operator $H = T - V$ in a rectangle $\Lambda \subset \mathbf{Z}^2$ under the condition $\sum_x V(x) = 2UN$. Let $\psi$ be the ground state wave function corresponding to the operator $H$. According to [2] the only possible distributions of $\psi$ along the coordinate lines are those presented in section 2. Take the first case. We then have that:

**i)** The distribution of $\psi$ along the central 45°-line that goes from the second to the fourth quadrant is LSD in the sense that

$$\psi(0,0) \geq \psi(-1,1) \geq \psi(1,-1) \geq \psi(-2,2) \geq ...$$

**ii)** The distribution of $\psi$ along any other 45°-line that goes from the second to the fourth quadrant will be LSD (RSD) according to the fact that the number of 45°-lines between it and the parallel central line is an odd (even) number.

**iii)** Along each 45°-degree line that goes from the second to the fourth quadrants $\psi$ attains its maximum over points on the central 45°-degree line that goes from the third to the first quadrants.

As a consequence we have that the support of the function $V(x)$ is composed by symmetric intervals with respect to the ce

**Proof**:

**i)** This assertion is already proved in section 2.

**ii)** Take one configuration of $\psi(x)$ that is at the sime time LSD along all coordinate lines in the horizontal direction and RSD along all coordinate lines in the vertical direction. Now, look at the distribution of values of $\psi(x)$ over $\bar{l}_c^{(2,4)}$. Since this distribution is LSD in the sense of section 2, in order to minimize the functional $\mathcal{F}$ in (4), both $Q_1$ and $Q_2$ (the two adjacent 45°-lines to $\bar{l}_c^{(2,4)}$, that will be respectively indicated as $\bar{l}_{-1}^{(2,4)}$ and $\bar{l}_1^{(2,4)}$) should be RSD. If they are not, rearrange them in this way, so that by Lemma 3 the energy is lowered. Now, move to the 45° degree line $\bar{l}_1^{(2,4)}$, whose neighbors are $\bar{l}_c^{(2,4)}$ and $\bar{l}_2^{(2,4)}$ and, since $\bar{l}_c^{(2,4)}$ is already arranged in the right way, rearrange $\bar{l}_2^{(2,4)}$ in a LSD way. When all 45°-degree lines are rearranged following this recipe, it may be possible that some of the LSD (RSD) arrangements in the horizontal (vertical) direction are spoiled. It is then necessary to rearrange the coordinate lines in the horizontal (vertical) direction again. This will lower the energy even more. The above procedure can then be repeatedly applied untill no more rearrangements are possible. This will then be the configuration of $\psi$ with the lowest energy.

**iii)** By inspection, after Lemma 2.

As a consequence of the theorem above, together with the fact that (2) and 3 were proved to be valid in the ground state in [2] we have that the support of the function $V(x)$, identical to the distribution of nuclei, will be composed by symmetric intervals with respect to the 45°-lines. This , together with the previous result that states symmetry of intervals where $W(x) \neq 0$ with respect to coordinate axii strongly suggest that the real configuration is some kind of lattice approximation of a circle.

# References


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