The Falicov-Kimball Model with Long–Range Hopping Matrices

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Abstract

The ground state nature of the Falicov-Kimball model with unconstrained hopping of electrons is investigated. We solve the eigenvalue problem in a pedagogical manner and give a complete account of the ground state energy both as a function of the number of electrons and nuclei and as a function of the total number of particles for any value of interaction $U \in \mathbb{R}$. We also study the energy gap and show the existence of a phase transition characterized by the absence of gap at the half–filled band for $U < 0$. The model in consideration was proposed and solved by Farkasŏvsky [F] for finite lattices and repulsive on-site interaction $U > 0$. Contrary to his proposal we conveniently scale the hopping matrix to guarantee the existence of the thermodynamic limit. We also solve this model with bipartite unconstrained hopping matrices in order to compare with the Kennedy–Lieb variational analysis [KL].

Key words: Falicov-Kimball model; Long-range hopping; Ground state; Phase Transition
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1 Introduction

The Falicov-Kimball model [FK] of correlated (spinless) electrons on a lattice $\Lambda \subset \mathbb{Z}^d$ is governed by the second-quantized Hamiltonian

$$\mathcal{H} = -\sum_{x,y\in\Lambda} t_{x,y}\, c_x^\dagger c_y + 2\,U \sum_{x\in\Lambda} w_x\, c_x^\dagger c_x \tag{1.1}$$

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where $c_x^\dagger$ and c_x are the creation and annihilation operators for the electrons at the site x, and $t_{x,y}$ is the matrix element for hopping between two sites. Each lattice site may be occupied by at most one fixed nucleus which interacts with the mobile electrons via a on-site interaction U. The interaction is repulsive when $U > 0$ and attractive if $U < 0$. The occupation number w_x is 0 or 1 according to whether the site x is occupied or not by a nucleus.

Although the w variables are referred as nuclei, this description is only one of many different model's interpretations. One may think of the Hamiltonian (1.1) as an approximation to the Hubbard model in which one of the two types of electrons are kept static. See references [KL, K] for a survey on this.

Compared to the Hubbard model, the Falicov–Kimball model has the advantage to be reducible to a single particle Hamiltonian. Since there are no interactions between the electrons, (1.1) is the second quantized form of the Schroedinger Hamiltonian on $\ell_2(\Lambda)$:

$$H = -T + 2\,U\,W \tag{1.2}$$

where T is the self–adjoint operator with matrix elements $t_{x,y} = t_{y,x}$ and W is the multiplication operator by w_x, i.e., the diagonal matrix $W = \mathrm{diag}\left(\{w_x\}_{x\in\Lambda}\right)$. Denoting L the number of sites in Λ ($L = |\Lambda|$), T and W are $L \times L$ matrices.

To discuss some of the known results on the ground state of (1.1), let Λ be the union of two disjoint sub-lattices $\mathcal{A}$ and $\mathcal{B}$ and let us assume that $t_{x,y}$ vanishes when x and y belongs to the same sub-lattice. It is also required that Λ is T–connected in the sense that T is an irreducible matrix (it cannot be written as a direct sum). For example, these conditions are met if T is the usual nearest neighbor matrix

$$t_{x,y} = \begin{cases} t & \text{if } |x-y| = 1 \\ 0 & \text{otherwise} \end{cases} \tag{1.3}$$

$t > 0$, since any $\Lambda \subset \mathbb{Z}^d$ connected by their links is T–connected. Note that T defines a bipartition of Λ: $x = (x_1, \cdots, x_d)$ belongs to $\mathcal{A}$ or $\mathcal{B}$ according to whether $x_1 + \cdots + x_d$ is an even or odd number.

Now we introduce some notations e definitions. Let

$$N_e = \sum_{x\in\Lambda} c_x^\dagger c_x \quad \text{and} \quad N_n = \sum_{x\in\Lambda} w_x \tag{1.4}$$

denote the total number of electrons and the total number of nuclei, respectively, and set $\mathcal{N} = N_e + N_n$. For each fixed configuration of nuclei $w = \{w_x\}_{x\in\Lambda}$ and N_e, $\mathcal{H}$ has a ground state energy $E(w, N_e)$. From this we define two other kinds of ground state energies:

$$E^{(2)}(N_n, N_e) = \min_{w:N_n \text{ fixed}} E(w, N_e) \tag{1.5}$$

and

$$E^{(1)}(\mathcal{N}) = \min_{N_n, N_e:\mathcal{N} \text{ fixed}} E^{(2)}(N_n, N_e)\ . \tag{1.6}$$

We shall also denote by w_Q, $Q \subset \Lambda$ the configuration of nuclei with $w_x = 1$ if $x \in Q$ and 0 otherwise.

Kennedy and Lieb [KL] have proven the following inequality

$$E^{(1)} \geq -\frac{1}{2}\,\mathrm{Tr}\left(T^2+U^2\right)^{1/2} + U\,\mathcal{N} - \frac{1}{2}U\,|\Lambda| \tag{1.7}$$

and concluded, from this, the following statements about the ground state of (1.1):

A. Let $(U,\mathcal{N})$ be such that $U>0$ and $\mathcal{N} \geq |\Lambda|$, with $|\Lambda|$ the number of sites in Λ. Then the ground state energy $E^{(1)}$ has a minimum value which saturates the inequality (1.7) at exactly the boundary $\mathcal{N}=|\Lambda|$. The ground state is doubly degenerated with the minimum of E attained at either $(w,N_e)=(w_{\mathcal{A}},|\mathcal{B}|)$ or $(w,N_e)=(w_{\mathcal{B}},|\mathcal{A}|)$.

B. Let $(U,\mathcal{N})$ be such that $U<0$ and $\mathcal{N} \leq 2\,|\mathcal{A}|$. Then the ground state energy $E^{(1)}$ has a minimum value given (1.7) at exactly the boundary $\mathcal{N}=2\,|\mathcal{A}|$. The minimum of $E^{(2)}$ is attained at $N_n=N_e=|\mathcal{A}|$. The ground state is unique unless $|\mathcal{A}|=|\mathcal{B}|=|\Lambda|/2$.

Remark 1.1 *Notice that, if $|\mathcal{A}| \neq |\mathcal{B}|$, the ground state energy has an asymmetric behavior when it passes from the* **A** *to the* **B** *condition These two ground state energies coincide with (1.7) at $\mathcal{N}=|\Lambda|$ only when $|\mathcal{A}|=|\mathcal{B}|=|\Lambda|/2$. In this situation the minimum of $E^{(2)}$ is attained at $N_n=N_e=|\Lambda|/2$. The ground state is doubly degenerated at the nuclei configuration $w_{\mathcal{A}}$ and $w_{\mathcal{B}}$. The point $N_e=|\Lambda|/2$ is called* half–filled band *because half of the available eigenstates of H are filled with electrons. Due to the fact that nucleus and electron have opposite charges, $N_n=N_e$ is often said to be the* neutral point *of $E^{(2)}$. It is also worth of attention that, when T is given by (1.3), the nuclei occupy alternate sites on the lattice forming a checker-board. We stress that* **A** *and* **B** *results are independent of the hopping matrix entries (irrespective to their signs and strengths) provided $t_{x,y}$ vanishes if x and y belongs to the same sub-lattice.*

Kennedy and Lieb [KL] have also proven existence of energy gap at half–filled band. They propose two gap definitions according to whether (1.6) or (1.5) is chosen as the ground state energy. Let $\mu(\mathcal{N}) := E^{(1)}(\mathcal{N}+1)-E^{(1)}(\mathcal{N})$ be the chemical potential and let

$$d^{(1)}(\mathcal{N}) := \mu(\mathcal{N})-\mu(\mathcal{N}-1) = E^{(1)}(\mathcal{N}+1)+E^{(1)}(\mathcal{N}-1)-2E^{(1)}(\mathcal{N}) \tag{1.8}$$

be the chemical potential discontinuity at $\mathcal{N}$. The system is said to have a *gap of the first kind* at $\mathcal{N}$ if there exist a constant $\varepsilon_1>0$, uniformly in Λ, such that $d^{(1)} \geq \varepsilon_1$. Analogously, the gap is said to be of *second kind* at (N_n,N_e) if

$$d^{(2)}(N_n,N_e) := E^{(2)}(N_n,N_e+1)+E^{(2)}(N_n,N_e-1)-2E^{(2)}(N_n,N_e) \geq \varepsilon_2 \tag{1.9}$$

for some constant $\varepsilon_2>0$, uniformly in Λ.

C. Let T be an irreducible matrix such that $\|T\| \leq \tau$ and $t_{x,y} \geq \delta$ for all non–vanishing entries, uniformly in Λ, for some constants $\tau<\infty$ and $\delta>0$. Under the conditions of item **A**, there is a first kind gap at $\mathcal{N}=|\Lambda|$ and second kind gaps at $(N_n,N_e)=(|\mathcal{A}|,|\mathcal{B}|)$ and at $(N_n,N_e)=(|\mathcal{B}|,|\mathcal{A}|)$ with $\varepsilon_2 \geq \varepsilon_1 > 0$ depending only on δ, τ, U.

D. Let T be as before. Under the conditions of item **B**, there are first kind gaps at $\mathcal{N} = 2\,|\mathcal{A}|$ and at $\mathcal{N} = 2\,|\mathcal{B}|$ and a second kind gaps at $(N_n, N_e) = (|\mathcal{A}|, |\mathcal{A}|)$ and at $(N_n, N_e) = (|\mathcal{B}|, |\mathcal{B}|)$ with $\varepsilon_2 \geq \varepsilon_1 > 0$ depending only on δ, τ, U.

The Falicov–Kimball model remains object of intense investigation. For a comprehensive survey of this model we quote a recent review by Gruber and Macris [GM] and references therein. Up to the present time, very few results about the ground state do not require half–filled band or neutral point condition. Other model restrictions which are frequently assumed concern with the spatial dimension d and the strength of interaction U. The model which has been investigated in more detail has T given by (1.3) with $\Lambda \subset \mathbb{Z}$ $(d = 1)$ (see [GM] for many intriguing questions on this). Also sufficiently large $|U|$ are assumed very often. There are not many results when T does not vanish at same sub-lattice.

In view of this scenario it seems worth to investigate one particular model where the eigenvalues and eigenvectors of H can be computed explicitly for all Λ. This program can be accomplished if the hopping matrix T has all non diagonal elements equal to a constant. We call this hopping matrix *mean field matrix* in analogy to what is usually called mean field in classical spin systems. We warn the reader that the Falicov–Kimball model with mean field hopping matrix cannot be confused with the mean field approximation of the Hubbard model.

The model Hamiltonian (1.1) with mean field hopping was introduced and solved by Farkasŏvsky [F], who called it simplified Hubbard model with unconstrained hopping of electrons. Its Hamiltonian is given by (1.1) or equivalently by (1.2) with the hopping matrix given by $(|\Lambda| = L)$

$$t_{x,y} = \frac{2\,t}{L} \tag{1.10}$$

for all $x, y \in \Lambda$ with $x \neq y$ and 0 otherwise.

Farkasŏvisky's solution of this model is obtained by a canonical transformation $\mathcal{U}$ that diagonalizes H. Unfortunately, there is no mention in reference [F] on how could $\mathcal{U}$ be computed. So, one of the purposes of this paper is to present a simple derivation of the eigenvalue problem of H.

What makes (1.10) solvable is the fact that the energy does not depend on the nuclei configuration $w = \{w_x\}_{x\in\Lambda}$:

$$E(w, N_e) = E^{(2)}(N_n, N_e) \tag{1.11}$$

since the probability of hopping from any site x to any other site y is evenly distributed. In view of this fact the model is not suitable to describe the positional order of nuclei induced by electrons (cristalization). However many questions about the ground state energy $E^{(1)}$, as a function of $\mathcal{N}$, can be formulated and answered. We believe that these answers expresses general features of the Falicov–Kimball model. We also believe that the solution of the eigenvalue problem can be useful in studying disordered systems.

Contrary to reference [F] we have made the hopping matrix size dependent ($t_{x,y} \to 0$ as $L \to \infty$) in order to guarantee the existence of thermodynamic limit. This simple fact allow us a complete description of the ground state for any value of the model parameters U, L and $\mathcal{N}$ (Farkasŏvsky discuss only the repulsive $U > 0$ case for finite L).

The following summarizes our analysis.

Theorem 1.2 *Let $\mathcal{H}$ be given by (1.1) with the hopping matrix T given by (1.10). Then, for $L > L_0$ with L_0 sufficiently large depending on U, we have:*

I. *If $U > 0$, the ground state energy $E^{(1)}$ is a monotone increasing function of $\mathcal{N}$ for all $0 < \mathcal{N} \leq 2L$. The minimum value of $E^{(2)}$ is attained at the following points:*

- *a. $(N_n, N_e) = (\mathcal{N} - 1, 1)$ if $0 < \mathcal{N} \leq \rho^* L$ with $\rho^* = \min(1/2 + 1/(4u), 1)$;*
- *b. $(N_n, N_e) = ([\rho^* L], \mathcal{N} - [\rho^* L])$ if $[\rho^* L] \leq \mathcal{N} \leq L$ ($[x]$ means the integer part of the number $x \in \mathbb{R}$);*
- *c. $(N_n, N_e) = (L, \mathcal{N} - L)$ if $L < \mathcal{N} \leq 2L$;*

Moreover, E^1 is constant in the domain $[\rho^* L] \leq \mathcal{N} \leq L$ (case b).

II. *If $U < 0$, the ground state energy $E^{(1)}$ is a monotone decreasing function of $\mathcal{N}$ for all $0 < \mathcal{N} \leq 2L$. Except by $1/L$ corrections, the minimum value of $E^{(2)}$ is attained at the neutral point $(N_n, N_e) = (\mathcal{N}/2, \mathcal{N}/2)$*

Remark 1.3 *Monotone behavior of the ground state energy $E^{(1)}$ seems, from our analysis, typical of the Falicov–Kimball model. This property would explain the minima tendency to be attained at the domain boundary in* **A** *and* **B** *results. The derivation of this property for nearest neighbor hopping matrix in $d = 1$ dimension is subject of a forthcoming paper [MB].*

Theorem 1.4 *Under the condition of Theorem 1.2, the mean–field Falicov–Kimball model has a first kind gap $d^{(1)} = 2U$ at the half–filled band $\mathcal{N} = L$, if $U > 0$ but no gap of first kind occurs if $U < 0$.*

In addition, there are three gaps of second kind at $(N_n, 1), (N_n, L - N_n)$ and $(N_n, L - N_n + 1)$ for all nuclei number $0 \leq N_n \leq L$ if $U > 0$ and at $(N_n, 1), (N_n, N_n)$ and $(N_n, N_n + 1)$, $0 \leq N_n \leq L$, if $U < 0$. The gap values are listed in (4.8) and (4.9).

Remark 1.5 *Absence of energy gap when $U < 0$ does not contradict Kennedy–Lieb's result. We note that the elements of the mean–field hopping matrix are not uniform in Λ. We also observe that this hopping matrix violates the bipartition condition required in item* **C**. *As we shall see, this condition does not affect our results on the gap which clearly indicate the existence of a phase transition.*

Finally, we illustrate the Kennedy–Lieb results state above with an exactly solvable model. Our lattice Λ may be arbitrarily decomposed into two sub-lattices $\mathcal{A}$ and $\mathcal{B}$. The model, called by us bipartite mean field, has non–vanishing hopping matrix elements $t_{x,y}$ equal to a constant if x, y connects the two sub–lattices. The Hamiltonian is thus given by (1.1) with

$$t_{x,y} = \begin{cases} \frac{2t}{L} & \text{if} \quad x, y \text{ is not in the same sub} - \text{lattice} \\ 0 & \qquad \text{otherwise} \end{cases} \tag{1.12}$$

The results of itens **A** – **D** may be appreciated in light of the eigenvalue problem for the present model. In particular, one sees that the equation (1.7) becomes equality if one of the the sub–lattices, let say $\mathcal{A}$, is constrained to be filled with nuclei ($|\mathcal{A}| = N_n$) for $0 \le \mathcal{N} \le 2L$ when $U < 0$ and for $|\mathcal{N}/L - 1| \ge 1/2$ when $U > 0$.

This paper is organized as follows. In Section 2 the eigenvalue problem of H with mean–field hopping matrix (1.10) is solved. Sections 3 and 4 give a complete description of the ground state energy and energy gaps for this particular model. This analysis is repeated for the bipartite mean–field model in Section 5. We finally draw some conclusions in the Section 6. Appendix A reviews some basic features about circulant matrices used in this text.

2 The Eigenvalue Problem

This section is devoted to the eigenvalue problem of the Schroedinger operator (1.2) with mean field hopping matrix (1.10).

For convenience, we write the interaction constant $U = t\,u$ and factorize $2\,t$ from the Hamiltonian matrix H. This factor is just a scale to the energy and may be fixed equal to 1 without any loss of generality. Equation (1.2) reads

$$H = -T + u\,W\ .$$

$H = H(w)$ is a $L \times L$ matrix with matrix elements $h_{x,y} = -1/L$ if $x \ne y$ and $h_{x,x} = u\,w_x$ which depends on the nuclei configuration w.

Now we claim that the spectrum of H given by the zeros of the characteristic polynomial

$$P(\lambda) = \det\left(H - \lambda\,\mathrm{I}\right) \tag{2.1}$$

is independent of the nuclei configuration.

To see this, let w and w' be two nucleus configurations differing by a permutation π, i.e., $w'_x = w_{\pi(x)}$. If Π denotes the permutation matrix determined by π, we have $\Pi^{-1}\,T\,\Pi = T$ and

$$H(w') = \Pi^{-1}\,H(w)\,\Pi\,. \tag{2.2}$$

Note that the nearest neighbor matrix T given by (1.3) is not invariant by the similarity transformation (2.2).

As a consequence of this fact $\det\left(H(w') - \lambda\,\mathrm{I}\right) = \det\left(H(w) - \lambda\,\mathrm{I}\right)$ and the eigenvalues of H depend only on the total number of nuclei N_n. We shall drop the subscript n of N_n in the sequel of this section.

To compute (2.1) let us pick the simplest matrix H. For any positive integers L and N, $L > N$, let J_1, J_2 and K be given by the following matrices

$$\begin{aligned} J_1 &= (u + 1/L)\ I_N - (1/L)\ 1\!\!1_N \\ J_2 &= (1/L)\,I_{L-N} - (1/L)\ 1\!\!1_{L-N} \\ K &= -(1/L)\ 1\!\!1_{N,L-N} \end{aligned} \tag{2.3}$$

where I_R is the identity matrix of size R, $1\!\!1_{R,S}$ is the $R \times S$ matrix with all elements equal to 1 and $1\!\!1_R = 1\!\!1_{R,R}$. We set

$$H_0 = \begin{pmatrix} J_1 & K \\ K^T & J_2 \end{pmatrix} . \tag{2.4}$$

Note that $H_0 = H(w_0)$ with the nuclei configuration $w_0 = (1, 1, \ldots, 1, 0, \ldots, 0)$.

In view of the above, the spectrum of $H(w)$ can be read from the spectrum of H_0 given as follows:

Proposition 2.1 *The spectrum of H_0 consists of the set $\{\lambda_1, \lambda_2, \lambda_+, \lambda_-\}$ where*

$$\begin{aligned} \lambda_1 &= 1/L \\ \lambda_2 &= 1/L + u \\ \lambda_\pm &= 1/L + \left[u - 1 \pm \Delta(N/L)\right]/2 \end{aligned} \tag{2.5}$$

with

$$\Delta(\rho) := \sqrt{(u+1)^2 - 4u\rho}\,, \tag{2.6}$$

have multiplicities $L - N - 1$, $N - 1$ and 1, respectively.

The corresponding eigenvectors $\mathbf{x} = (\mathbf{u}, \mathbf{v}) \in \mathbb{C}^N \times \mathbb{C}^{L-N}$ are $\mathbf{x}_{1,j} = (\mathbf{u}_{N,j}\,,\, \mathbf{0})$, $j = 1, \ldots, N-1$, $\mathbf{x}_{2,k} = (\mathbf{0}\,,\, \mathbf{u}_{L-N,k})$, $k = 1, \ldots, L-N-1$, and $\mathbf{x}_\pm = (\mathbf{1}\,,\, \mathbf{u}_\pm)$ where $\mathbf{0} = (0, \ldots, 0)$ is the zero–vector, $\mathbf{1} = (1, \ldots, 1)$ is the one–vector,

$$\mathbf{u}_\pm = \frac{u + 1 - 2N/L \pm \Delta(N/L)}{2(1 - N/L)}\,\mathbf{1} \tag{2.7}$$

and $\mathbf{u}_{R,j} = (1, \omega_R^j, \omega_R^{2j}, \ldots, \omega_R^{Nj})$, $j = 1, \ldots R-1$, with $\omega_R = e^{2\pi i/R}$.

The proof of Proposition 2.1 will follow from two lemmas. The first reduces the problem to matrices of the form $\alpha I + \beta\, 1\!\!1$. The second describes the properties of such matrices.

Lemma 2.2

$$\det\left(H_0 - \lambda I\right) = \det\left(J_1 - \lambda I\right) \cdot \det\left[\left(J_2 - \lambda I\right) - K^T \left(J_1 - \lambda I\right)^{-1} K\right] . \tag{2.8}$$

Proof. Let

$$M = \begin{pmatrix} A & K \\ K^T & B \end{pmatrix},$$

be such that A, B and K are $N \times N$, $(L-N) \times (L-N)$ and $N \times (L-N)$ matrices, respectively, with A symmetric and invertible. M can be brought to a block diagonal form by using a non–unitary transformation

$$\begin{pmatrix} A & 0 \\ 0 & B - K^T A^{-1} K \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -K^T A^{-1} & 1 \end{pmatrix} \begin{pmatrix} A & K \\ K^T & B \end{pmatrix} \begin{pmatrix} 1 & -A^{-1} K \\ 0 & 1 \end{pmatrix} . \tag{2.9}$$

Taking the determinant of both sides of equation (2.9) with $A = J_1 - \lambda I$ and $B = J_2 - \lambda I$ gives (2.2). □

Lemma 2.3 *1. The linear space $\mathcal{C}$ of all $R \times R$ matrices of the form $\alpha I + \beta \mathbb{1}$ is closed under sum, product and inverse operations.*

2. *The inverse of a matrix $C = \alpha I + \beta \mathbb{1}$ is given by*

$$C^{-1} = \frac{1}{\alpha} I - \frac{\beta}{\alpha(\alpha + \beta R)} \mathbb{1} \tag{2.10}$$

provided $\alpha \neq 0$ and $\alpha \neq -\beta R$.

3. *Any matrix $C = \alpha I + \beta \mathbb{1}$ can be reduced to a diagonal form*

$$F^{-1} C F = \mathrm{diag}\{\alpha + \beta R, \alpha, \ldots, \alpha\}$$

where F is the Fourier matrix

$$F_{k,l} := \frac{1}{\sqrt{R}} \omega_R^{(k-1)(l-1)} , \qquad k, l = 1, \ldots R$$

with $\omega_R = e^{2\pi i/R}$.

In other words, C has a simple eigenvalue $\lambda_1 = \alpha + \beta N$ corresponding to the eigenvector $\mathbf{1} = (1, 1, \ldots, 1)$ and a $(R-1)$–fold eigenvalue $\lambda_2 = \alpha$ associated to eigenvectors $\mathbf{u}_{R,j} = (1, \omega_R^j, \omega_R^{2j}, \ldots, \omega_R^{(R-1)j})$, $j = 1, \ldots, (R-1)$.

4. *$\det C = (\alpha + \beta R)\, \alpha^{R-1}$.*

The proof of Lemma 2.3 is in the Appendix A.

Proof of Proposition 2.1 We use Lemma 2.2 to reduce the calculation of the characteristic function $P_0(\lambda) = \det(H_0 - \lambda I)$ to algebraic calculations of matrices of $\mathcal{C}$.

Using item *1.* and *2.* of Lemma 2.3 and definitions (2.3), we have

$$(J_1 - \lambda I)^{-1} = \frac{1}{u + 1/L - \lambda} I_N + \frac{1/L}{(u + 1/L - \lambda)(u - (N-1)/L - \lambda)} \mathbb{1}_N$$

and, in view of $\mathbb{1}_{R,S}\, \mathbb{1}_{S,R} = S\, \mathbb{1}_R$,

$$K^T (J_1 - \lambda I)^{-1} K = \frac{N/L^2}{u - (N-1)/L - \lambda} \mathbb{1}_{L-N}$$

which gives

$$(J_2 - \lambda I) - K^T (J_1 - \lambda I)^{-1} K = (1/L - \lambda)\, I_{L-N} - \frac{(u + 1/L - \lambda)/L}{u - (N-1)/L - \lambda} \mathbb{1}_{L-N} . \tag{2.11}$$

We then use item *4.* of Lemma 2.3 and equations (2.3) and (2.11) to write

$$\det(J_1 - \lambda I) = (u - (N-1)/L - \lambda)\ (u + 1/L - \lambda)^{N-1} \tag{2.12}$$

and, with a little of algebra,

$$\det\Big((J_2-\lambda I)-K^T\left(J_1-\lambda I\right)^{-1}K\Big)=\frac{(1/L-\lambda)^{L-N-1}}{u-(N-1)/L-\lambda}\,R(\lambda) \tag{2.13}$$

where

$$\begin{aligned} R(\lambda) &= \lambda^2-(u-1-2/L)\lambda-u(L-N-1)/L-1/L+1/L^2 \\ &= (\lambda-\lambda_+)(\lambda-\lambda_-)\,. \end{aligned}$$

The eigenvalues of H_0 then follows from (2.12), (2.13) and Lemma 2.2.

The corresponding eigenvectors of H_0 can be obtained from item *3.* of Lemma 2.3. A vector $\mathbf{x}$ in $\mathbb{C}^L$ is written as $(\mathbf{u},\mathbf{v})$ where $\mathbf{u}\in\mathbb{C}^N$ and $\mathbf{v}\in\mathbb{C}^{L-N}$. Using Lemma 2.3 and the notation of Proposition 2.1, the eigenvectors corresponding to the λ_1 and λ_2 are, by inspection, given by $(\mathbf{u}_{N,j},\mathbf{0}), j=1,\ldots,N-1$ and $(\mathbf{0},\mathbf{u}_{L-N,k}), k=1,\ldots,L-N-1$, respectively. Notice $K\,\mathbf{u}_{N,j}=\mathbf{0}$ for all $j=1,\ldots,N-1$ in view of the property (A.7) in the Appendix A. By inspection also, one can verify that the eigenvectors corresponding to $\lambda_\pm$ are $(\mathbf{1},\mathbf{u}_\pm)$ with $\mathbf{u}_\pm$ given by (2.7).

This concludes the proof of Proposition 2.1. □

3 Ground States

For fixed nuclei configuration w, let $\mu_1\le\mu_2\le\cdots\le\mu_L$ be the sequence of ordered eigenvalues of (1.2), counting multiplicities, and let N_e be the total number of electrons in the system.

Due to the exclusion principle, each energy level (eigenvalues μ_j) can be occupied by at most one electron. In the ground state the first N_e lowest energy levels of H are occupied by electrons and the $L-N_e$ remaining levels are left empty. The ground state energy E of the model Hamiltonian (1.1) at (w,N_e) is thus determined by the sum of the lowest eigenvalues:

$$E(w,N_e):=\sum_{j=1}^{N_e}\mu_j\,. \tag{3.1}$$

We shall here prove Theorem 1.2 on the ground state energy $E^{(1)}$ of the Hamiltonian (1.1) with mean field hopping matrix (1.10) whose eigenvalues have been studied in the previous section.

Since we have proven the spectrum of H, $\sigma(H)=\{\lambda_1,\lambda_2,\lambda_+,\lambda_-\}$, depends only on the total number of nuclei, we have

$$E^{(2)}(N_n,N_e)=E(w,N_e)$$

for all w. Consequently, we shall only be concerned with the minimum value of $E^{(2)}$ for fixed number of particles $\mathcal{N}=N_n+N_e$.

Our discussion about ground state energy begins by the eigenvalues ordering. We observe that the spectrum $\sigma(H)$ depends on the nuclei density $\rho_n=N_n/L$ through the function

$$\Delta^2(\rho):=(u+1)^2-4\,u\,\rho \tag{3.2}$$

which, in view of $0 \le \rho \le 1$, satisfies

$$(|u|-1)^2 \le \Delta^2 \le (|u|+1)^2 \ .$$

Since $\lambda_\pm = 1/L + (u-1 \pm \Delta)/2$, this implies

$$1/L + (u-1+|\,|u|-1\,|)\,/2 \le \lambda_+ \le 1/L + (u+|u|)\,/2$$

and

$$\lambda_- \le 1/L + (u-1-|\,|u|-1\,|)\,/2$$

from which the eigenvalues ordering follows.

We distinguish two cases:

I. if $u > 0$ we have

$$\lambda_- \le \lambda_1 \le \lambda_+ \le \lambda_2\,;$$

II. if $u < 0$ we have

$$\lambda_- \le \lambda_2 \le \lambda_+ \le \lambda_1\,.$$

Proof of part **I** *of Theorem 1.2.* Let $u > 0$ and $\mathcal{N} \le L$. In this case we have

$$\mu_1 = \lambda_- \ , \ \ \mu_2 = \cdots = \mu_{L-N_n} = \lambda_1 \ , \ \ \mu_{L-N_n+1} = \lambda_+ \ , \ \ \mu_{L-N_n+2} = \cdots = \mu_L = \lambda_2 \tag{3.3}$$

and the ground state energy is thus given by

$$\begin{aligned} E^{(2)}(N_n, N_e) &= \lambda_- + (N_e - 1)\,\lambda_1 \\ &= \lambda_- + (\mathcal{N} - N_n - 1)\,\lambda_1 \\ &= \mathcal{N}/L + g(\rho_n) \end{aligned} \tag{3.4}$$

where

$$g(\rho) := \frac{1}{2}\,(u - 1 - \Delta(\rho)) - \rho \tag{3.5}$$

and Δ as in (3.2). We remind that, under the condition $\mathcal{N} \le L$, the multiplicity $L - N_n - 1$ of λ_1 is greater than or equal to the number of electrons $N_e - 1$. This explain why we have taken only two eigenvalues in (3.4).

Equation (3.4) and (3.5) reduces the problem of minimizing $E^{(2)}(N_n, N_e) = E^{(2)}(N_n, \mathcal{N} - N_n)$ with respect to N_n to the problem of minimizing g as a function of ρ_n. The function $g : [0,1] \to \mathbb{R}$ has the following properties:

1. $g(\rho) \le g(0) = -1$ with $g(1) = -1$ if $u \ge 1$;
2. g attains to a unique minimum value at

   $$\rho^* = \min\left(\frac{1}{2} + \frac{1}{4\,u}, 1\right)\ ;$$

   (note that $\rho^* = 1$ if $u \le 1/2$);

3. the minimum value is given by

$$g(\rho^*) = \begin{cases} u-2 & \text{if} \quad 0<u<1/2 \\ -1-1/(4\,u) & \text{if} \quad u \geq 1/2\,, \end{cases} \tag{3.6}$$

Items $1,2$ and 3 can be obtained explicitly. Note that the derivative

$$g'(\rho) = \frac{u}{\Delta(\rho)} - 1 \tag{3.7}$$

vanishes only at ρ^* provided $u \geq 1/2$. If $u < 1/2$, g attains its minimum value at the domain boundary $\rho = 1$.

¿From equation (3.4) and properties $1,2$ and 3 we conclude that the ground state $E^{(1)}(\mathcal{N})$ has only one eigenvalue λ_- occupied by one electron if $\mathcal{N} \leq \rho^* L$ and there will be more electrons contributing to the ground state if $\mathcal{N} > \rho^* L$. Note that $\lambda_- = \lambda_-(\rho_n)$ is negative if $\rho_n \leq \rho^*$ provided $L > 2$. This follows from the fact that $\lambda_-(\rho_n) \leq \lambda_-(\rho^*) = 1/L + (u-1-\Delta(\rho^*))/2 = 1/L - 1/2$ since, from (3.7), $\Delta(\rho^*) = u$. We shall always assume L sufficiently large.

In summary,

$$E^{(1)}(\mathcal{N}) = \begin{cases} \lambda_-\left((\mathcal{N}-1)/L\right) & \text{if} \quad \mathcal{N} < \rho^* L \\ \mathcal{N}/L + g\left([\rho^* L]/L\right) & \text{if} \quad \rho^* L \leq \mathcal{N} \leq L \end{cases} \tag{3.8}$$

where $[x]$ means the closest integer of $x \in \mathbb{R}$. We emphasize that $E^{(1)}(\mathcal{N})$ is a monotone increasing function of $\mathcal{N}$, since λ_- is a monotone increasing function of the nuclei number, and piecewise constant if $\rho^* L \leq \mathcal{N} \leq L$.

Now, let $u > 0$ and $\mathcal{N} > L$. The ground state energy $E^{(2)}(N_n, N_e)$ in this case is given by

$$\begin{aligned} E^{(2)}(N_n, N_e) &= \lambda_- + (L - N_n - 1)\,\lambda_1 + \lambda_+ + (N_e - (L - N_n + 1))\,\lambda_2 \\ &= \lambda_- + (L - N_n - 1)\,\lambda_1 + \lambda_+ + (\mathcal{N} - L - 1)\,\lambda_2 \\ &= (\mathcal{N} - N_n)/L + (\mathcal{N} - L)u - 1 \end{aligned} \tag{3.9}$$

which attains to a minimum value at $(N_n, N_e) = (L, \mathcal{N} - L)$ corresponding to the maximal nuclear occupation. We thus have

$$E^{(1)}(\mathcal{N}) = (\mathcal{N} - L)(1/L + u) - 1 \tag{3.10}$$

for $L < \mathcal{N} \leq 2L$. The combination of (3.8) and (3.10) leads to a monotonic increasing ground state energy $E^{(1)}$ as a function of $\mathcal{N}$ in the whole domain.

This concludes the analysis of the case **I**. □

Proof of part **II** *of Theorem 1.2.* Here, we have

$$\mu_1 = \lambda_-\,, \quad \mu_2 = \cdots = \mu_{N_n} = \lambda_2\,, \quad \mu_{N_n+1} = \lambda_+\,, \quad \mu_{N_n+2} = \cdots = \mu_L = \lambda_2\,. \tag{3.11}$$

We shall divide our analysis in two sub-cases. Let $u < 0$ and $N_e \leq N_n$. In view of the eigenvalue ordering, we have

$$\begin{aligned} E^{(2)}(N_n, N_e) &= \lambda_- + (N_e - 1)\,\lambda_2 \\ &= \lambda_- + (\mathcal{N} - N_n - 1)\,\lambda_2 \\ &= \mathcal{N}/L + u(\mathcal{N} - 1) + h(\rho_n) \end{aligned} \tag{3.12}$$

where

$$h(\rho) = g(\rho) - uL\rho \,. \tag{3.13}$$

Once again, the problem of minimizing $E^{(2)}(N_n, N_e)$ under the condition $N_e \leq N_n$ is reduced to the problem of minimizing h in the domain $1/L \leq \rho \leq 1$. Note that the lower limit $1/L$ is due to the fact the equation (3.9) is valid only if $1 \leq N_e \leq \rho_n L$. The following description of h gives the answer to this problem.

Proposition 3.1 *Given $u < 0$, there is $L_0 = L_0(u)$ such that, for all $L > L_0$, $h : [1/L, 1] \to \mathbb{R}$ given by (3.13) is a strictly monotone increasing function of ρ.*

Proof. Proposition 3.1 is implied if $h'(\rho) > 0$ for all ρ in $[1/L, 1]$. From (3.13) and (3.7) this is implied by

$$\frac{u}{\Delta(\rho)} > uL + 1 \,. \tag{3.14}$$

To show that condition (3.14) holds for any value $u \in (-\infty, 0)$, we must break this open interval into three pieces: $(-\infty, -1-1/L) \cup (-1-1/L, -1+1/L) \cup (-1+1/L, -1/L)$. Note that we have to take L large in order get u arbitrarily close to 0. This leads to $L > -1/u$.

Let us assume $-1 + 1/L < u < -1/L$. Using the inequality $\Delta(\rho) > u + 1$, equation (3.14) can be replaced by a more restrictive condition

$$\frac{u}{u+1} > uL + 1 \,.$$

This is equivalent to $L\,u^2 + L\,u + 1 = L\,(u + 1 - 1/L)(u + 1/L) < 0$ which is always true for $u \in (-1 + 1/L, -1/L)$.

Suppose now $u < -1 - 1/L$. Then we analogously use $\Delta(\rho) > -(u + 1)$ to replace (3.14) by a more restrictive condition

$$L\,u^2 + (L + 2)\,u + 1 > 0 \,. \tag{3.15}$$

Since the roots $u = -1/2 - 1/L \pm [1/4 + 1/L^2]^{1/2}$ of the quadratic equation are close to -1 and 0, (3.15) is always satisfied if $u < -1/2 - 1/L - [1/4 + 1/L^2]^{1/2} < -1 - 1/L$.

It remains to verify condition (3.14) for $-1 - 1/L < u < -1 + 1/L$. In this case we use $\rho > 1/L$ to replace (3.14) by

$$\frac{u}{\Delta(1/L)} = \frac{u}{\sqrt{(u+1)^2 - 4u/L}} > uL + 1 \,. \tag{3.16}$$

Since $u = \mathcal{O}(1)$ and $(u+1) = \mathcal{O}(1/L)$, the left hand side of this inequality is $\mathcal{O}\left(\sqrt{L}\right)$ and the right hand side $\mathcal{O}\,(L)$. Recall $u \leq -1/L$ and both sides of (3.16) are negative. Therefore, we can always find L sufficiently large so that condition (3.14) is verified concluding the proof of the Proposition. □

Proposition 3.1 implies that the ground state energy $E^{(2)}$ under the condition $N_e \leq N_n$ has a minimum value at $N_n = N_e = \mathcal{N}/2$ given by

$$E^{(1)}_{<}(\mathcal{N}) = \mathcal{N}/L + u(\mathcal{N} - 1) + h(\mathcal{N}/(2L)) \tag{3.17}$$

Finally, let us consider $u<0$ and $N_e > N_n$. The ground state energy in this case is given by

$$\begin{aligned} E^{(2)}(N_n, N_e) &= \lambda_- + (N_n-1)\,\lambda_2 + \lambda_+ + (N_e - N_n - 1)\lambda_1 \\ &= \mathcal{N}/L - 1 + (Lu-1)N_n/L \end{aligned} \tag{3.18}$$

Since $E^{(2)}(N_n, \mathcal{N}-N_n)$ is a monotone decreasing function of $\rho_n = N_n/L$, it attains to a minimum value at $N_n = N_e - 1 = \mathcal{N} - N_n - 1$ given by

$$E^{(1)}_{>}(\mathcal{N}) = \mathcal{N}/L - 1 + (Lu-1)(\mathcal{N}-1)/(2L)\,. \tag{3.19}$$

The ground state for the case **II** is thus given by

$$\begin{aligned} E^{(1)}(\mathcal{N}) &= \min\left(E^{(1)}_{<}(\mathcal{N})\,,\, E^{(1)}_{>}(\mathcal{N})\right) \\ &= \frac{u}{2}(\mathcal{N}-1) + \frac{\mathcal{N}}{2L} - \frac{m}{2} \end{aligned} \tag{3.20}$$

where $m := \max\left(2 - 1/L, 1 + \Delta(\mathcal{N}/(2L))\right)$.

Note that $E^{(1)}$ is a monotone decreasing function of $\mathcal{N}$ if L is sufficiently large. We point out that the minimum of $E^{(2)}$ is attained at approximately neutral (symmetric) point $N_n + \mathcal{O}(1/L) = N_e + \mathcal{O}(1/L) = \mathcal{N}/2$ for all values of $u<0$ and $0 \le \mathcal{N} \le 2L$.

This concludes the proof of Theorem 1.2. □

4 Gaps

Let $\{e_L(\rho)\}_{L\ge 0}$ be the sequence of ground state energy density functions defined by

$$e_L(\rho) = \frac{E^{(1)}(\rho\, L)}{L} \tag{4.1}$$

and let $e(\rho) = \lim_{L\to\infty} e_L(\rho)$ be its thermodynamic limit.

¿From our previous analysis, the ground state energy $E^{(1)}$ can be written in the form (see equations (3.8), (3.10) and (3.20))

$$E^{(1)}(\rho\, L) = a_0(u,\rho,L) + a_1(u,\rho) + a_2(u,\rho)\, L \tag{4.2}$$

where, for fixed u, a_0, a_1 and a_2 are bounded functions of $\rho \in [0,2]$ with $a_0 \to 0$ as $L \to \infty$.

Hence, given two positive integer numbers L, M, $L < M$,

$$\left|\frac{E^{(1)}(\rho\, L)}{L} - \frac{E^{(1)}(\rho\, M)}{M}\right| \le \left|\frac{a_0(L)}{L} - \frac{a_0(M)}{M}\right| + a_1\left|\frac{1}{L} - \frac{1}{M}\right| \le C\frac{1}{L} \tag{4.3}$$

for some constant $C = C(u) < \infty$, uniformly on L, and this shows that $\{e_L\}_{L\ge 0}$ forms a Cauchy sequence which converges to $e(\rho)$.

It also follows from (3.8), (3.10) and (3.20) that:

a. if $u > 0$, we have

$$e(\rho) = \begin{cases} 0 & \text{if} \quad 0 \le \rho \le 1 \\ (\rho - 1)u & \text{if} \quad 1 < \rho \le 2\,. \end{cases} \tag{4.4}$$

(Note that $a_2 = 0$ when $0 \le \rho \le 1$);

b. if $u < 0$, we have $e(\rho) = u\,\rho/2$ for all $0 \le \rho \le 2$.

By a similar computation, one can show that the sequence of chemical potentials $\{\mu_L(\rho)\}_{L\ge 0}$ given by

$$\mu_L(\rho) := E^{(1)}(\rho\, L + 1) - E^{(1)}(\rho\, L) = \frac{e_L(\rho + 1/L) - e_L(\rho)}{1/L} \tag{4.5}$$

converges to the derivative of the ground state energy density $e'(\rho)$ for all $\rho \in [0,1) \cap (1,2]$ provided $u > 0$. As a consequence, there exists a positive gap of first kind at $\rho = 1$:

$$\lim_{\rho \searrow 1} \mu(\rho) - \lim_{\rho \nearrow 1} \mu(\rho) = u\,. \tag{4.6}$$

For $u < 0$ the sequence of chemical potentials $\{\mu_L(\rho)\}_{L\ge 0}$, converges to $e'_L(\rho) = u/2$ for all $\rho \in [0,2]$ and there is no first kind gap in this regime.

Now, let us consider the second kind gap. From the definitions (1.9) and (3.1) we have

$$d^{(2)}(N_n, N_e) = \mu_{N_e+1} - \mu_{N_e} \tag{4.7}$$

(For this, recall (1.11)).

For $u > 0$, it follows from the equation (3.3) several cases:

$$\begin{array}{llcll} 1. & d^{(2)}(N_n, 1) & = & \dfrac{-u + 1 + \Delta(\rho_n)}{2} & \\ 2. & d^{(2)}(N_n, N_e) & = & 0 & \text{if} \quad 1 < N_e < L - N_n \\ 3. & d^{(2)}(N_n, L - N_n) & = & \dfrac{u - 1 + \Delta(\rho_n)}{2} & \\ 4. & d^{(2)}(N_n, L - N_n + 1) & = & \dfrac{u + 1 - \Delta(\rho_n)}{2} & \\ 5. & d^{(2)}(N_n, N_e) & = & 0 & \text{if} \quad N_e > L - N_n + 1 \end{array} \tag{4.8}$$

We thus find three gaps for $u > 0$: second kind gaps occur at $N_e = 1, L - N_n$ and $L - N_n + 1$ for each $0 \le N_n \le L$.

For $u < 0$ equation (3.11) gives the following:

$$\begin{array}{llcll} 1. & d^{(2)}(N_n, 1) & = & \dfrac{u + 1 + \Delta(\rho_n)}{2} & \\ 2. & d^{(2)}(N_n, N_e) & = & 0 & \text{if} \quad 1 < N_e < N_n \\ 3. & d^{(2)}(N_n, N_n) & = & \dfrac{-u - 1 + \Delta(\rho_n)}{2} & \\ 4. & d^{(2)}(N_n, N_n + 1) & = & \dfrac{-u + 1 - \Delta(\rho_n)}{2} & \\ 5. & d^{(2)}(N_n, N_e) & = & 0 & \text{if} \quad N_e > N_n + 1 \end{array} \tag{4.9}$$

¿From these we find that, for $u<0$, second kind gaps occur at $N_e=1, N_n$ and N_n+1 for each $0\le N_n\le L$ and this concludes the proof of Theorem 1.4. $\square$

5 Bipartite Mean Field Model

We shall briefly in this section analyze the ground state of the Hamiltonian $\mathcal{H}$ with bipartite mean–field hopping matrix T given by (1.12).

We begin by solving the eigenvalue problem. Let us decompose the vector space $\mathbb{C}^L$, $L=|\Lambda|$, into two subspace $\mathbb{C}^N$ and $\mathbb{C}^M$ corresponding to each sub-lattice $\mathcal{A}$ and $\mathcal{B}$ where $N=|\mathcal{A}|$ and $M=|\mathcal{B}|$. The nuclei occupation number in a sub–lattice $\mathcal{X}\subset\Lambda$ will be denoted by $n_{\mathcal{X}}$. We shall frequently write $n=n_{\mathcal{A}}$ and $m=n_{\mathcal{B}}$. From these notations we have $L=N+M$ and $N_n=n+m$.

The Hamiltonian $H=H(w)$, acting on $\mathbb{C}^L$, can thus be written as a block matrix

$$H=\begin{pmatrix} J_{\mathcal{A}} & K \\ K^T & J_{\mathcal{B}} \end{pmatrix} \tag{5.1}$$

where $J_{\mathcal{X}}=u\,\mathrm{diag}\{w_x, x\in\mathcal{X}\}$, $\mathcal{X}=\mathcal{A},\mathcal{B}$ and $K=-(1/L)\,1\!\!1_{N,M}$.

As before, we can find a permutation matrix Π such that $H_0=\Pi^{-1}H\Pi$ has the diagonal block matrices $J_{\mathcal{X}}$ of the form $\mathrm{diag}\{u,\ldots,u,0,\ldots,0\}$. Hence, in view of Lemmas 2.2 and 2.3, the characteristic polynomial $P(\lambda)$ of H_0 is given by

$$P(\lambda)=\det\left(H_0-\lambda I\right)=\det A\,\det C \tag{5.2}$$

where $A=(J_{\mathcal{A}}-\lambda I)$ and $C=(J_{\mathcal{B}}-\lambda I)-K^T\,(J_{\mathcal{A}}-\lambda I)^{-1}\,K$, can be written as

$$C=\begin{pmatrix} E & G \\ G^T & F \end{pmatrix} \tag{5.3}$$

with

$$\begin{aligned} E &= (u-\lambda)\,I_m-\alpha\,1\!\!1_m \\ F &= -\lambda\,I_{M-m}-\alpha\,1\!\!1_{M-m} \\ G &= -\alpha\,1\!\!1_{m,M-m} \end{aligned} \tag{5.4}$$

and

$$\alpha=\frac{1}{L^2}\frac{(u-\lambda)\,N-u\,n}{\lambda\,(u-\lambda)}\,. \tag{5.5}$$

We now repeat the calculation given in the proof of Proposition 2.1. Once again, by Lemmas 2.2 and 2.3

$$\det C=\det E\,\det H \tag{5.6}$$

where

$$\begin{aligned} H &= F-G^{-1}E^{-1}G \\ &= -\lambda\,I_{M-m}-\frac{\alpha(u-\lambda)}{u-\lambda-\alpha\,m}\,1\!\!1_{M-m} \end{aligned} \tag{5.7}$$

Putting all pieces together, by using item *4* of Lemma 2.3 we have

$$\begin{array}{rcl} \det A & = & (u-\lambda)^n\,(-\lambda)^{N-n} \\ \det E & = & (u-\lambda)^{m-1}\,(u-\lambda-\alpha\, m) \\ \det H & = & -(-\lambda)^{M-m-1}\,\dfrac{\lambda(u-\lambda)+\alpha[u(M-m)-\lambda\, M]}{u-\lambda-\alpha\, m}\,. \end{array} \tag{5.8}$$

The characteristic polynomial $P(\lambda) = \det A\, \det E\, \det H$ can thus be written as

$$P(\lambda) = (u-\lambda)^{N_n-2}\,(-\lambda)^{L-N_n-2}\,S(\lambda) \tag{5.9}$$

(recall $L = N+M$ and $N_n = n+m$) with

$$S(\lambda) = \lambda^2\,(u-\lambda)^2 - \left(\frac{N}{L}\lambda - \frac{N-n}{L}\,u\right)\left(\frac{M}{L}\lambda - \frac{M-m}{L}\,u\right)\,. \tag{5.10}$$

We have proven the following

Proposition 5.1 *The spectrum of H given by (5.1) is the set $\{\lambda_1, \lambda_2, \lambda_{+,+}, \lambda_{+,-}, \lambda_{-,+}, \lambda_{-,-}\}$ where $\lambda_1 = 0$, $\lambda_2 = u$ and $\lambda_{\pm,\pm}$, the four solutions of the equation $S(\lambda) = 0$, have multiplicities $L-N_n-2$, N_n-2 and 1, respectively.*

Remark 5.2 *Although the eigenvalues $\lambda_{\pm,\pm}$ can be evaluated analytically, their expressions are too large to be useful. Numerical computation indicates that for any values of parameters $\rho := N/L$, $\eta_{\mathcal{A}} := n/L$ and $\eta_{\mathcal{B}} := m/L$ in the interval $(0,1/2)$, we have the following ordering*

$$\begin{array}{ll} \lambda_{-,-} < \lambda_1 < \lambda_{+,-} < \lambda_{-,+} < \lambda_2 < \lambda_{+,+} & \text{if} \quad u>0 \\ \lambda_{-,-} < \lambda_2 < \lambda_{+,-} < \lambda_{-,+} < \lambda_1 < \lambda_{+,+} & \text{if} \quad u<0 \end{array} \tag{5.11}$$

The solutions of $S(\lambda) = 0$ can be easily found if two roots are equal to 0 and u. This equation can be easily solved also when the second term of the right hand side of (5.10) is a square of a linear function of λ times a constant. We shall consider three choices of parameters having these properties:

Example 5.3 *1. If $\rho \le 1/2$ ($N \le M$), $\eta_{\mathcal{A}} = \rho = N_n/L$ ($n = N$) and $\eta_{\mathcal{B}} = 0$ ($m = 0$), the characteristic polynomial*

$$S(\lambda) = \lambda\,(\lambda-u)\,(\lambda\,(\lambda-u)+\rho(1-\rho))$$

has the following roots: $\lambda_{+,-} = \lambda_1 = 0$, $\lambda_{-,+} = \lambda_2 = u$, $\lambda_{-,-} = \lambda_-$ and $\lambda_{+,+} = \lambda_+$ where

$$\lambda_\pm = \frac{u}{2} \pm \sqrt{\left(\frac{u}{2}\right)^2 + \rho(1-\rho)} \tag{5.12}$$

2. *If $\rho = 1/2$ ($N = M = L/2$) and $\eta_{\mathcal{A}} = \eta_{\mathcal{B}} \equiv \eta = N_n/(2L)$ ($n = m$), we have*

$$S(\lambda) = \lambda^2(\lambda - u)^2 - (\lambda/2 - (1/2 - \eta)u)^2$$

which gives

$$\begin{aligned} \lambda_{+,\pm} &= (u + 1/2 \pm \Delta_+)/2 \\ \lambda_{-,\pm} &= (u - 1/2 \pm \Delta_-)/2 \end{aligned} \tag{5.13}$$

where

$$\Delta_\pm(\eta) = \sqrt{(u \mp 1/2)^2 \pm 4\, u\, \eta} \tag{5.14}$$

3. *If $\rho = N/L$, $\eta_{\mathcal{A}} = \rho/2$ ($n = N/2$) and $\eta_{\mathcal{B}} = (1-\rho)/2$ ($m = M/2$), we have*

$$S(\lambda) = \lambda^2(\lambda - u)^2 - \rho(1-\rho)\,(\lambda - u/2)^2$$

which has the following roots

$$\lambda_{\pm,\pm} = \frac{u \pm \Theta_\pm}{2} \tag{5.15}$$

where $\Theta_\pm = \Theta_\pm(\rho)$ is given by

$$\Theta_\pm^2 = u^2 + 2\rho(1-\rho) \pm 2\sqrt{\rho^2(1-\rho)^2 + u^2\rho(1-\rho)} \tag{5.16}$$

(Note that here $N_n = n + m = L/2$)

For comparison with the variational method used by Lieb–Kennedy and with the results stated in Section 3, we shall compute the ground state energy with these eigenvalues. Our analysis here, opposed to the previous sections, will be brief and very selective.

Let N, M, n and m be as in the Example 5.3.1. In this case we have $\lambda_- \leq \lambda_1 \leq \lambda_2 \leq \lambda_+$ if $u > 0$ and $\lambda_- \leq \lambda_2 \leq \lambda_1 \leq \lambda_+$ if $u < 0$.

Proceeding as in the Section 3, the ground state energy $E^{(2)}$ at (N_n, N_e) is given by

I. For $u > 0$,

a. if $\mathcal{N} = N_n + N_e \leq L$, we have

$$\begin{aligned} E^{(2)}(N_n, N_e) &= \lambda_-(\rho) + (N_e - 1)\lambda_1 \\ &= \lambda_-(\rho) \end{aligned} \tag{5.17}$$

where $\rho = N/L = N_n/L$;

b. if $\mathcal{N} > L$, we have

$$\begin{aligned} E^{(2)}(N_n, N_e) &= \lambda_-(\rho) + (N_e - L + N_n)\,\lambda_2 \\ &= \lambda_-(\rho) + (\mathcal{N} - L)\,u \end{aligned} \tag{5.18}$$

Now, the ground state $E^{(2)}$ will be minimized with respect to (N_n, N_e) with $\mathcal{N} = N_n + N_e$ fixed. Note that the eigenvalue λ_-, given by (5.12), is a monotone decreasing function of ρ in $0 \leq \rho \leq 1/2$ and a monotone increasing function in $1/2 \leq \rho \leq 1$ for all $u \in \mathbb{R}$. This gives

c. if $\mathcal{N} \leq L$,

$$E^{(1)}(\mathcal{N}) = \lambda_-(\rho^*) \tag{5.19}$$

where $\rho^* = \min((\mathcal{N}-1)/L, 1/2)$;

d. if $\mathcal{N} > L$

$$E^{(1)}(\mathcal{N}) = \lambda_-(\hat{\rho}) + (\mathcal{N} - L)\, u \tag{5.20}$$

where $\hat{\rho} = \max(1/2, \mathcal{N}/L - 1)$.

The minimum is attained at $(N_n, N_e) = (\mathcal{N}-1, 1)$ if $\mathcal{N} < L/2$, $(N_n, N_e) = (L/2, \mathcal{N} - L/2)$ if $L/2 \leq \mathcal{N} \leq 3L/2$ and at $(N_n, N_e) = (\mathcal{N} - L, L)$ if $\mathcal{N} > 3L/2$. As the number of sites at the sub–lattice $\mathcal{A}$ coincide with the number of nucleus, $|\mathcal{A}| = N = N_n$, the minimum value of $E^{(2)}$ is attained at the partition of Λ into two evenly divided sub–lattices, $|\mathcal{A}| = |\mathcal{B}|$, for $L/2 \leq \mathcal{N} \leq 3L/2$. We recall that the sub–lattice $\mathcal{A}$ is completely occupied by nuclei and the sub–lattice $\mathcal{B}$ is empty in this example.

II. For $u < 0$, we have

a. if $N_e \leq N_n$,

$$E^{(2)}(N_n, N_e) = \lambda_-(\rho) + (N_e - 1)\, u \tag{5.21}$$

b. if $N_e > N_n$,

$$E^{(2)}(N_n, N_e) = \lambda_-(\rho) + (N_n - 1)\, u \tag{5.22}$$

Since the minimum of $E^{(2)}$ occurs at $N_n = N_e = \mathcal{N}/2$, this gives

$$E^{(1)}(\mathcal{N}) = -\lambda_+(\mathcal{N}/(2L)) + \mathcal{N}/2\, u \tag{5.23}$$

$\square$

Let N, M, n and m be as in the Example 5.3.2. Using the fact that, for $u > 0$,

$$|u - 1/2| \leq \Delta_\pm \leq u + 1/2 \tag{5.24}$$

and Proposition 5.1, we have $\mu_1 = \lambda_{-,-}$, $\mu_2 = \cdots = \mu_{L-N_n-1} = 0$, $\mu_{L-N_n} = \lambda_{+,-}$, $\mu_{L-N_n+1} = \lambda_{-,+}$, $\mu_{L-N_n+2} = \cdots = \mu_{L-1} = u$ and $\mu_L = \lambda_{+,+}$.

We also have

$$|u + 1/2| \leq \Delta_\pm \leq 1/2 - u\ ,$$

if $u < 0$, which gives $\mu_1 = \lambda_{-,-}$, $\mu_2 = \cdots = \mu_{N_n-1} = u$, $\mu_{N_n} = \lambda_{+,-}$, $\mu_{N_n+1} = \lambda_{-,+}$, $\mu_{N_n+2} = \cdots = \mu_{L-1} = 0$ and $\mu_L = \lambda_{+,+}$.

Observe that $\lambda_{+,-} \leq \lambda_{-,+}$ for any $u \in \mathbb{R}$ and $0 \leq \eta \leq 1/2$ because

$$\Delta_+ + \Delta_- \geq \left\{2(u^2+1/4) + 2|u^2-1/4|\right\}^{1/2} \geq 1\,.$$

Proceeding as in the Section 3, the ground state energy $E^{(2)}$ at (N_n, N_e) is given by

I. For $u > 0$, we have

a. if $\mathcal{N} = N_n + N_e \leq L$, with $N_e \neq L$,

$$\begin{aligned} E^{(2)}(N_n,N_e) &= \lambda_{-,-}(\eta) + (N_e-1)\lambda_1 \\ &= (u - 1/2 - \Delta_-(\eta))/2 \end{aligned} \tag{5.25}$$

(recall $\eta \equiv N_n/(2L)$);

b.

$$E^{(2)}(0,L) = \lambda_{-,-}(0) + \lambda_{+,-}(0) = -\frac{1}{2}\,; \tag{5.26}$$

c. if $\mathcal{N} = N_n + N_e > L$,

$$\begin{aligned} E^{(2)}(N_n,N_e) &= \lambda_{-,-}(\eta) + \lambda_{+,-}(\eta) + \lambda_{-,+}(\eta) + (N_e - L + N_n - 1)\,u \\ &= (u - 1/2 - \Delta_+(\eta))/2 + (\mathcal{N} - L)\,u \end{aligned} \tag{5.27}$$

We note, from definition (5.14), that Δ_σ is a *monotone increasing function* of η if $u > 0$ and $\sigma = +$ (*or* if $u < 0$ and $\sigma = -$). On the other hand, Δ_σ is a *monotone decreasing function* of η if $u > 0$ and $\sigma = -$ (*or* if $u < 0$ and $\sigma = +$). Minimizing $E^{(2)}$ with respect to (N_n, N_e) with $\mathcal{N} = N_n + N_e$ fixed, gives

d.

$$E^{(1)}(\mathcal{N}) = (u - 1/2 - \Delta_-(0))/2 = -1/2 \tag{5.28}$$

if $\mathcal{N} \leq L$ and

e.

$$\begin{aligned} E^{(1)}(\mathcal{N}) &= (u - 1/2 - \Delta_+(1/2))/2 + (\mathcal{N} - L)\,u \\ &= -1/2 + (\mathcal{N} - L)\,u \end{aligned} \tag{5.29}$$

if $\mathcal{N} > L$.

Note that the minimum is attained at $(N_n, N_e) = (0, \mathcal{N})$ if $\mathcal{N} \leq L$ and at $(N_n, N_e) = (L, \mathcal{N} - L)$ if $\mathcal{N} > L$. In other words, the ground state has no nucleus occupying the lattice sites of Λ if $\mathcal{N} \leq L$ and Λ is fully occupied by nuclei if $\mathcal{N} > L$.

II. For $u < 0$, we have

a. if $N_e \leq N_n$,

$$\begin{aligned} E^{(2)}(N_n,N_e) &= \lambda_{-,-}(\eta) + (N_e - 1)\,u \\ &= -(u + 1/2 + \Delta_-(\eta))/2 + (\mathcal{N} - N_n)\,u \end{aligned} \tag{5.30}$$

b. if $N_e > N_n$,

$$\begin{aligned} E^{(2)}(N_n, N_e) &= \lambda_{-,-}(\eta) + (N_n - 2)\, u + \lambda_{+,-}(\eta) + \lambda_{-,+}(\eta) \\ &= -(u + 1/2 + \Delta_+(\eta))/2 + N_n\, u \end{aligned} \tag{5.31}$$

To minimize $E^{(2)}$ in this case one has to deal with two contributions to the ground state energy. Note in the equations (5.30) and (5.31) that there is one term depending on $\eta = N_n/(2L)$ and other depending on N_n. As N_n varies, these two contributions moves the ground state energy into opposite directions. Despite this, we claim that, if L is large enough, the second contribution always dominates and the following description holds (see Section 3 for similar analysis):

c.

$$E^{(1)}(\mathcal{N}) = -\frac{1}{4} - \frac{1}{2}\ \max(\, \Delta_+(\zeta), \Delta_-(\zeta)\,) + \frac{(\mathcal{N} - 1)}{2}\, u \tag{5.32}$$

where $\zeta = \mathcal{N}/(4L)$. Note that the minimum is attained at the neutral point $N_n = N_e = \mathcal{N}/2$. In addition, note that $\Delta_+(\zeta) = \Delta_-(\zeta)$ at $\zeta = 1/4$ ($\mathcal{N} = L$). Since $\Delta_\sigma(\zeta)$ increases or decreases according to whether σ is positive or negative,

$$E^{(1)}(\mathcal{N}) = -\frac{1}{4} - \frac{1}{2}\Delta_\sigma(\zeta) + \frac{(\mathcal{N} - 1)}{2}\, u \tag{5.33}$$

with $\sigma = -$ if $\zeta \le 1/4$ and $\sigma = +$ if $\zeta > 1/4$.

$\square$

Let N, M, n and m be as in the Example 5.3.3. Note that, for all $u \in \mathbb{R}$ different from zero, $\Theta_\sigma(\rho)$, given by (5.16), is a monotone function of ρ, $0 \le \rho \le 1/2$, which increases if $\sigma = +$ and decreases if $\sigma = -$. This follows from the fact that $\Theta_\pm > 0$ and

$$\Theta'_\pm(\rho) = \frac{1 - 2\rho}{\Theta_\pm}\left[1 \pm \frac{1}{2\theta}\left(2(1 - 2\rho) + u^2\right)\right]$$

where $\theta = \left(\rho^2(1-\rho)^2 + u^2\rho(1-\rho)\right)^{1/2}$. Note, in addition, that $\Theta_\pm(0) = u$ and $\Theta'_\pm(0) = \pm\infty$.

This behavior of $\Theta_\pm$ allows us to deduce the expressions of the ground state energies $E^{(1)}$ and $E^{(2)}$ from those already obtained for the Example 2 by making the following replacement:

$$\begin{array}{rcl} \pm 1/2 - \Delta_\pm & \longleftrightarrow & -\Theta_\pm \\ \pm 1/2 + \Delta_\pm & \longleftrightarrow & \Theta_\pm \end{array} \tag{5.34}$$

For the item **II**.c , e.g.,

$$E^{(1)}(\mathcal{N}) = -\frac{1}{2}\ \max\left(\Theta_+(\rho), \Theta_-(\rho)\right) + \frac{\mathcal{N} - 1}{2}\, u \tag{5.35}$$

holds for all $u < 0$, where $\rho = N/(2L)$. We recall that the minimum of $E^{(2)}$ is attained at $N_n = N_e$. Since the nuclei number $N_n = L/2$, we conclude that $\mathcal{N} = N_n + N_e = L$ is the only accessible point in this example. $\square$

6 Conclusions

The nature of the ground state of the Falicov–Kimball model with long range hopping matrices (mean–field matrices) was investigated. The eigenvalue problem of this model has been entirely solved allowing us to obtain the profile of the ground state energy. We have investigated the ground state energy $E^{(2)}$ as a function of the number of nuclei and electrons (N_n, N_e), and $E^{(1)}$ as a function of the total number of particles $\mathcal{N} = N_n + N_e$, for all values of the interaction U. This analysis revels general features of the Falicov–Kimball model which may be conjecture to be true irrespective to whether bipartition and half–filled band hold. The aim of this section is to point out some of these features.

Kennedy–Lieb's results on the Falicov–Kimball model (items **A-D** in the introduction) require the lattice to be bipartite. Let us compute, for comparison, equation (1.7) for the bipartite mean–field model. In this case, we have $T^2 = (M/L^2)\ 1\!\!1_N \oplus (N/L^2)\ 1\!\!1_M$ which gives (with $U = t\,u$ and $2t = 1$)

$$T^2 + U^2 = \left(\frac{u^2}{4} I_N + \frac{M}{L^2}\, 1\!\!1_N\right) \oplus \left(\frac{u^2}{4} I_M + \frac{N}{L^2}\, 1\!\!1_M\right)$$

and, by using Lemma 2.3,

$$\left(T^2 + U^2\right)^{1/2} = \left(\frac{|u|}{2} I_N + \frac{\Gamma}{N}\, 1\!\!1_N\right) \oplus \left(\frac{|u|}{2} I_M + \frac{\Gamma}{M}\, 1\!\!1_M\right)$$

where

$$\Gamma = \sqrt{\left(\frac{u}{2}\right)^2 + \frac{NM}{L^2}} - \frac{|u|}{2} \tag{6.1}$$

is equal to λ_+ if $u < 0$ or $-\lambda_-$ if $u > 0$ with $\lambda_\pm$ as given in (5.12).

¿From this, we have $1/2\,\mathrm{Tr}\,(T^2 + U^2)^{1/2} = |u|L/4 + \Gamma$ which, when substituting in equation (1.7) ($\times 2$ in view of t), reproduces the ground state energy $E^{(1)}$ of the Example 5.3.1 for $\mathcal{N} \geq L$ if $u > 0$ and $\mathcal{N} \leq 2|\mathcal{A}|$ if $u < 0$ (see equations (5.20) and (5.23)). Note that the equation (1.7) turns out to be equality in this example for $0 \leq \mathcal{N} \leq 2L$ if $u < 0$ and for $|\mathcal{N}/L - 1| \leq 1/2$ if $u > 0$.

Worth of mentioning here is the monotone behavior of $E^{(1)}$ as a function of $\mathcal{N}$. Monotonicity has been holden generically in all examples considered (satisfying bipartition or not) with the only exception being the Example 5.3.1 for $u > 0$ and $0 \leq \mathcal{N} \leq L/2$ (see equation (5.19)). This exception, as we believe, is related to the fact that the number of nuclei is related to the size of the sub–lattice: $|\mathcal{A}| = N_n$ in this example.

For $u > 0$ there is an interval of values of $\mathcal{N}$, extending up to the half–filled band point $\mathcal{N} = L$, where $E^{(1)}$ remains constant (see equations (3.8), (5.19) and (5.28)). We believe that this behavior is generically true and is related to the existence of first kind gap at $\mathcal{N} = L$ for $u > 0$. As $\mathcal{N} = N_n + N_e$ varies in this interval the minimum of $E^{(2)}$ is attained with the nuclei number N_n kept fixed. At $\mathcal{N} = L$ all eigenvalues $\mu \leq 0$ ($\mu \leq 1/L$ for mean field hopping matrix) have been filled with electrons. As a consequence, if there is a second kind gap in the spectrum of $H = T + u\,\mathrm{diag}(\{\sigma_x\})$, as usually do happen for typical hopping matrices T, the ground state energy density given by (4.1) develops a kink at $\rho = \mathcal{N}/L = 1/2$ (see equation (4.4)) giving rise a discontinuity in the chemical potential.

We finally discuss why there is no first kind gap if $u < 0$ for the mean field models considered here. The key equation (3.11) shows $\mu_1 \le \cdots \le \mu_{N_n} \le u < 0$ and $\mu_j \ge 0$ if $j > N_n$. So, for any number of particles $\mathcal{N} = N_n + N_e$, the minimum of energy is attained when all negative eigenstates are filled with electrons: $N_n = N_e$. The sum of these eigenvalues thus gives a smooth bulk (order L) contribution to $E^{(1)}$. Equations (3.20), (5.23), (5.33) and (5.35), show that $e(\rho) = \lim_{L\to\infty} E^{(1)}(L\,\rho)/L$ is a smooth function of ρ, $0 \le \rho \le 1$ implying absence of first kind gap. However, if sub–dominant terms of $E^{(1)}$ are taking into account in equations (3.20) and (5.33), $\lim_{L\to\infty} \left(E^{(1)}(L\,\rho) - L\,e(\rho)\right)$ is continuous but non–differentiable function of ρ at $\rho = 1/2$. This fact is the scar of a gap sweeped out by the long range hopping. Opposed to the result by Kennedy–Lieb, the mean field Falicov–Kimball model presents a phase transition at $u = 0$. Observe that there is no contradiction with item **D** of the introduction since the elements of the mean field hopping matrix are non–uniform in L.

A Matrices of the Form $\alpha I + \beta 1\!\!1$

Proof of Lemma 2.3. Clearly, the collection of matrices $\mathcal{C}$ form a vector space. This collection also forms a commutative algebra with the product of two matrices $C = \alpha I + \beta 1\!\!1$ and $D = \gamma I + \delta 1\!\!1$ given by

$$CD = DC = \alpha\gamma\, I + (\alpha\delta + \beta\gamma + \beta\delta R) 1\!\!1 \,. \tag{A.1}$$

¿From equation (A.1), D is the inverse of C, $D = C^{-1}$, if

$$\alpha\gamma = 1 \qquad \text{and} \qquad \alpha\delta + \beta\gamma + \beta\delta R \tag{A.2}$$

hold. Solving these two equations we get the coefficients of I and $1\!\!1$ of the item *2*.

To prove item *3* we notice that matrices of the form $\alpha I + \beta 1\!\!1$ are circulant matrices

$$\tilde{C} = \operatorname{circ}(c_1, c_2, \ldots, c_R) = \begin{pmatrix} c_1 & c_2 & c_3 & \ldots & c_R \\ c_R & c_1 & c_2 & \ldots & c_{R-1} \\ c_{R-1} & c_R & c_1 & \ldots & c_{R-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_2 & c_3 & c_4 & \ldots & c_1 \end{pmatrix} \tag{A.3}$$

with

$$c_1 = \alpha + \beta \qquad \text{and} \qquad c_2 = c_3 = \cdots = c_R = \beta \,. \tag{A.4}$$

Circulant matrices can always be diagonalized by Fourier matrices F (see e.g. [D]):

$$\Lambda = F^{-1}\,\tilde{C}\,F \tag{A.5}$$

where $\Lambda = \operatorname{diag}\{\lambda_1, \lambda_2, \ldots, \lambda_R\}$ with

$$\lambda_j = c_1 + c_2\omega_R^{j-1} + \cdots + c_R\omega_R^{(R-1)(j-1)} \,. \tag{A.6}$$

Substituting (A.4) in (A.6) we get

$$\lambda_1 = \alpha + \beta R \quad \text{and} \quad \lambda_2 = \cdots = \lambda_R = \alpha$$

in view of the fact that

$$1 + \omega_R^{j-1} + \omega_R^{2(j-1)} + \cdots + \omega_R^{(R-1)(j-1)} = 0 \tag{A.7}$$

for all $j = 2, \ldots, R$.

For completeness, let us verify that (A.5) is true for matrices of the form $C = \alpha I + \beta \mathbb{1}$. Here we need only to Fourier transform the matrix $\mathbb{1}$. Writing F as the matrix $[\mathbf{1}\, \mathbf{u}_{R,1} \cdots \mathbf{u}_{R,R-1}]$ with the vectors defined in Lemma 2.3 as columns and using (A.7) give

$$F^{-1}\, \mathbb{1}\, F = \mathrm{diag}(R, 0, \ldots 0)$$

from which the eigenvalues of C can be read.

Finally, item *4* follows from item *3* and this completes the proof of the proposition. □

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