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SEGREGATION IN THE FALICOV-KIMBALL MODEL

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Abstract. The Falicov-Kimball model is a simple quantum lattice model that describes light and heavy electrons interacting with an on-site repulsion; alternatively, it is a model of itinerant electrons and fixed nuclei. It can be seen as a simplification of the Hubbard model; by neglecting the kinetic (hopping) energy of the spin up particles, one gets the Falicov-Kimball model.

We show that away from half-filling, i.e. if the sum of the densities of both kinds of particles is less than 1, the particles segregate at zero temperature and for large enough repulsion. In the language of the Hubbard model, this means creating two regions with a positive and a negative magnetization.

Our key mathematical results are lower and upper bounds for the sum of the lowest eigenvalues of the discrete Laplace operator in an arbitrary domain, with Dirichlet boundary conditions. The lower bound consists of a bulk term, independent of the shape of the domain, and of a term proportional to the boundary. Therefore, one lowers the kinetic energy of the itinerant particles by choosing a domain with a small boundary. For the Falicov- Kimball model, this corresponds to having a single 'compact' domain that has no heavy particles.

Keywords: Falicov-Kimball model, segregation, phase separation.

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Contents

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1. Introduction

1.1. **The Falicov-Kimball model.**

Introduced thirty years ago to describe the semiconductor-metal transition in SmB_6 and related materials [FK], the Falicov-Kimball model is a simple lattice model with rich and interesting properties. The system consists of two species of spinless electrons with different effective masses: one species has infinite mass (so the particles do not move — we call them 'classical particles'), while the second species represents itinerant spinless electrons whose kinetic energy is represented by a hopping matrix. The Hamiltonian in a finite domain $\Omega \subset \mathbb{Z}^d$ is

$$H_\Omega^U(\{w_x\}) = -\sum_{\substack{x,y\in\Omega \\ |x-y|=1}} c_x^\dagger c_y + 2d\sum_{x\in\Omega} n_x + U\sum_{x\in\Omega} w_x n_x. \tag{1.1}$$

Here, $c_x^\dagger$, c_x, denote creation, annihilation operators of an electron at site x; $n_x = c_x^\dagger c_x$; $w_x = 0,1$ is the number of classical particles ('heavy electrons') at x, and $U \geqslant 0$ is an on-site repulsion between the two species of particles. $H_\Omega^U(\{w_x\})$ represents the energy of the electrons under a potential Uw_x. The term $2d\sum n_x$ in (1.1) is for convenience only. It makes H_Ω^U positive, and this term only adds $2d$ times the electron number, N. At zero temperature, one is typically interested in the configurations of classical particles that minimize the ground state energy of the electrons.

The model was reinvented in [KL] as a simplification of the Hubbard model, by neglecting the hoppings of electrons of spin $\uparrow$, say. This simplification changes the nature of the model somewhat, mainly because the continuous SU(2) symmetry is lost. Connections between the two models are therefore not immediate; however, the greater knowledge obtained for the Falicov-Kimball model may help in understanding the Hubbard model.

Rigorous results in [KL] include a proof that equilibrium states display long-range order of the chessboard type when both species of particles have density 1/2; this holds for all dimension greater than 1 and for *all* $U \neq 0$ (including $U < 0$), provided the temperature is low enough. Absence of long-range order when the inverse temperature β is small, or βU is small, was also established in [KL]. An extension of these results for large U and small temperature was proposed in [LM, MM, DFF].

One may increase the density of one species and decrease the density of the other species while maintaining the half-filling condition, namely that the total density is 1. (However, as was shown in [KL], the lowest energy is achieved when both species have density 1/2.) The one-dimensional case was considered in [Lem]; if classical particles and electrons have respective densities $\frac{p}{q}$ and $1-\frac{p}{q}$, the ground state is the 'most homogeneous configuration' for U large enough; this configuration is periodic with a period no greater than q. Away from half-filling the particles segregate: classical particles occupy one side of the chain, leaving room for electrons on the other side. There are several results in 2D. Gruber et. al. [GJL] performed a $1/U$ expansion and found periodic phases when the density of the classical particles is 1/3, 1/4, 1/5. This was made rigorous by Kennedy [Ken]. These results are reviewed in [GM]. The knowledge of the 2D phase diagram for large U was further extended in [Ken2, Hal, HK]. New ground states for various rational densities were uncovered; for some densities they are periodic, but there are also densities where coexistence of configurations with different periods have minimum energy. The results are summarized in Fig. 1 in [HK].

1.2. **Away from half-filling.**

The purpose of our study is to explore the situation away from half-filling; i.e., we take the total density to differ from 1. Hole-particle symmetries for both species of particles [KL] imply that the results for positive U and densities $(n_{\rm e}, n_{\rm c})$ of electrons and heavy (classical) particles, transpose to (a) positive U and densities $(1-n_{\rm e}, 1-n_{\rm c})$, and (b) negative U and densities $(n_{\rm e}, 1-n_{\rm c})$ or $(1-n_{\rm e}, n_{\rm c})$. For simplicity, we take the total density $n_{\rm e}+n_{\rm c}$ to be strictly less than 1.

We start our study by taking the limit $U \to \infty$. Electrons are described by wave functions that vanish on sites occupied by the classical particles, and the question is to find the arrangement of classical particles that minimizes the energy of the electrons. This amounts to minimizing the sum of the lowest eigenvalues of the discrete Laplace operator with Dirichlet boundary conditions. This is explained in Section 2, where it is shown that the energy per site of N electrons in a finite domain $\Lambda \subset \mathbb{Z}^d$ with volume $|\Lambda|$, is bounded below by the energy per site of the electrons in the infinite lattice with density $n = N/|\Lambda|$.

One can refine this lower bound by including a term proportional to $|\partial\Lambda|$, the volume of the boundary $\partial\Lambda$ of Λ (Section 3). This implies that the configuration of the heavy, fixed electrons that minimizes the ground state energy of the movable electrons has, more or less, one large hole with relatively small perimeter. Thus the movable particles are separated from the fixed ones. This behavior was conjectured in [FF] and is opposite to the checkerboard configuration, in which both kinds of particles are inextricably mixed. Segregation was shown to occur in the ground state of the $d=1$ model in [Lem], and of the $d=\infty$ model in [FGM]. The present paper proves that this holds for all dimensions, and in particular for the relevant physical situations $d=2$ and $d=3$.

Segregation is more difficult to understand on a heuristical level than the chessboard phase. The latter is a *local* phenomenon that results from effective interactions between nearest neighbor sites, while the former is a *global* phenomenon involving extended wave functions. This remark should also apply to the Hubbard model, for which antiferromagnetism is much better understood than ferromagnetism.

The fact that the sum of the lowest N eigenvalues of the Laplacian in a domain of volume $|\Lambda|$ is bounded below by the infinite volume value at the same density is not unexpected and holds also in the continuum. Indeed, the original idea, due to Li and Yau [LY] (see also [LL] Sections 12.3 and 12.11), was demonstrated in the continuum, and we only adapted it to the lattice context. However, the fact that the error term is proportional to $|\partial\Lambda|$, the area of the boundary, is a completely different story. Its proof, at least the one given here, is complicated. More to the point, such a bound *does not hold in the continuum.* One can easily construct a continuum domain with finite volume $|\Lambda|$, but with $|\partial\Lambda| = \infty$, and for which all eigenvalues are finite.

Taking U large instead of infinite decreases the energy, but the gain is at most proportional to $|\partial\Lambda|$, as explained in Section 4. Therefore the infinite–U segregation effect outweighs this gain and the particles are still separated. Finally, an upper bound derived in Section 5 shows that the energy of electrons in Λ really consists of a bulk term independent of the shape of Λ, plus a term of the order of the boundary.

These results are summarized in Theorem 1.1 below. One can use them to discuss the electronic free energy at inverse temperature β, for a *fixed* configuration of classical particles, see Theorem 1.2. The conclusion of this paper involves a discussion of first-order phase transitions at finite temperature, of what happens when classical particles have a small hopping term, and of the possible links with ferromagnetism in systems of interacting electrons with spins.

In order to present the main result of this paper, we need a few definitions. For $k \in (-\pi,\pi]^d$, we set

$$\varepsilon_k = 2d - 2\sum_{i=1}^{d} \cos k_i. \tag{1.2}$$

The energy per site $e(n)$ of a density n of free electrons in the infinite volume $\mathbb{Z}^d$ is

$$e(n) = \frac{1}{(2\pi)^d} \int_{\varepsilon_k < \varepsilon_{\rm F}} \varepsilon_k \, {\rm d}k, \tag{1.3}$$

where the Fermi level $\varepsilon_{\rm F} = \varepsilon_{\rm F}(n)$ is defined by the equation

$$n = \frac{1}{(2\pi)^d} \int_{\varepsilon_k < \varepsilon_{\rm F}} {\rm d}k. \tag{1.4}$$

We can specify the configuration $(w_x)_{x\in\mathbb{Z}^d}$ of classical particles by the domain $\Lambda \subset \mathbb{Z}^d$ consisting of those sites *without* particles (holes), that is, $w(x) = 1$ if $x \notin \Lambda$ and $w(x) = 0$ if $x \in \Lambda$. Let h_Λ^U denote the one-particle Hamiltonian whose action on a square summable, complex function φ on $\mathbb{Z}^d$ is

$$[h_\Lambda^U \varphi](x) = -\sum_{y,|y-x|=1} \varphi(y) + 2d\varphi(x) + U\chi_{\Lambda^{\rm c}}(x)\varphi(x). \tag{1.5}$$

Here, $\chi_{\Lambda^{\rm c}}(x)$ is the characteristic function that is 1 if x belongs to the complement $\Lambda^{\rm c}$ of Λ, and is 0 if $x \notin \Lambda^{\rm c}$. We define $E_{\Lambda,N}^U$ to be the ground state energy of N electrons for the configurations defined by Λ, i.e.

$$E_{\Lambda,N}^U = \inf_{\{\varphi_1,\dots,\varphi_N\}} \sum_{i=1}^{N} (\varphi_i, h_\Lambda^U \varphi_i), \tag{1.6}$$

where the infimum is taken over N orthonormal functions, i.e. $(\varphi_i,\varphi_j) = \delta_{ij}$. There exist normalized minimizers if the Fermi level is below U; they are not identically zero inside Λ, and decay exponentially outside.

Notice that $E_{\Lambda,N}^U$ is increasing in U, since $(\varphi, h_\Lambda^U \varphi)$ is increasing in U for any φ.

We define the boundary by $\partial\Lambda = \{x \in \Lambda : {\rm dist}\,(x,\Lambda^{\rm c}) = 1\}$, where $\Lambda^{\rm c}$ is the complement of Λ, i.e., the points in $\mathbb{Z}^d$ not in Λ. The following theorem summarizes the results obtained in this paper. It contains upper *and* lower bounds for the ground state energy. We set $n = N/|\Lambda|$.

Theorem 1.1. *There are functions $\alpha(n) > 0$ and $\gamma(U)$ with $\lim_{U\to\infty} U\gamma(U) = 8d^2$, such that for all finite domains Λ,*

$$\bigl(2dn - e(n)\bigr)|\partial\Lambda| \;\geqslant\; E_{\Lambda,N}^U - |\Lambda| e(n) \;\geqslant\; \bigl(\alpha(n) - \gamma(U)\bigr)|\partial\Lambda|.$$

For $n \leqslant |S_d|/(4\pi)^d$, $\alpha(n)$ can be taken to be

$$\alpha(n) = \frac{2^{d-3}}{\pi^d d^3 |S_d|^{2/d}} n^{1+\frac{2}{d}}.$$

Here, $|S_d|$ is the volume of the unit sphere in d dimensions.

An explicit expression for $\gamma(U)$ can be found in Proposition 4.1. The theorem states that the 'good' configurations Λ for which electrons have low energy must have small boundaries. As a consequence, the system displays phase separation in the ground state.

Notice that the upper bound is symmetric under the transformation $n \mapsto 1-n$ (i.e. it respects the particle-hole symmetry for the case $U=\infty$), and it is saturated for $U=\infty$ by configurations with isolated holes. Indeed, in this case the eigenstates consist of δ functions on the holes, with eigenvalues equal to $2d$, and $\partial\Lambda = \Lambda$. The lower bound satisfies $\alpha(1-n) = \alpha(n)$ and therefore also respects the particle-hole symmetry.

The lower bound is first explained in Section 2 for $U = \infty$ and without the term involving the boundary. The latter requires more effort and is derived using Lemmas 3.2–3.5 in Section 3. Proposition 4.1 then extends it to the case of finite U. The upper bound is proved in Section 5.

1.3. **Electrons at low temperature.** It is natural to consider the situation at positive temperature. The relevant object is the Gibbs state obtained by averaging over the configurations of classical particles, and by taking the trace of the Gibbs operator $\exp\{-\beta H_\Omega^U(\{w_x\})\}$. We expect the system to display a first-order phase transition in the grand-canonical ensemble; densities of both types of particles should have discontinuities as functions of the chemical potentials. But a rigorous treatment of this phase transition is beyond reach at present. However, we do obtain some properties of the system when the configuration of the classical particles is fixed, and the electrons are at positive temperature. Namely, one can extend the estimates of the ground state energy to estimates of the electronic free energy. The results are described in this section, and their derivation can be found in Section 6.

Let us consider a box Ω with periodic boundary conditions. The configuration of classical particles is specified by the set of holes $\Lambda \subset \Omega$ (later, in Corollary 1.3, we shall average over Λ). With μ being the chemical potential, the grand-canonical *electronic* free energy (equal to $-|\Omega|/\beta$ times the pressure) is

$$F_{\Omega,\Lambda}^U(\beta,\mu) = -\frac{1}{\beta}\log \operatorname{Tr} \exp\bigl\{-\beta H_{\Omega,\Lambda}^U + \beta\mu N_\Omega\bigr\}. \tag{1.7}$$

Here, $H_{\Omega,\Lambda}^U = H_\Omega^U(\{w_x\})$ as defined in (1.1), $N_\Omega = \sum_{x\in\Omega} n_x$ is the number of electrons in Ω, and the trace is in the Fock space of antisymmetric wave functions on Ω.

A simple 'guess' for $F_{\Omega,\Lambda}^U$ is obtained by considering independent electrons, which are either in Λ or else in Λ^{c}. In the latter case the effective chemical potential is $\mu - U$. Our 'guess' would then be

$$F_{\Omega,\Lambda}^U(\beta,\mu) \approx |\Lambda| f(\beta,\mu) + (|\Omega| - |\Lambda|) f(\beta,\mu-U), \tag{1.8}$$

where $f(\beta,\mu)$ is the free energy per site for free electrons:

$$f(\beta,\mu) = -\frac{1}{\beta}\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d} \mathrm{d}k \, \log\bigl(1 + \mathrm{e}^{-\beta(\varepsilon_k - \mu)}\bigr). \tag{1.9}$$

Formula (1.8) is, indeed, correct when U is large — in the sense that the error is proportional only to $|\partial\Lambda|$. More precisely,

Theorem 1.2. *There are functions $\bar\alpha(\beta,\mu) > 0$ with $\lim_{\beta\to\infty}\bar\alpha(\beta,\mu) > 0$ if $0 < \mu < 4d$, and $\bar\gamma(U)$ with $\lim_{U\to\infty} U\bar\gamma(U) = 16d^2 + 2^{d+3}d^4$, such that for all finite domains Ω and $\Lambda \subset \Omega$,*

$$\begin{aligned} C_{d,\mu}|\partial\Lambda| + C'_{d,\mu}|\Omega|^{1-\frac{1}{d}} &\geqslant F_{\Omega,\Lambda}^U(\beta,\mu) - \bigl\{|\Lambda| f(\beta,\mu) + (|\Omega| - |\Lambda|) f(\beta,\mu-U)\bigr\} \\ &\geqslant \bigl(\bar\alpha(\beta,\mu) - \bar\gamma(U)\bigr)|\partial\Lambda|, \end{aligned}$$

with

$$\begin{aligned} C_{d,\mu} &= \Big(\frac{4\pi\sqrt{d}}{|S_d|^{1/d}} + 2d(2d+1) \Big) \frac{1}{1+\mathrm{e}^{-\beta\mu}}, \\ C'_{d,\mu} &= \frac{4\pi\sqrt{d}}{|S_d|^{1/d}} \frac{1}{1+\mathrm{e}^{-\beta(\mu-U)}}. \end{aligned}$$

The term $|\Omega|^{1-\frac{1}{d}}$ on the left side is not exactly proportional to $|\partial\Lambda|$. However, we have in mind that $|\Lambda|$ and $|\Omega|$ are comparable, in which case $|\Omega|^{1-\frac{1}{d}}$ is no greater than $|\partial\Lambda|$ (up to a factor).

Notice that the upper bound vanishes as $\mu \to -\infty$, i.e. when the density tends to 0. In the limit $U \to \infty$, Theorem 1.2 takes a simpler form, namely

$$C_{d,\mu}|\partial\Lambda| \;\geqslant\; F^{U=\infty}_{\Omega,\Lambda}(\beta,\mu) - |\Lambda| f(\beta,\mu) \;\geqslant\; \bar\alpha(\beta,\mu)|\partial\Lambda|. \tag{1.10}$$

This extension of Theorem 1.1 to the case of positive (electronic) temperatures is explained in Section 6. The lower bound follows from Propositions 6.1 and 6.2, while the upper bound is stated in Proposition 6.3.

Our next step is to find upper and lower bounds for the total grand-canonical 'free energy' by averaging over Λ (i.e., averaging over the positions of the classical particles). This can be done with the aid of the Ising model free energy $f_{\rm Ising}(\beta,h)$,

$$f_{\rm Ising}(\beta,h) = -\frac{1}{\beta} \lim_{|\Omega|\to\infty} \frac{1}{|\Omega|} \sum_{\{s_x=\pm1\}} \exp\Big\{ -\beta \sum_{\substack{\{x,y\}\subset\Omega \\ |x-y|=1}} s_x s_y - \beta h \sum_{x\in\Omega} s_x \Big\}, \tag{1.11}$$

where the sum if over configurations of classical spins on Ω.

Corollary 1.3. *If U is large enough (so that $\bar\alpha(\beta,\mu) - \bar\gamma(U) > 0$), we have Ising bounds for the full free energy,*

$$\begin{aligned} &\tfrac12 [f(\beta,\mu) + f(\beta,\mu-U)] + \tfrac14 \bar{\bar\alpha} + \tfrac{\bar{\bar\alpha}}{4d} f_{\rm Ising}\big(\tfrac{1}{4d}\bar{\bar\alpha}\beta, \tfrac{2d}{\bar{\bar\alpha}} [f(\beta,\mu) - f(\beta,\mu-U)] \big) \\ &\qquad\qquad \leqslant -\frac{1}{\beta} \lim_{|\Omega|\to\infty} \frac{1}{|\Omega|} \log \sum_{\Lambda\subset\Omega} \mathrm{e}^{-\beta F^U_{\Omega,\Lambda}(\beta,\mu)} \\ &\leqslant \tfrac12 [f(\beta,\mu) + f(\beta,\mu-U)] + \tfrac12 d C_{d,\mu} + \tfrac12 C_{d,\mu} f_{\rm Ising}\big(\tfrac12 C_{d,\mu}\beta, \tfrac{1}{C_{d,\mu}} [f(\beta,\mu) - f(\beta,\mu-U)] \big) \end{aligned}$$

where $\bar{\bar\alpha} = \bar\alpha(\beta,\mu) - \bar\gamma(U)$.

The proof can be found at the end of Section 6.

Another consequence of Theorem 1.2 concerns the equilibrium state; namely, it allows for a precise meaning of segregation. We consider the probability that sites x and y are *both* occupied by classical particles, or both are unoccupied. Namely, we consider

$$\langle \delta_{w_x,w_y} \rangle_\Omega = \frac{\sum_{\Lambda\subset\Omega: w_x=w_y} \exp\big\{ -\beta F^U_{\Omega,\Lambda}(\beta,\mu) \big\}}{\sum_{\Lambda\subset\Omega} \exp\big\{ -\beta F^U_{\Omega,\Lambda}(\beta,\mu) \big\}} \tag{1.12}$$

where the sums are over subsets Λ of Ω such that $|\Lambda| = [(1-n_{\rm c})|\Omega|]$ ($[z]$ denotes the integer part of $z \in \mathbb{R}$). The restriction $w_x = w_y$ means that either both x and y belong to Λ, or both belong to the complement of Λ.

Segregation means that up to a small fraction of sites that are close to the boundary between classical particles and empty sites, any two sites at finite distance are either both hosts of a classical particle, or are both empty. The fraction of sites close to the boundary vanishes in the thermodynamic limit. Hence we *expect* that

$$\lim_{\beta\to\infty} \lim_{|x-y|\to\infty} \lim_{|\Omega|\to\infty} \langle \delta_{w_x,w_y} \rangle_\Omega = 1, \tag{1.13}$$

but we are unable to prove it. Notice that using Theorem 1.1, one can conclude that

$$\lim_{|x-y|\to\infty} \lim_{|\Omega|\to\infty} \lim_{\beta\to\infty} \langle \delta_{w_x,w_y} \rangle_\Omega = 1. \tag{1.14}$$

Indeed, taking the limit of zero temperature at finite volume, the sum over Λ becomes restricted to the ground state configuration(s), whose boundary fraction $|\partial\Lambda|/|\Lambda|$ tends to zero in the thermodynamic limit.

We can however take advantage of Theorem 1.2 to obtain a result that is better than (1.14):

Corollary 1.4. *If U is large enough (depending on μ and d only), the ground state of the Falicov-Kimball model displays segregation, in the sense that*

$$\lim_{|x-y|\to\infty} \lim_{\beta\to\infty} \lim_{|\Omega|\to\infty} \langle \delta_{w_x,w_y} \rangle_\Omega = 1.$$

The proof of this corollary can be found at the end of Section 6.

2. The discrete Laplace operator in a finite domain

We start our investigations by taking the limit $U \to \infty$. Let us denote $h_\Lambda \equiv h_\Lambda^{U=\infty}$, the corresponding Hamiltonian, which acts on functions $\varphi \in L^2(\Lambda)$ as follows: if $x \in \Lambda$,

$$[h_\Lambda \varphi](x) = -\sum_{y\in\Lambda, |x-y|=1} \varphi(y) + 2d\,\varphi(x). \tag{2.1}$$

We are looking for a lower bound for the sum $E_{\Lambda,N}$ of the first N eigenvalues of h_Λ.

This problem was considered by Li and Yau [LY] for the Laplace operator in the continuum. Let $\Lambda \subset \mathbb{R}^d$ be a bounded domain. They prove that the sum S_N of the first N eigenvalues of the Laplace operator with Dirichlet boundary conditions is bounded below,

$$S_N > (2\pi)^2 \frac{d}{d+2} |S_d|^{-\frac{2}{d}} N^{1+\frac{2}{d}} |\Lambda|^{-\frac{2}{d}}, \tag{2.2}$$

where $|S_d|$ and $|\Lambda|$ are the volumes of respectively the d-dimensional sphere and of Λ.

The corresponding inequality in the discrete case — our Theorem 1.1 without the boundary correction — constitutes the heart of this paper, and we explain below the proof of Li and Yau; see also [LL], Theorem 12.3.

The Fourier transform of a function $\varphi \in L^2(\mathbb{Z}^d, \mathbb{C})$ is defined by

$$\hat\varphi(k) = \sum_{x\in\mathbb{Z}^d} \varphi(x)\,\mathrm{e}^{\mathrm{i}kx}, \quad k \in [-\pi,\pi]^d, \tag{2.3}$$

and the inverse transform is

$$\varphi(x) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \mathrm{d}k\, \hat\varphi(k)\,\mathrm{e}^{-\mathrm{i}kx}. \tag{2.4}$$

Using the Fourier transform, a little thought shows that the energy of a particle in a state φ in $L^2(\Lambda)$ is

$$(\varphi, h_\Lambda\, \varphi) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \mathrm{d}k\, |\hat\varphi(k)|^2 \varepsilon_k, \tag{2.5}$$

with ε_k defined in (1.2) and with $\varphi(x) = 0$ if $x \notin \Lambda$ in (2.3).

Let us consider N orthonormal functions $\varphi_1, \dots, \varphi_N$, and let $E_\Lambda(\varphi_1, \dots, \varphi_N)$ be their energy. We have

$$E_\Lambda(\varphi_1, \dots, \varphi_N) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \mathrm{d}k\, \rho(k) \varepsilon_k, \tag{2.6}$$

with

$$\rho(k) = \sum_{j=1}^N |\hat\varphi_j(k)|^2. \tag{2.7}$$

The function $\rho(k)$ satisfies the following equations:

$$0 \leqslant \rho(k) \leqslant |\Lambda|, \tag{2.8a}$$

$$\frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \mathrm{d}k\, \rho(k) = N. \tag{2.8b}$$

Indeed, positivity of ρ is immediate and the last equation is Plancherel's identity. The upper bound (2.8a) for $\rho(k)$ can be seen by writing

$$\rho(k) = (f, P f), \tag{2.9}$$

where P is the projector onto $\{\varphi_j\}_{j=1}^N$,

$$P_{x,y} = \sum_{j=1}^N \varphi_j(x) \varphi_j^*(y), \tag{2.10}$$

and f is the vector

$$f_x = \mathrm{e}^{-\mathrm{i}kx} \chi_\Lambda(x). \tag{2.11}$$

Then, since $P \leqslant \mathbb{1}$, we have $\rho(k) \leqslant \|f\|^2 = |\Lambda|$.

Clearly, we have the lower bound

$$E_{\Lambda,N} \geqslant \inf_{\substack{\rho:\, 0 \leqslant \rho \leqslant |\Lambda| \\ (2\pi)^{-d} \int \rho = N}} \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \mathrm{d}k\, \rho(k)\, \varepsilon_k. \tag{2.12}$$

We can use the bathtub principle ([LL], Theorem 1.14) to find the infimum: it is given by the function

$$\rho_{\min}(k) = \begin{cases} |\Lambda| & \text{if } \varepsilon_k \leqslant \varepsilon_{\mathrm{F}} \\ 0 & \text{otherwise,} \end{cases} \tag{2.13}$$

where the Fermi level ε_{F} is given by the relation $\frac{1}{(2\pi)^d} \int_{\varepsilon_K < \varepsilon_{\mathrm{F}}} \mathrm{d}k = N/|\Lambda|$. Thus the right side of (2.12) is precisely equal to $|\Lambda|\, e(N/|\Lambda|)$.

3. Lower bound involving the boundary

In the previous section, we showed that $E_{\Lambda,N}$ is bounded below by its bulk term. Now we strengthen this inequality and prove that $E_{\Lambda,N}$ also includes a term proportional to the boundary of Λ. This can be checked for $d = 1$ by explicit computation, but higher dimensions require more elaborate treatment.

We start with a lemma that applies when the density n is small enough (or, by hole-particle symmetry, when it is close to 1).

Lemma 3.1. *If $n \leqslant |S_d|/(4\pi)^d$, we have*

$$E_{\Lambda,N} \geqslant |\Lambda| e(n) + \frac{2^{d-3} n^{1+\frac{2}{d}}}{\pi^d d^3 |S_d|^{2/d}} |\partial\Lambda|.$$

Proof. Recall that

$$E_{\Lambda,N} = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \mathrm{d}k\, \rho(k) \varepsilon_k \tag{3.1}$$

with $\rho(k) = \sum_{j=1}^N |\hat{\varphi}(k)|^2$. We want to show that $\rho(k)$ cannot be too close to $\rho_{\min}(k)$ in (2.13). By completeness of the set of eigenvectors $\{\varphi_j\}$, we have

$$\rho(k) = |\Lambda| - \sum_{j=N}^{|\Lambda|} |\hat{\varphi}(k)|^2. \tag{3.2}$$

We use now the Schrödinger equation; namely, eigenvectors of h_Λ satisfy

$$-\sum_e \varphi_j(x+e) + \chi_{\Lambda^c}(x) \sum_{e:x+e\in\Lambda} \varphi_j(x+e) + 2d\varphi_j(x) = e_j \varphi_j(x). \tag{3.3}$$

Taking the Fourier transform, we get

$$\varepsilon_k \hat{\varphi}_j(k) + (b_k, \varphi_j) = e_j \hat{\varphi}_j(k), \tag{3.4}$$

where b_k is a 'boundary vector',

$$b_k(x) = \chi_{\partial\Lambda}(x)\, \mathrm{e}^{-\mathrm{i}kx} \sum_{e:x+e\notin\Lambda} \mathrm{e}^{-\mathrm{i}ke}. \tag{3.5}$$

Notice that $|\partial\Lambda| \leqslant \|b_k\|^2 \leqslant (2d)^2 |\partial\Lambda|$ if $|k|_1 \leqslant \frac{\pi}{2}$. From (3.4), we have

$$|\hat{\varphi}_j(k)|^2 = \frac{|(b_k, \varphi_j)|^2}{(\varepsilon_k - e_j)^2} \geqslant \frac{1}{(4d)^2} |(b_k, \varphi_j)|^2. \tag{3.6}$$

Let us introduce $\tilde{N}$ such that $e_{\tilde{N}} \leqslant \frac{1}{2}$ and $e_{\tilde{N}+1} > \frac{1}{2}$. We first consider the situation where $N \leqslant \tilde{N}$. We seek to obtain $\rho(k) \leqslant |\Lambda| - \text{const}|\partial\Lambda|$, and this will be achieved if

$$\|P_+ b_k\|^2 \geqslant \text{const}|\partial\Lambda|, \tag{3.7}$$

where P_+ is the projector onto the states $(\varphi_{\tilde{N}+1}, \dots, \varphi_{|\Lambda|})$. To see this, we first remark that

$$(b_k, h_\Lambda b_k) = \sum_{\{x,y\}:|x-y|=1} |b_k(x) - b_k(y)|^2 \geqslant \|b_k\|^2. \tag{3.8}$$

We used the fact that each site x of $\partial\Lambda$ has at least one neighbor y outside of Λ, and we obtained an inequality by restricting the sum over such pairs. Using first $e_j \leqslant 4d$ and then the previous inequality, we have

$$\begin{aligned} 4d \sum_{j=\tilde{N}+1}^{|\Lambda|} |(b_k, \varphi_j)|^2 &\geqslant \sum_{j=\tilde{N}+1}^{|\Lambda|} |(b_k, \varphi_j)|^2 e_j \\ &\geqslant \|b_k\|^2 - \sum_{j=1}^{\tilde{N}} |(b_k, \varphi_j)|^2 e_j \geqslant \tfrac{1}{2} \|b_k\|^2. \end{aligned} \tag{3.9}$$

Since $n \leqslant |S_d|/(4\pi)^d$ we have $|k|_1 \leqslant \frac{\pi}{2}$, and therefore

$$\rho(k) \leqslant |\Lambda| - \frac{|\partial\Lambda|}{2(4d)^3}. \tag{3.10}$$

We can write a lower bound by proceeding as in Section 2, but using the previous bound for $\rho(k)$, instead of $|\Lambda|$. The bathtub principle then gives

$$E_{\Lambda,N} - |\Lambda| e(n) \geqslant \frac{1}{(2\pi)^d} \int_{\varepsilon_{\rm F} < \varepsilon_k < \varepsilon'_{\rm F}} {\rm d}k\, \varepsilon_k \Bigl(|\Lambda| - \frac{|\partial\Lambda|}{2(4d)^3} \Bigr) - \frac{1}{(2\pi)^d} \int_{\varepsilon_k < \varepsilon_{\rm F}} {\rm d}k\, \varepsilon_k \frac{|\partial\Lambda|}{2(4d)^3}, \tag{3.11}$$

where we introduce $\varepsilon'_{\rm F}$ such that

$$N = \frac{1}{(2\pi)^d} \Bigl(|\Lambda| - \frac{|\partial\Lambda|}{2(4d)^3} \Bigr) \int_{\varepsilon_k < \varepsilon'_{\rm F}} {\rm d}k. \tag{3.12}$$

We bound the first integral of (3.11) using $\varepsilon_k > \varepsilon_{\rm F}$, and we obtain

$$E_{\Lambda,N} - |\Lambda| e(n) \geqslant \frac{|\partial\Lambda|}{2(4d)^3} \frac{1}{(2\pi)^d} \int_{\varepsilon_k < \varepsilon_{\rm F}} {\rm d}k (\varepsilon_{\rm F} - \varepsilon_k). \tag{3.13}$$

One can derive a more explicit expression for the lower bound. First,

$$\int_{\varepsilon_k < \varepsilon_{\rm F}} {\rm d}k (\varepsilon_{\rm F} - \varepsilon_k) \geqslant \tfrac{1}{2} \varepsilon_{\rm F} \int_{\varepsilon_k \leqslant \frac{1}{2}\varepsilon_{\rm F}} {\rm d}k. \tag{3.14}$$

Second we use $1 - \frac{\theta^2}{2} \leqslant \cos\theta \leqslant 1 - \frac{4}{\pi^2}\theta^2$, to get

$$\frac{8}{\pi^2} |k|^2 \leqslant \varepsilon_k \leqslant |k|^2. \tag{3.15}$$

One can use the upper bound of (3.15) to get

$$\int_{\varepsilon_k < \frac{1}{2}\varepsilon_{\rm F}} {\rm d}k \geqslant |S_d| (\tfrac{1}{2}\varepsilon_{\rm F})^{d/2}. \tag{3.16}$$

Recall that $|S_d|$ is the volume of the unit sphere in d dimensions. The lower bound of (3.15) allows to write

$$\varepsilon_{\rm F} \geqslant \frac{2^5 n^{2/d}}{|S_d|^{2/d}}. \tag{3.17}$$

Then one gets the bound

$$\int_{\varepsilon_k < \varepsilon_{\rm F}} {\rm d}k (\varepsilon_{\rm F} - \varepsilon_k) \geqslant \frac{2^{4+2d} n^{1+\frac{2}{d}}}{|S_d|^{2/d}}. \tag{3.18}$$

Hence the boundary correction to $E_{\Lambda,N}$ is bounded below by $\alpha(n)|\partial\Lambda|$ with

$$\alpha(n) = \frac{2^{d-3}}{\pi^d d^3 |S_d|^{2/d}} n^{1+\frac{2}{d}}. \tag{3.19}$$

Recall that we supposed $N \leqslant \tilde N$, where $\tilde N$ is the index of the largest eigenvalue that is smaller than $\frac{1}{2}$. Were it not the case, we can write, with $\tilde n = \tilde N/|\Lambda|$,

$$E_{\Lambda,N} = \sum_{j=1}^{\tilde N} e_j + \sum_{j=\tilde N+1}^{N} e_j \geqslant |\Lambda| e(\tilde n) + \alpha(\tilde n)|\partial\Lambda| + \tfrac{1}{2}|\Lambda|(n - \tilde n). \tag{3.20}$$

We used the previous inequality to bound the first sum, and $e_j \geqslant \frac{1}{2}$ for the second sum. This is greater than $|\Lambda| e(n) + \alpha(n)|\partial\Lambda|$ provided

$$e(\tilde{n}) + \alpha(\tilde{n})\frac{|\partial\Lambda|}{|\Lambda|} + \tfrac{1}{2}(n-\tilde{n}) \;\geqslant\; e(n) + \alpha(n)\frac{|\partial\Lambda|}{|\Lambda|}. \tag{3.21}$$

A sufficient condition is that $\frac{1}{2}n - e(n) - \alpha(n)$ is an increasing function of n. Computing the derivative (the derivative of $e(n)$ is $\varepsilon_{\rm F}(n)$, that is smaller than $(2\pi)^2 n^{2/d}/|S_d|^{2/d}$ using (3.15)), and requiring it to be positive leads to the condition

$$n \;\leqslant\; \frac{|S_d|}{\{2(2\pi)^2 + \frac{2^{d-2}}{\pi^d d^3}(1+\frac{2}{d})\}^{d/2}}. \tag{3.22}$$

The right side is greater than $|S_d|/(4\pi)^d$. □

It may seem obvious that the extra energy due to the presence of the boundary increases as n increases, until it reaches $\frac{1}{2}$. But we can provide no proof for this, and hence we need a new derivation for the lower bound with higher densities. We proceed in two steps. First we give a lemma that works when the boundary has few nearest neighbors; the proof is similar to that of the previous lemma. Then we give three lemmas, with more intricate demonstrations, and that establish the lower bound for boundaries where at least a density of sites have nearest neighbors. We need some notation to characterize the configuration around a site x of the boundary.

Let e, e' be unit vectors in $\mathbb{Z}^d$; the notation $e \parallel i$ means that e is parallel to the i-th direction; equivalently, the components of e are given by $e_k = \pm\delta_{ik}$. We introduce integers $q_{x,i}$ and $q_{x,ij}$; for $x \in \partial\Lambda$, we set

$$\begin{aligned} q_{x,i} &= \#\{e \parallel i : x+e \notin \Lambda\} \\ q_{x,ij} &= \#\{(e,e') : e \parallel i, e' \parallel j,\, x+e \in \partial\Lambda,\, x+e+e' \notin \Lambda\}. \end{aligned} \tag{3.23}$$

Notice that $0 \leqslant q_{x,i} \leqslant 2$ and $0 \leqslant q_{x,ij} \leqslant 4$. Also, $q_{x,ii} = \#\{e \parallel i, x+e \in \partial\Lambda, x+2e \notin \Lambda\}$, and $0 \leqslant q_{x,ii} \leqslant 2$. We also define $q_x = \sum_i q_{x,i}$.

The following lemma applies to domains where most boundary sites x satisfy $q_{x,ij} \equiv 0$, in which case x has no neighbors that belong to the boundary. Here, $q_{x,ij} \equiv 0$ means that, at x, $q_{x,ij} = 0$ for all $1 \leqslant i,j \leqslant d$.

Lemma 3.2. *For all $\Lambda \subset \mathbb{Z}^d$ with*

$$\#\{x \in \partial\Lambda : q_{x,ij} \not\equiv 0\} \;\leqslant\; \frac{1}{32d^4}|\partial\Lambda|,$$

there exists $\alpha(n) > 0$ such that

$$E_{\Lambda,N} \;\geqslant\; |\Lambda| e(n) + \alpha(n)|\partial\Lambda|.$$

Remark: $\lim_{n\to 0}\alpha(n) = 0$ and $\alpha(1-n) = \alpha(n)$ by particle-hole symmetry.

Proof. We can suppose $N \leqslant \frac{|\Lambda|}{2}$. Particle-hole symmetry implies that if $\varphi_j(x)$ is an eigenvector with eigenvalue e_j, then $(-1)^x\varphi_j(x)$ is an eigenvector with eigenvalue $4d - e_j$. We consider the following function $\rho(k)$:

$$\rho(k) = \begin{cases} \sum_{j=1}^{N} |\hat\varphi_j(k)|^2 & \text{if } N \leqslant \tilde{N} \\ \sum_{j=1}^{\tilde{N}} |\hat\varphi_j(k)|^2 + \frac{N-\tilde{N}}{|\Lambda|-2\tilde{N}} \sum_{j:e_j=2d} |\hat\varphi_j(k)|^2 & \text{if } N > \tilde{N}; \end{cases} \tag{3.24}$$

here, $\tilde{N}$ is such that $e_{\tilde{N}} < 2d$, $e_{\tilde{N}+1} \geqslant 2d$.

The goal is to prove that $\rho(k)$ cannot approach $\rho_{\min}$ in (2.13). Since $\sum_{j=1}^{|\Lambda|} |\hat\varphi_j(k)|^2 = |\Lambda|$, we have

$$\rho(k) \leqslant |\Lambda| - \Big\{ \sum_{j=|\Lambda|-\tilde N+1}^{|\Lambda|} |\hat\varphi_j(k)|^2 + \frac12 \sum_{j:e_j=2d} |\hat\varphi_j(k)|^2 \Big\}. \tag{3.25}$$

We introduce

$$S(k) = \sum_{j=|\Lambda|-\tilde N+1}^{|\Lambda|} |(b_k,\varphi_j)|^2 + \frac12 \sum_{j:e_j=2d} |(b_k,\varphi_j)|^2, \tag{3.26}$$

with b_k the boundary vector defined in (3.5). By the inequality (3.6), it is enough to show that $S(k)$ is bounded below by a quantity of the order of $|\partial\Lambda|$. We have

$$S(k) = \bigl(b_k, P_+\, b_k\bigr) + \tfrac12 (b_k, P_0\, b_k), \tag{3.27}$$

where P_+ is the projector onto the subspace spanned by all φ_j with $e_j > 2d$, and P_0 is the projector corresponding to the eigenvalue $2d$.

We want to show that $S(k) \geqslant \text{const}|\partial\Lambda|$ for small $|k|$. This amounts to prove that the vector b_k cannot lie entirely in the subspace spanned by $\{\varphi_j\}_{1\leqslant j\leqslant N}$.

Notice that if $x \in \partial\Lambda$ and $q_{x,ij} \equiv 0$, then x has no neighbors in $\partial\Lambda$. Using the assumption of Lemma 3.2, as well as $|b_k(x)| \leqslant 2d$ and $|\partial\Lambda| \leqslant \|b_k\|^2$, we get

$$\begin{aligned}(b_k, h_\Lambda\, b_k) &= \sum_{\{x,y\}:|x-y|=1} |b_k(x) - b_k(y)|^2 \\ &\geqslant 2d \sum_{x\in\partial\Lambda} |b_k(x)|^2 - 2d \sum_{\substack{x\in\partial\Lambda \\ q_{x,ij}\neq 0}} |b_k(x)|^2 \\ &\geqslant \bigl(2d - \frac{1}{4d}\bigr) \|b_k\|^2.\end{aligned} \tag{3.28}$$

The last inequality uses the assumption of Lemma 3.2, and the fact that $|b_k(x)|$ is at most $2d$ and at least 1.

Next we consider $\|(h_\Lambda - 2d)b_k\|^2$. We have, for $x \in \Lambda$,

$$\bigl[(h_\Lambda - 2d)b_k\bigr](x) = -\sum_e b_k(x+e), \tag{3.29}$$

and therefore, if $|k|_1 \leqslant \frac{\pi}{2}$,

$$\|(h_\Lambda - 2d)b_k\|^2 \geqslant \sum_{x\in\Lambda}\sum_e |b_k(x+e)|^2 = \sum_x (2d - q_x)|b_k(x)|^2. \tag{3.30}$$

We write $b_k = b' + b''$, with $b''(x) = b_k(x)$ if $q_x = 2d$, 0 otherwise. Notice that $b' \perp b''$. Clearly, $P_0 b'' = b''$, and therefore

$$S(k) = (b', P_+\, b') + \tfrac12 (b', P_0\, b') + \tfrac12 \|b''\|^2. \tag{3.31}$$

Furthermore, from (3.28) and (3.30), b' satisfies

$$(b', (h_\Lambda - 2d) b') \geqslant -\frac{1}{4d}\|b_k\|^2, \qquad (b', (h_\Lambda - 2d)^2 b') \geqslant \|b'\|^2. \tag{3.32}$$

Because $|e_j - 2d| \leqslant 2d$, the last inequality implies

$$-\sum_j |(\varphi_j, b')|^2 (e_j - 2d) + 2 \sum_{j:e_j>2d} |(\varphi_j, b')|^2 (e_j - 2d) = \sum_j |(\varphi_j, b')|^2 |e_j - 2d| \geqslant \frac{\|b'\|^2}{2d}. \tag{3.33}$$

With the first inequality in (3.32), this yields

$$\sum_{j:e_j>2d} |(\varphi_j, b')|^2 (e_j - 2d) \geqslant \frac{\|b'\|^2}{4d} - \frac{\|b_k\|^2}{8d}, \tag{3.34}$$

hence

$$\sum_{j:e_j>2d} |(\varphi_j, b')|^2 \geqslant \frac{\|b'\|^2}{8d^2} - \frac{\|b_k\|^2}{16d^2}. \tag{3.35}$$

Back to (3.31), we obtain

$$S(k) \geqslant \frac{\|b'\|^2}{8d^2} + \tfrac{1}{2}\|b''\|^2 - \frac{\|b_k\|^2}{16d^2} \geqslant \frac{\|b_k\|^2}{16d^2}. \tag{3.36}$$

We can combine this bound with (3.25) and (3.6); we have then for all $|k|_1 < \frac{\pi}{2}$

$$\rho(k) \leqslant |\Lambda| - \frac{|\partial\Lambda|}{(4d)^4}. \tag{3.37}$$

We introduce $\varepsilon'_{\mathrm{F}}$ such that

$$\frac{1}{(2\pi)^d}\Big(|\Lambda| - \frac{|\partial\Lambda|}{(4d)^4}\Big) \int_{\varepsilon_k<\varepsilon'_{\mathrm{F}}, |k|_1<\frac{\pi}{2}} \mathrm{d}k + \frac{|\Lambda|}{(2\pi)^d} \int_{\varepsilon_k<\varepsilon'_{\mathrm{F}}, |k|_1>\frac{\pi}{2}} \mathrm{d}k = N, \tag{3.38}$$

and we have

$$\begin{aligned} E_{\Lambda,N} - |\Lambda| e(\tfrac{N}{|\Lambda|}) \geqslant{}& \frac{1}{(2\pi)^d}\Big(|\Lambda| - \frac{|\partial\Lambda|}{(4d)^4}\Big) \int_{\varepsilon_{\mathrm{F}}<\varepsilon_k<\varepsilon'_{\mathrm{F}}, |k|_1<\frac{\pi}{2}} \mathrm{d}k\, \varepsilon_k \\ &+ \frac{|\Lambda|}{(2\pi)^d} \int_{\varepsilon_{\mathrm{F}}<\varepsilon_k<\varepsilon'_{\mathrm{F}}, |k|_1>\frac{\pi}{2}} \mathrm{d}k\, \varepsilon_k - \frac{1}{(2\pi)^d} \frac{|\partial\Lambda|}{(4d)^4} \int_{\varepsilon_k<\varepsilon_{\mathrm{F}}, |k|_1<\frac{\pi}{2}} \mathrm{d}k\, \varepsilon_k. \end{aligned} \tag{3.39}$$

We bound the first two integrals using $\varepsilon_k > \varepsilon_{\mathrm{F}}$; from the definitions of ε_{F} and $\varepsilon'_{\mathrm{F}}$ we have

$$\frac{|\partial\Lambda|}{(2\pi)^d} \int_{\varepsilon_k<\varepsilon'_{\mathrm{F}}, |k|_1<\frac{\pi}{2}} \mathrm{d}k = \frac{|\Lambda|}{(2\pi)^d} \int_{\varepsilon_{\mathrm{F}}<\varepsilon_k<\varepsilon'_{\mathrm{F}}} \mathrm{d}k. \tag{3.40}$$

As a result, we obtain the bound we were looking for,

$$E_{\Lambda,N} - |\Lambda| e(\tfrac{N}{|\Lambda|}) \geqslant \frac{|\partial\Lambda|}{(4d)^4} \frac{1}{(2\pi)^d} \int_{\varepsilon_k<\varepsilon_{\mathrm{F}}, |k|_1<\frac{\pi}{2}} \mathrm{d}k\, \big(\varepsilon_{\mathrm{F}} - \varepsilon_k\big). \tag{3.41}$$

$\square$

We present now another lemma that claims the lower bound for $E_{\Lambda,N}$, and that involves a new assumption. We shall see below in Lemmas 3.4 and 3.5 that for all volumes, at least one of these lemmas applies.

Lemma 3.3. *Let $\delta > 0$ and $n \geqslant |S_d|/(4\pi)^d$. We assume that*

$$\|(h_\Lambda - e_N) b_{k_0}\|^2 \geqslant \delta |\partial\Lambda|,$$

for some k_0 *belonging to the Fermi surface, i.e.* $\varepsilon_{k_0} = \varepsilon_{\mathrm{F}}$ *where* ε_{F} *is the Fermi energy for density* $n = \frac{N}{|\Lambda|}$. *Then we have*

$$E_{\Lambda,N} - |\Lambda| e(n) \geqslant \eta\, |\partial\Lambda|$$

with $\eta = |S_d|^5 \delta^{30d+2} / (2^{271d+23} \pi^{10d+2} d^{130d+9})$.

The constant η that appears as a lower bound seems ridiculously small, but we cannot do better. Notice that this lower bound is much smaller than the one obtained in Lemma 3.1 at low density, with $n = |S_d|/(4\pi)^2$. We expect however that the lower bound is an increasing function of n for $0 \leqslant n \leqslant 1$, although we cannot prove it.

Proof. We have

$$E_{\Lambda,N} - |\Lambda| e(n) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \mathrm{d}k \Big[\Delta_-(k) \varepsilon_k - \Delta_+(k) \varepsilon_k \Big], \tag{3.42}$$

where

$$\begin{aligned} \Delta_+(k) &= \big(|\Lambda| - \rho(k) \big)\, \chi\, \big[\varepsilon_k < \varepsilon_{\mathrm{F}} \big] \\ \Delta_-(k) &= \rho(k)\, \chi\, \big[\varepsilon_k > \varepsilon_{\mathrm{F}} \big]. \end{aligned}$$

Notice that $\int \mathrm{d}k\, \Delta_-(k) = \int \mathrm{d}k\, \Delta_+(k)$. Then we both have

$$E_{\Lambda,N} - |\Lambda| e(n) \geqslant \begin{cases} \frac{1}{(2\pi)^d} \int \mathrm{d}k\, \Delta_-(k) (\varepsilon_k - \varepsilon_{\mathrm{F}}) \\ \frac{1}{(2\pi)^d} \int \mathrm{d}k\, \Delta_+(k) (\varepsilon_{\mathrm{F}} - \varepsilon_k). \end{cases} \tag{3.43}$$

And by Hölder, this implies

$$E_{\Lambda,N} - |\Lambda| e(n) \geqslant \Big(\frac{1}{(2\pi)^d} \int \mathrm{d}k\, [\Delta_\pm(k)]^{1/5} \Big)^5 \Big/ \Big(\frac{1}{(2\pi)^d} \int \mathrm{d}k\, |\varepsilon_k - \varepsilon_{\mathrm{F}}|^{-\frac14} \Big)^4. \tag{3.44}$$

One shows in Lemma A.1 (a) that the integral of $|\varepsilon_k - \varepsilon_{\mathrm{F}}|^{-\frac14}$ is bounded by 2.

Recall that $\{\varphi_j\}_{1 \leqslant j \leqslant |\Lambda|}$ are the eigenvectors of h_Λ. Let P_-, resp. P_+, be the projectors onto the first N eigenvectors, resp. the last $|\Lambda| - N$ eigenvectors. By (3.6), one has inequalities

$$\begin{aligned} \Delta_+(k) &\geqslant \frac{1}{(4d)^2} \|P_+ b_k\|^2 \qquad \text{if } \varepsilon_k < \varepsilon_{\mathrm{F}}, \\ \Delta_-(k) &\geqslant \frac{1}{(4d)^2} \|P_- b_k\|^2 \qquad \text{if } \varepsilon_k > \varepsilon_{\mathrm{F}}. \end{aligned} \tag{3.45}$$

Let us introduce sets A and A' by

$$\begin{aligned} A &= \{ k : \varepsilon_k < \varepsilon_{\mathrm{F}} \text{ and } |k - k_0| < \tfrac{\delta^3}{2^{25} d^{25/2}} \}, \\ A' &= \{ k : \varepsilon_k > \varepsilon_{\mathrm{F}} \text{ and } |k - k_0| < \tfrac{\delta^3}{2^{25} d^{25/2}} \}. \end{aligned} \tag{3.46}$$

We obtain a lower bound by substituting (3.45) into (3.44), and restricting the integrals to A and A'. Namely,

$$
\begin{aligned}
E_{\Lambda,N} - |\Lambda| e(n) &\geqslant \frac{1}{2^8 d^2} \Big(\frac{1}{(2\pi)^d} \int_A \mathrm{d}k \, \|P_+ b_k\|^{2/5} \Big)^5, \\
E_{\Lambda,N} - |\Lambda| e(n) &\geqslant \frac{1}{2^8 d^2} \Big(\frac{1}{(2\pi)^d} \int_{A'} \mathrm{d}k \, \|P_- b_k\|^{2/5} \Big)^5.
\end{aligned}
$$

Let $\tilde b_k = b_k / \|b_k\|$. From the assumption of the lemma, and using $\|h_\Lambda - \varepsilon\| \leqslant 4d$ and Lemma A.1 (d), we have that for all $k \in A \cup A'$,

$$
\frac{\|b_k\|^2}{|\partial\Lambda|} \geqslant \frac{\delta}{2^5 d^2}. \tag{3.47}
$$

Extracting a factor $|\partial\Lambda|$, and using the above inequality, we can write

$$
\begin{aligned}
E_{\Lambda,N} - |\Lambda| e(n) &\geqslant |\partial\Lambda| \frac{\delta}{2^{13} d^4 (2\pi)^{5d}} \Big(\int_A \mathrm{d}k \, \|P_+ \tilde b_k\|^{2/5} \Big)^5, \\
E_{\Lambda,N} - |\Lambda| e(n) &\geqslant |\partial\Lambda| \frac{\delta}{2^{13} d^4 (2\pi)^{5d}} \Big(\int_{A'} \mathrm{d}k \, \|P_- \tilde b_k\|^{2/5} \Big)^5.
\end{aligned} \tag{3.48}
$$

Consider $k \in A$. The assumption of the lemma for k_0, together with the bound for the gradient in Lemma A.1 (e), implies

$$
\frac{(b_k, (h_\Lambda - e_N)^2 b_k)}{|\partial\Lambda|} \geqslant \frac{\delta}{2}. \tag{3.49}
$$

Therefore

$$
(\tilde b_k, (h_\Lambda - e_N)^2 \tilde b_k) \geqslant \frac{\delta}{8d^2}. \tag{3.50}
$$

This can be rewritten as

$$
\sum_{j=1}^{|\Lambda|} |(\varphi_j, \tilde b_k)|^2 (e_j - e_N)^2 \geqslant \frac{\delta}{8d^2}, \tag{3.51}
$$

that is,

$$
\sum_{j=1}^{|\Lambda|} |(\varphi_j, \tilde b_k)|^2 (e_j^2 + e_N^2) \geqslant \frac{\delta}{8d^2} + 2e_N (\tilde b_k, h_\Lambda \tilde b_k). \tag{3.52}
$$

Hence

$$
(\tilde b_k, h_\Lambda \tilde b_k) \leqslant e_N + \sum_{j=1}^{|\Lambda|} |(\varphi_j, \tilde b_k)|^2 \Big(\frac{e_j^2}{2e_N} - \frac{e_N}{2} \Big) - \frac{\delta}{2^5 d^3}. \tag{3.53}
$$

The quantity in the brackets is negative for $j \leqslant N$. Observing that $e_N \geqslant \frac{e(|S_d|/(4\pi)^d)}{|S_d|/(4\pi)^d} \geqslant 1/2^{d+1}\pi^2$ (because $n \geqslant |S_d|/(4\pi)^d$ and using Lemma A.1 (c)), the bracket is bounded by $2^{d+4}\pi^2 d^2$. Therefore,

$$
(\tilde b_k, h_\Lambda \tilde b_k) \leqslant e_N + 2^{d+4}\pi^2 d^2 \, \|P_+ \tilde b_k\|^2 - \frac{\delta}{2^5 d^3}. \tag{3.54}
$$

On the other hand, for $k' \in A'$,

$$(\tilde{b}_{k'}, h_\Lambda \tilde{b}_{k'}) \geqslant \sum_{j=N+1}^{|\Lambda|} |(\varphi_j, \tilde{b}_{k'})|^2 e_j \geqslant e_{N+1} - 4d \|P_- \tilde{b}_{k'}\|^2. \tag{3.55}$$

Since $|k - k'| \leqslant \delta^3 / 2^{24} d^{25/2}$, we have from Lemma A.1 (g) and (3.47)

$$(\tilde{b}_{k'}, h_\Lambda \tilde{b}_{k'}) - (\tilde{b}_k, h_\Lambda \tilde{b}_k) \leqslant \frac{\delta}{2^6 d^3}. \tag{3.56}$$

Therefore

$$e_{N+1} - 4d \|P_- \tilde{b}_{k'}\|^2 \leqslant e_N + 2^{d+4} \pi^2 d^2 \|P_+ \tilde{b}_k\|^2 - \frac{\delta}{2^5 d^3} + \frac{\delta}{2^6 d^3}. \tag{3.57}$$

Clearly, $e_N \leqslant e_{N+1}$; then

$$\|P_+ \tilde{b}_k\|^2 + \tfrac{1}{2^{d+2} \pi^2 d} \|P_- \tilde{b}_{k'}\|^2 \geqslant \frac{\delta}{2^{d+10} \pi^2 d^5}. \tag{3.58}$$

We use now (3.48). The worst situation happends when $\|P_+ \tilde{b}_k\|^2$ is equal to the right side of the previous equation. Using Lemma A.1 (b) we finally get the lower bound of Lemma 3.3. □

Now we show that we can use Lemma 3.3 for all Λ such that Lemma 3.2 does not apply.

Let $a_x = \big((2d - \varepsilon) q_{x,i} \big)_{1 \leqslant i \leqslant d}$ and $Q_x = \big((1 + \delta_{ij}) q_{x,ij} \big)_{1 \leqslant i,j \leqslant d}$. More generally, we let a denote a vector with entries $(2d - \varepsilon) q_{x,i}$, and Q a matrix with entries $2 q_{x,ii}$ in the diagonal and $q_{x,ij}$ off the diagonal, that correspond to a possible configuration around x. With $c = (\cos k_i)_{1 \leqslant i \leqslant d}$, we introduce

$$F(c; a, Q) = (a, c) + \tfrac{1}{2} \operatorname{Tr} Q - (c, Qc). \tag{3.59}$$

This function appears when establishing a lower bound for $\|(h_\Lambda - \varepsilon) b_k\|^2$.

Let $\mathcal{Q}$ be the set of all matrices Q (for which there exists some compatible configuration); we introduce

$$\mathcal{Q}'' = \{ Q \in \mathcal{Q} : Q_{ii} \equiv 2 \text{ and } Q_{ij} + Q_{ji} = 4 \text{ for all } i \neq j \} \tag{3.60}$$

and

$$\mathcal{Q}' = \{ Q \notin \mathcal{Q}'' : Q_{ij} \not\equiv 0 \}. \tag{3.61}$$

The reason behind the definition of $\mathcal{Q}'$ is that we can provide a lower bound only if $F(c; a, Q)$ is not uniformly zero when k moves along the Fermi surface (i.e. with $\varepsilon_k = \varepsilon_{\mathrm{F}}$); and we can show that $F(c; a, Q)$ is not uniformly zero only for $Q \in \mathcal{Q}'$, see Lemma 3.5 below.

For given ε_{F}, we define

$$\mu(\varepsilon_{\mathrm{F}}) = \min_{a, Q \in \mathcal{Q}'} \min_{\varepsilon \in [0, 2d]} \max_{c : \varepsilon_k = \varepsilon_{\mathrm{F}}} |F(c; a, Q)|. \tag{3.62}$$

We state a lower bound involving $\mu(\varepsilon_{\mathrm{F}})$, and check below in Lemma 3.5 that $\mu(\varepsilon_{\mathrm{F}})$ is strictly positive for $\varepsilon_{\mathrm{F}} > 0$.

Lemma 3.4. *Let $d \geqslant 2$. For all finite Λ satisfying*

$$\#\{ x \in \partial\Lambda : q_{x,ij} \not\equiv 0 \} \geqslant \frac{1}{32 d^4} |\partial\Lambda|,$$

we have

$$\max_{k:\varepsilon_k=\varepsilon_{\mathrm{F}}} \|(h_\Lambda-\varepsilon)b_k\|^2 \;\geqslant\; \frac{\mu(\varepsilon_{\mathrm{F}})}{2^6 d^5 5^{d^2}}|\partial\Lambda|.$$

The factor $\frac{1}{32d^4}$ is arbitrary here, and has been taken such in order to complement the condition of Lemma 3.2.

Proof. Let us introduce

$$q_k(x) = \chi_{\partial\Lambda}(x) \sum_{e:x+e\notin\Lambda} \mathrm{e}^{-\mathrm{i}ke}\,. \tag{3.63}$$

By the definition of the discrete Laplacian,

$$\big[(h_\Lambda-\varepsilon)b_k\big](x) = \mathrm{e}^{-\mathrm{i}kx}\Big\{(2d-\varepsilon)q_k(x) - \sum_e \mathrm{e}^{-\mathrm{i}ke}\,q_k(x+e)\Big\}. \tag{3.64}$$

Let us denote by $r_k(x)$ the quantity inside the brackets above. Clearly, $\|(h_\Lambda-\varepsilon)b_k\|^2 = \|r_k\|^2$. Let $\mathcal{R}_a$, $a=1,\dots,2^d$, represents all combinations of inversions of some coordinates. We have the following inequality:

$$\frac{1}{2^d}\sum_{a=1}^{2^d}\|r_{\mathcal{R}_a k}\|^2 \;\geqslant\; \Big\|\frac{1}{2^d}\sum_{a=1}^{2^d} r_{\mathcal{R}_a k}\Big\|^2. \tag{3.65}$$

Indeed, starting from the RHS, we have in essence (with $0\leqslant a_i\leqslant 1$ and $\sum_i a_i = 1$)

$$\begin{aligned}\Big(\sum_i a_i\vec{v}_i,\sum_i a_i\vec{v}_i\Big) &= \sum_{i,j} a_i a_j(\vec{v}_i,\vec{v}_j)\\ &\leqslant \Big(\sum_i \sqrt{a_i}\sqrt{a_i}\|\vec{v}_i\|\Big)^2\\ &\leqslant \Big[\Big(\sum_i a_i\Big)^{1/2}\Big(\sum_i a_i\|\vec{v}_i\|^2\Big)^{1/2}\Big]^2\end{aligned} \tag{3.66}$$

which is the LHS of (3.65).

The RHS of (3.65) is clearly smaller than $\max_{k:\varepsilon_k=\varepsilon_{\mathrm{F}}}\|(h_\Lambda-\varepsilon)b_k\|^2$. One computes now $\sum_{a=1}^{2^d} r_{\mathcal{R}_a k}(x)$ for $x\in\partial\Lambda$. First,

$$\frac{1}{2^d}\sum_{a=1}^{2^d}(2d-\varepsilon)q_{\mathcal{R}_a k}(x) = (2d-\varepsilon)\sum_{i=1}^d q_{x,i}\cos k_i. \tag{3.67}$$

Second,

$$\begin{aligned}&-\frac{1}{2^d}\sum_{a=1}^{2^d}\sum_{e:x+e\in\partial\Lambda}\mathrm{e}^{-\mathrm{i}\mathcal{R}_a k\,e}\sum_{e':x+e+e'\notin\Lambda}\mathrm{e}^{-\mathrm{i}\mathcal{R}_a k\,e'}\\ &\qquad= -\sum_{i=1}^d q_{x,ii}\cos(2k_i) - \frac12\sum_{i,j:i\neq j} q_{x,ij}\big[\cos(k_i+k_j)+\cos(k_i-k_j)\big] \qquad (3.68)\\ &\qquad= -2\sum_{i=1}^d q_{x,ii}\cos^2 k_i + \sum_{i=1}^d q_{x,ii} - \sum_{i,j:i\neq j} q_{x,ij}\cos k_i\cos k_j.\end{aligned}$$

We used $\cos(2k_i) = 2\cos^2 k_i - 1$, and the bracket in the second line is $[\cdot] = 2\cos k_i\cos k_j$.

Gathering (3.67) and (3.68), we obtain

$$\frac{1}{2^d}\sum_{a=1}^{2^d} r_{\mathcal{R}_a k}(x) = F(c; a_x, Q_x). \tag{3.69}$$

One can check that whenever $Q_x \notin \mathcal{Q}'$ and differs from 0, there exists a neighbor y that belongs to $\mathcal{Q}'$. Then the condition of the lemma implies that

$$\#\{x \in \partial\Lambda : Q_x \in \mathcal{Q}'\} \geqslant \frac{1}{2^6 d^5}|\partial\Lambda|. \tag{3.70}$$

Furthermore, $\mathcal{Q}'$ has less than 5^{d^2} elements since $0 \leqslant Q_{ij} \leqslant 4$; then for any Λ that satisfies the assumption of the lemma there exists $Q \in \mathcal{Q}'$ such that

$$\#\{x \in \partial\Lambda : Q_x = Q\} \geqslant \frac{1}{2^6 d^5 5^{d^2}}|\partial\Lambda|. \tag{3.71}$$

We get a lower bound for $\|(h_\Lambda - \varepsilon)b_k\|^2$ by considering only those sites, i.e.

$$\max_{k:\varepsilon_k=\varepsilon_{\mathrm{F}}} \|(h_\Lambda - \varepsilon)b_k\|^2 \geqslant \sum_{x\in\partial\Lambda:Q_x=Q} \max_{c:\varepsilon_k=\varepsilon_{\mathrm{F}}} |F(c; a_x, Q_x)| \geqslant \frac{\mu(\varepsilon_{\mathrm{F}})}{2^6 d^5 5^{d^2}}|\partial\Lambda| \tag{3.72}$$

uniformly in $\varepsilon \in [0, 2d]$. ☐

There remains to be checked that $\mu(\varepsilon_{\mathrm{F}})$ differs from 0.

Lemma 3.5. *For all $\varepsilon_{\mathrm{F}} > 0$, we have $\mu(\varepsilon_{\mathrm{F}}) \neq 0$.*

Proof. We proceed *ab absurdo* and explore ways where $F(c; a, Q)$ could be uniformly zero.

The constraint $\varepsilon_k = \varepsilon_{\mathrm{F}}$ takes a simple form, namely $(u, c) = d - \frac{1}{2}\varepsilon_{\mathrm{F}}$. Furthermore, c satisfies $|c|_\infty \leqslant 1$; if $\varepsilon_{\mathrm{F}} \neq 0$, we can find δc such that $|c+\delta c|_\infty \leqslant 1$ and $(u, c+\delta c) = d - \frac{1}{2}\varepsilon_{\mathrm{F}}$ — in which case δc must be perpendicular to u. The condition $F(c+\delta c; a, Q) = F(c; a, Q)$ for all $\delta c \perp u$ implies that $a - 2Qc \parallel u$. This should also be true when c is replaced with $c + \delta c$, hence $Q\delta c \parallel u$ for all $\delta c \perp u$. Now take $(\delta c)_k = \delta_{ik} - \delta_{jk}$. We have

$$\begin{aligned}(Q\delta c)_i &= Q_{ii} - Q_{ij} \\ (Q\delta c)_j &= -Q_{jj} + Q_{ji},\end{aligned} \tag{3.73}$$

and these two components must be equal, since $Q\delta c$ is parallel to u. Hence $Q_{ii} + Q_{jj} = Q_{ij} + Q_{ji}$, or

$$2q_{x,ii} + 2q_{x,jj} = q_{x,ij} + q_{x,ji}. \tag{3.74}$$

In this case $F(c; a, Q)$ takes the form

$$F(c; a, Q) = (2d - \varepsilon)\sum_{i=1}^d q_{x,i}c_i - (2d - \varepsilon_{\mathrm{F}})\sum_{i=1}^d q_{x,ii}c_i + \sum_{i=1}^d q_{x,ii}. \tag{3.75}$$

Since $Q \in \mathcal{Q}'$ we have $q_{x,ij} \not\equiv 0$; if $(u, c) = 0$, one can take $c = 0$, and $F(c; a, Q)$ is strictly positive, so we can suppose $(u, c) \neq 0$.

Let $s = \sum_i q_{x,ii}/(u, c)$, and v the vector with components

$$v_i = (2d - \varepsilon)q_{x,i} - (2d - \varepsilon_{\mathrm{F}})q_{x,ii} + s. \tag{3.76}$$

Then $F(c; a, Q) = (v, c)$. If we require this to be zero for $c \parallel u$, then we need $v \perp u$. But we also require $(v, c + \delta c) = (v, c)$ for all $\delta c \perp u$, hence $v \parallel u$. So v must be zero, i.e.

$$(2d - \varepsilon)q_{x,i} - (2d - \varepsilon_{\mathrm{F}})q_{x,ii} + s = 0 \tag{3.77}$$

for all $1 \leqslant i \leqslant d$.

We also have $q_{x,i} + q_{x,ii} \leqslant 2$, and $q_{x,ii}$ cannot be always equal to 2. If $s \neq 0$, one checks that necessarily $q_{x,ii} \equiv 1$, which is impossible because $Q \in \mathcal{Q}'$. Hence $F(c; a, Q)$ cannot be uniformly zero when moving along the Fermi surface. □

4. Finite U

We consider now the Falicov-Kimball model with finite repulsion U, and establish a lower bound for the ground state energy of N electrons in a configuration specified by Λ. More precisely, we show that when decreasing the repulsion U, one does not lower the energy more than const $\cdot |\partial\Lambda|/U$.

For any Λ, the spectrum of $h^U_{\Omega,\Lambda}$ is included in $[0, 4d] \cup [U, U + 4d]$. When $U > 4d$, eigenstates with energy in $[0, 4d]$ shows exponential decay outside of Λ; and eigenstates with energy in $[U, U + 4d]$ show exponential decay inside Λ. Hence Λ and $\Omega \setminus \Lambda$ are essentially decorrelated, and the situation is close to that with $U = \infty$.

The following proposition compares the energies of electrons with finite and infinite U. It is useful to introduce $\eta(U)$,

$$\eta(U) = \Big(\frac{2d}{U - 2d}\Big)^2 \sum_{j=1}^{d} \Big[\frac{(U - 2d)^2}{U(U - 4d)}\Big]^j = \frac{(U - 2d)^{2d}}{(U(U - 4d))^d} - 1. \tag{4.1}$$

Notice that $\lim_{U\to\infty} U^2 \eta(U) = 4d^3$, as it easily comes out from the middle expression.

Proposition 4.1. *If $U > 4d$, we have*

$$E^U_{\Lambda,N} \geqslant E_{\Lambda,N} - \gamma(U)|\partial\Lambda|,$$

with

$$\gamma(U) = \frac{8d^2}{U - 2d} + d\, 2^{d+2} \eta(U).$$

Proof. First, we remark that eigenvectors of $h^U_{\Omega,\Lambda}$ with eigenvalue smaller than $4d$ have exponential decay outside of Λ. Indeed, for $x \notin \Lambda$ the Schrödinger equation can be written

$$\varphi_j(x) = \frac{\sum_e \varphi_j(x + e)}{U + 2d - e_j}. \tag{4.2}$$

If $e_j \leqslant 4d$, we have

$$\sum_{j=1}^{|\Lambda|} |\varphi_j(x)|^2 \leqslant \frac{\sum_{j=1}^{|\Lambda|} 2d \sum_e |\varphi_j(x + e)|^2}{(U - 2d)^2}. \tag{4.3}$$

Using this inequality, we can proceed by induction on the distance between x and Λ. The induction hypothesis is that the following holds true

$$\sum_{j=1}^{|\Lambda|} |\varphi_j(x)|^2 \leqslant \Big(\frac{2d}{U - 2d}\Big)^{2n} \tag{4.4}$$

for any x such that dist $(x, \Lambda) \geqslant n$. As a result, we have

$$\sum_{j=1}^{|\Lambda|} |\varphi_j(x)|^2 \leqslant \Big(\frac{2d}{U - 2d}\Big)^{2\,\mathrm{dist}\,(x,\Lambda)}. \tag{4.5}$$

Let us introduce

$$\tilde\rho_{xy} = \sum_{j=1}^N \chi_\Lambda(x)\,\varphi_j^*(x)\,\varphi_j(y)\,\chi_\Lambda(y). \tag{4.6}$$

We show that $E^U_{\Lambda,N}$ is bounded below by $\operatorname{Tr}\tilde\rho h_\Lambda$, up to a contribution no greater than const $|\partial\Lambda|/U$. Recall that h_Λ is the Hamiltonian with infinite repulsions. If P_Λ is the projector onto the domain Λ, let $\tilde\varphi_j = P_\Lambda \varphi_j$.

$$\begin{aligned} E^U_{\Lambda,N} &= \sum_{j=1}^N \Big(\sum_{\{x,y\}:|x-y|=1} |\varphi_j(x)-\varphi_j(y)|^2 + U \sum_{x\notin\Lambda} |\varphi_j(x)|^2 \Big) \\ &\geqslant \sum_{j=1}^N \Big(\sum_{\{x,y\}:|x-y|=1} |\tilde\varphi_j(x)-\tilde\varphi_j(y)|^2 + \sum_{\substack{\{x,y\}\not\subset\Lambda \\ |x-y|=1}} |\varphi_j(x)-\varphi_j(y)|^2 - \sum_{\substack{x\in\Lambda,y\notin\Lambda \\ |x-y|=1}} |\varphi_j(x)|^2 \Big) \\ &\geqslant \operatorname{Tr}\tilde\rho h_\Lambda - 2\sum_{j=1}^N \sum_{\substack{x\in\Lambda,y\notin\Lambda \\ |x-y|=1}} |\varphi_j(x)|\,|\varphi_j(y)|. \end{aligned} \tag{4.7}$$

By the Schwarz inequality, the last term is smaller than

$$2\Big(\sum_{\substack{x\in\Lambda,y\notin\Lambda \\ |x-y|=1}} \sum_{j=1}^N |\varphi_j(x)|^2 \Big)^{1/2} \Big(\sum_{\substack{x\in\Lambda,y\notin\Lambda \\ |x-y|=1}} \sum_{j=1}^N |\varphi_j(y)|^2 \Big)^{1/2} \leqslant \frac{8d^2}{U-2d}|\partial\Lambda|. \tag{4.8}$$

We used (4.5) with dist (x,Λ) being respectively 0 and 1, in order to control the quantities in both brackets.

Recall that e_j denotes the j-th eigenvalue of the Hamiltonian h_Λ; that is, with infinite repulsions. Let us introduce the projector P_j onto the corresponding eigenstate. Then

$$\operatorname{Tr}\tilde\rho h_\Lambda = \sum_{j=1}^{|\Lambda|} e_j \operatorname{Tr}\tilde\rho P_j \equiv \sum_{j=1}^{|\Lambda|} e_j\, n_j, \tag{4.9}$$

where the n_j satisfy $0 \leqslant n_j \leqslant 1$, and $\sum_j n_j = \operatorname{Tr}\tilde\rho$. By the bathtub principle [LL], we obtain the lower bound

$$\operatorname{Tr}\tilde\rho h_\Lambda \geqslant \sum_{j=1}^{\operatorname{Tr}\tilde\rho} e_j. \tag{4.10}$$

There remains to show that $\operatorname{Tr}\tilde\rho$ is close to N. We have

$$\begin{aligned} N - \operatorname{Tr}\tilde\rho &= \sum_{x\notin\Lambda}\sum_{j=1}^N |\varphi_j(x)|^2 \leqslant \sum_{n=1}^\infty \#\{x : \operatorname{dist}(x,\Lambda)=n\} \Big(\frac{2d}{U-2d}\Big)^{2n} \\ &\leqslant |\partial\Lambda| \sum_{n=1}^\infty 2^d \binom{n+d-1}{d-1} \Big(\frac{2d}{U-2d}\Big)^{2n} = 2^d \eta(U) |\partial\Lambda|. \end{aligned} \tag{4.11}$$

We bounded $\#\{\cdot\} \leqslant 2^d\binom{n+d-1}{d-1}|\partial\Lambda|$. Since $e_j \leqslant 4d$, we obtain the proposition. □

5. Upper bound

We establish now an upper bound for the sum of the first N eigenvalues in a finite domain Λ, for the case of infinite repulsion. The bound carries over to finite U, since $E^U_{\Lambda,N}$ is increasing in U.

The strategy is to average h_Λ over a huge box. The 'strength' of the averaged Hamiltonian depends on the number of bonds in Λ, which is roughly $2d|\Lambda| - |\partial\Lambda|$. The averaged Hamiltonian is, up to a factor, the hopping matrix in the huge box, and its ground state energy is easy to compute in the thermodynamic limit. This can be compared to $E_{\Lambda,N}$ by concavity of the sum of lowest eigenvalues of self-adjoint operators. The result is

Proposition 5.1. *The sum of the first N eigenvalues of the Laplace operator in a domain Λ with Dirichlet boundary conditions, satisfies the upper bound*

$$E_{\Lambda,N} \leqslant |\Lambda| e(n) + |\partial\Lambda|(2dn - e(n)).$$

Proof. Let L be a multiple of $|\Lambda|$, and N_L be such that $N_L/L^d = N/|\Lambda|$. We consider a box $\{1,\dots,L\}^d$. We introduce $\tilde\varepsilon = \frac{1}{2}(e_N + e_{N+1})$. Let $\mathcal{R}_a$, $a = 1,\dots,L^d d!$, represent a translation possibly followed by an axis permutation. We define the averaged Hamiltonian

$$\bar h_{L,\Lambda} = \frac{1}{L^d d!} \sum_{a=1}^{L^d d!} \Big(h_{\mathcal{R}_a\Lambda} - \tilde\varepsilon \mathbb{1}_{\mathcal{R}_a\Lambda} \Big). \tag{5.1}$$

Then

$$\begin{aligned} S_{N_L}(\bar h_{L,\Lambda}) &\geqslant \frac{1}{L^d d!} \sum_{a=1}^{L^d d!} S_{N_L}\big(h_{\mathcal{R}_a\Lambda} - \tilde\varepsilon \mathbb{1}_{\mathcal{R}_a\Lambda}\big) \\ &= S_N(h_\Lambda - \tilde\varepsilon \mathbb{1}_\Lambda). \end{aligned} \tag{5.2}$$

Indeed, all summands in the above equation are equal, and the Hamiltonian $h_\Lambda - \tilde\varepsilon\mathbb{1}_\Lambda$ has no more than N negative eigenvalues, and at least $L^d - |\Lambda|$ zero eigenvalues. The RHS is equal to $E_{\Lambda,N} - N\tilde\varepsilon$.

Let Q_i be the number of sites in Λ that have i neighbors in Λ. We have $|\Lambda| = \sum_{i=0}^{2d} Q_i$ and $|\partial\Lambda| = \sum_{i=0}^{2d-1} Q_i$; and the number of bonds in Λ is $\frac{1}{2}\sum_{i=0}^{2d} iQ_i$. Then the averaged Hamiltonian is

$$\big(\bar h_{L,\Lambda}\big)_{xy} = -\frac{t}{L^d}\delta_{|x-y|=1} + (2d - \tilde\varepsilon)\frac{|\Lambda|}{L^d}\delta_{xy}, \tag{5.3}$$

with

$$t = \frac{1}{2d}\sum_{i=0}^{2d} iQ_i. \tag{5.4}$$

Let $Q = \sum_{i=0}^{2d} \frac{2d-i}{2d} Q_i$; then $t = |\Lambda| - Q$ and $Q \leqslant |\partial\Lambda|$. One easily checks that

$$\bar h_{L,\Lambda} = \frac{|\Lambda|}{L^d} h_{\{1,\dots,L\}^d} + \frac{Q}{L^d}\big(2d\mathbb{1}_{\{1,\dots,L\}^d} - h_{\{1,\dots,L\}^d}\big) - \tilde\varepsilon\frac{|\Lambda|}{L^d}\mathbb{1}_{\{1,\dots,L\}^d}. \tag{5.5}$$

Notice that all operators commute. In (5.2), the terms involving $\tilde\varepsilon$ cancel, since $S_{N_L}(\mathbb{1}_{\{1,\dots,L\}^d}) = N_L$, and $N_L\frac{|\Lambda|}{L^d} = N$. Now, as $L \to \infty$,

$$\frac{1}{L^d} S_{N_L}(h_{\{1,\dots,L\}^d}) \to e(n). \tag{5.6}$$

Therefore (5.2) implies

$$|\Lambda| e(n) + Q(2dn - e(n)) \;\geqslant\; E_{\Lambda,N}. \tag{5.7}$$

$\square$

6. Positive electronic temperature

This section considers the electronic free energy at positive temperature, for a fixed configuration of classical particles. We will see that the inequalities satisfied by the sums over lowest eigenvalues have an extension to free energies.

6.1. Lower bound for $U = \infty$.

We start with $U \to \infty$. Let $F_\Lambda(\beta,\mu) = -\frac{1}{\beta}\log \operatorname{Tr} \mathrm{e}^{-\beta H_\Lambda}$ where the trace is taken in the Fock space of antisymmetric wave functions on Λ, and $H_\Lambda \equiv H^{U=\infty}_{\Omega,\Lambda}$ is the second quantized form of the one-particle Hamiltonian h_Λ defined by (2.1).

Proposition 6.1. *For all finite Λ, one has the lower bound*

$$F_\Lambda(\beta,\mu) - |\Lambda| f(\beta,\mu) \;\geqslant\; \bar\alpha(\beta,\mu)|\partial\Lambda|,$$

where $\bar\alpha(\beta,\mu) > 0$ satisfies $\lim_{\beta\to\infty} \bar\alpha(\beta,\mu) > 0$ if $0 < \mu < 4d$.

Proof. The fermionic free energy $F_\Lambda(\beta,\mu)$ can be expressed in terms of the eigenvalues of h_Λ,

$$F_\Lambda(\beta,\mu) = -\frac{1}{\beta}\sum_{j=1}^{|\Lambda|} \log\bigl(1 + \mathrm{e}^{-\beta(e_j-\mu)}\bigr). \tag{6.1}$$

In order to compare this with the corresponding infinite-volume expression (1.9), we partition the Brillouin zone $[-\pi,\pi]^d$ according to the level sets of the function ε_k; more precisely, we define measures μ_j, $1 \leqslant j \leqslant |\Lambda|$, by

$$\mathrm{d}\mu_j(k) = \frac{|\Lambda|}{(2\pi)^d}\; \chi\bigl[\varepsilon_{\mathrm F}(\tfrac{j-1}{|\Lambda|}) < \varepsilon(k) < \varepsilon_{\mathrm F}(\tfrac{j}{|\Lambda|})\bigr]\,\mathrm{d}k. \tag{6.2}$$

Notice that $\int \mathrm{d}\mu_j(k) = 1$ and $\frac{1}{|\Lambda|}\sum_{j=1}^{|\Lambda|} \mathrm{d}\mu_j(k) = \frac{\mathrm{d}k}{(2\pi)^d}$. Next we introduce e_j^*, that are equal to ε_k averaged over μ_j:

$$e_j^* = \int \mathrm{d}\mu_j(k)\,\varepsilon_k. \tag{6.3}$$

The ground state energy (1.3) of a density $N/|\Lambda|$ of electrons in $\mathbb{Z}^d$ can then be written as

$$e(N/|\Lambda|) = \frac{1}{|\Lambda|}\sum_{j=1}^N e_j^*. \tag{6.4}$$

From the lower bound without a boundary term, we have

$$\sum_{j=1}^N e_j > \sum_{j=1}^N e_j^*, \tag{6.5}$$

for all $N < |\Lambda|$, and equality when $N = |\Lambda|$.

Actually, inequality (6.5) can be strengthened by introducing a term depending on the boundary of Λ. In Theorem 1.1, $\alpha(n)$ can be taken to be increasing in n for $n \leqslant \frac{1}{2}$. Also,

$\alpha(1-n)=\alpha(n)$. Therefore there exists a function $a(\varepsilon)$, with $a(\varepsilon)>0$ for $0<\varepsilon<2d$, $a(4d-\varepsilon)=-a(\varepsilon)$, and

$$\alpha(n)=\frac{1}{(2\pi)^d}\int_{\varepsilon_k<\varepsilon_{\mathrm{F}}}\mathrm{d}k\,a(\varepsilon_k). \tag{6.6}$$

Next we define

$$e'_j=\int\mathrm{d}\mu_j(k)\,\big(\varepsilon_k+\tfrac{|\partial\Lambda|}{|\Lambda|}a(\varepsilon_k)\big); \tag{6.7}$$

then the following is stronger than (6.5) and holds true,

$$\sum_{j=1}^N e_j\;\geqslant\;\sum_{j=1}^N e'_j. \tag{6.8}$$

With $a(\varepsilon)$ chosen appropriately both sequences (e_j) and (e'_j) are increasing, and the inequality above is an equality when $N=|\Lambda|$. The sequence (e_j) is said to 'majorize' (e'_j). We can apply an inequality due to Hardy, Littlewood and Pólya (and independently found by Karamata); see [Mit] page 164. For any concave function g, we have

$$\sum_{j=1}^{|\Lambda|}g(e_j)\;\geqslant\;\sum_{j=1}^{|\Lambda|}g(e'_j). \tag{6.9}$$

(Conversely, if (6.9) holds for all concave g, then (e_j) majorizes (e'_j).) We use this inequality with

$$g(e)=-\frac{1}{\beta}\log(1+\mathrm{e}^{-\beta(e-\mu)}), \tag{6.10}$$

which is concave. We get

$$F_\Lambda(\beta,\mu)\;\geqslant\;\sum_{j=1}^{|\Lambda|}g(e'_j)\;\geqslant\;\frac{|\Lambda|}{(2\pi)^d}\int_{[-\pi,\pi]^d}\mathrm{d}k\,g\big(\varepsilon_k+\tfrac{|\partial\Lambda|}{|\Lambda|}a(\varepsilon_k)\big), \tag{6.11}$$

where the last step is Jensen's inequality. Then

$$\frac{1}{|\Lambda|}F_\Lambda(\beta,\mu)-f(\beta,\mu)\;\geqslant\;\frac{1}{(2\pi)^d}\int\mathrm{d}k\,\big\{g\big(\varepsilon_k+\tfrac{|\partial\Lambda|}{|\Lambda|}a(\varepsilon_k)\big)-g(\varepsilon_k)\big\}. \tag{6.12}$$

In the limit $\beta\to\infty$, we have

$$g(e)=\begin{cases}e-\mu & \text{if } e<\mu\\ 0 & \text{if } e\;\geqslant\;\mu.\end{cases} \tag{6.13}$$

As a result, for all $0<\mu<4d$ we get a lower bound for large β that is uniform in the limit $\beta\to\infty$.

One also gets a lower bound by using concavity of g, that holds for all temperatures, but that is not uniform in β:

$$\begin{aligned}\frac{1}{|\Lambda|}F_\Lambda(\beta,\mu) - f(\beta,\mu) &\geqslant \frac{1}{(2\pi)^d}\int \mathrm{d}k \int_{\varepsilon_k}^{\varepsilon_k + \frac{|\partial\Lambda|}{|\Lambda|}a(\varepsilon_k)} \mathrm{d}e\, g'(e) \\ &= \frac{1}{(2\pi)^d}\int \mathrm{d}k \Big\{ \tfrac{|\partial\Lambda|}{|\Lambda|} a(\varepsilon_k) g'(\varepsilon_k) - O(a(\varepsilon_k)^2) \Big\} \\ &= \frac{|\partial\Lambda|}{|\Lambda|}\frac{1}{(2\pi)^d}\int_{\varepsilon_k<2d} \mathrm{d}k\, a(\varepsilon_k) \Big\{ g'(\varepsilon_k) - g'(4d-\varepsilon_k) - O(a(\varepsilon_k))\Big\}.\end{aligned} \tag{6.14}$$

The integrand in the last line is strictly positive if $a(\varepsilon_k)$ is small enough, and chosen to vanish appropriately as $\varepsilon_k \to 2d$. ☐

6.2. **Lower bound with finite U.** We extend now the results of the previous section to the case of finite repulsion U. As we noted in Section 4, when $U > 4d$ all eigenstates have exponential decay, either in Λ or in $\Omega \setminus \Lambda$. We show that the total free energy in Ω is equal to a term involving $\Omega \setminus \Lambda$ only, plus a term involving Λ only, up to a correction of order $|\partial\Lambda|/U$.

Proposition 6.2.

$$F^U_{\Omega,\Lambda}(\beta,\mu) \geqslant F_\Lambda(\beta,\mu) + F_{\Omega\setminus\Lambda}(\beta,\mu-U) - \bar\gamma(U)|\partial\Lambda|$$

with

$$\bar\gamma(U) = (2dU + 4d + 8d^2)2^d\eta(U) + \frac{(4d)^2}{U-2d},$$

and $\eta(U)$ *is defined in* (4.1). *Notice that* $\lim_{U\to\infty} U\bar\gamma(U) = 16d^2 + 8d^4 2^d$.

Proof. Let us introduce

$$\tilde\varphi_j(x) = \begin{cases} \varphi_j(x) & \text{if } 1 \leqslant j \leqslant |\Lambda| \text{ and } x\in\Lambda, \text{ or if } |\Lambda| < j \leqslant |\Omega| \text{ and } x \notin \Lambda \\ 0 & \text{otherwise.}\end{cases} \tag{6.15}$$

We assume $N > |\Lambda|$ (otherwise, replace $|\Lambda|$ by N in the next expressions, and ignore the sums whose initial number is greater than the final one). Then

$$\begin{aligned}\sum_{j=1}^N e^U_j = \sum_{j=1}^{|\Lambda|}\Big(&\sum_{\substack{\{x,y\}\\|x-y|=1}} |\tilde\varphi_j(x) - \tilde\varphi_j(y)|^2 + \sum_{\substack{\{x,y\}\not\subset\Lambda\\|x-y|=1}} |\varphi_j(x)-\varphi_j(y)|^2 \\ &- \sum_{\substack{x\in\Lambda, y\notin\Lambda\\|x-y|=1}} |\varphi_j(x)|^2 + U\sum_{x\notin\Lambda}|\varphi_j(x)|^2\Big) \\ + \sum_{j=|\Lambda|+1}^N \Big(&\sum_{\substack{\{x,y\}\\|x-y|=1}} |\tilde\varphi_j(x) - \tilde\varphi_j(y)|^2 + \sum_{\substack{\{x,y\}\not\subset\Lambda^{\rm c}\\|x-y|=1}} |\varphi_j(x)-\varphi_j(y)|^2 \\ &- \sum_{\substack{x\notin\Lambda, y\in\Lambda\\|x-y|=1}} |\varphi_j(x)|^2 + U\sum_{x\notin\Lambda}|\varphi_j(x)|^2\Big).\end{aligned} \tag{6.16}$$

We proceed as in Section 4 and define

$$\begin{aligned}\tilde\rho_{xy} &= \sum_{j=1}^{|\Lambda|} \chi_\Lambda(x)\varphi_j^*(x)\varphi_j(y)\chi_\Lambda(y),\\ \tilde\rho'_{xy} &= \sum_{j=|\Lambda|+1}^{N} \chi_{\Lambda^c}(x)\varphi_j^*(x)\varphi_j(y)\chi_{\Lambda^c}(y).\end{aligned} \tag{6.17}$$

Then

$$\sum_{j=1}^N e_j^U \;\geqslant\; \operatorname{Tr}\tilde\rho h_\Lambda + \operatorname{Tr}\tilde\rho'[h_{\Omega\setminus\Lambda}+U] - 2\sum_{j=1}^N \sum_{\substack{x\in\Lambda, y\notin\Lambda\\ |x-y|=1}} |\varphi_j(x)|\,|\varphi_j(y)|. \tag{6.18}$$

The inequality (4.10) is still valid, for both $\tilde\rho$ and $\tilde\rho'$. Hence

$$\sum_{j=1}^N e_j^U \;\geqslant\; \sum_{j=1}^{\operatorname{Tr}\tilde\rho} e_j + \sum_{j=|\Lambda|+1}^{|\Lambda|+1+\operatorname{Tr}\tilde\rho'} (\bar e_j + U) - 2\sum_{j=1}^N \sum_{\substack{x\in\Lambda, y\notin\Lambda\\ |x-y|=1}} |\varphi_j(x)|\,|\varphi_j(y)|. \tag{6.19}$$

Here, $\bar e_j$, $|\Lambda| < j \;\leqslant\; |\Omega|$ are the eigenvalues of the operator $h_{\Omega\setminus\Lambda}$.

We define

$$\delta_j = \begin{cases} 4d\sum_{x\notin\Lambda}|\varphi_j(x)|^2 + 2\sum_{\substack{x\in\Lambda, y\notin\Lambda\\ |x-y|=1}}|\varphi_j(x)|\,|\varphi_j(y)| & \text{if } 1 \;\leqslant\; j \;\leqslant\; |\Lambda| \\ (4d+U)\sum_{x\in\Lambda}|\varphi_j(x)|^2 + 2\sum_{\substack{x\in\Lambda, y\notin\Lambda\\ |x-y|=1}}|\varphi_j(x)|\,|\varphi_j(y)| & \text{if } |\Lambda| < j \;\leqslant\; |\Omega|. \end{cases} \tag{6.20}$$

Then (6.19) takes the simpler form

$$\sum_{j=1}^N e_j^U \;\geqslant\; \sum_{j=1}^{|\Lambda|}(e_j - \delta_j) + \sum_{j=|\Lambda|+1}^{N} (\bar e_j + U - \delta_j). \tag{6.21}$$

The sequence in the RHS is not necessarily increasing, but one gets a lower bound by rearranging the terms. Hence one can apply Hardy, Littlewood, Pólya inequality. Indeed, it also works when the total sum over elements of the sequences are not equal, provided the concave function is increasing — which is the case with $g(e)$. One obtains

$$\sum_{j=1}^{|\Omega|} g(e_j^U) \;\geqslant\; \sum_{j=1}^{|\Lambda|} g(e_j - \delta_j) + \sum_{j=|\Lambda|+1}^{|\Omega|} g(\bar e_j + U - \delta_j). \tag{6.22}$$

We use now $g(e-\delta) \;\geqslant\; g(e) - \delta$, and we find

$$F^U_{\Omega,\Lambda}(\beta,\mu) \;\geqslant\; F_\Lambda(\beta,\mu) + F_{\Omega\setminus\Lambda}(\beta,\mu-U) - \sum_{j=1}^{|\Omega|}\delta_j. \tag{6.23}$$

The remaining effort consists in estimating the sum of δ_j, using exponential decay of eigenfunctions φ_j either in Λ or in $\Omega \setminus \Lambda$. Retracing (4.11) and (4.8), we get

$$\begin{aligned}\sum_{j=1}^{|\Lambda|} \delta_j &\leqslant 4d\, 2^d \eta(U)|\partial\Lambda| + \frac{8d^2}{U-2d}|\partial\Lambda|, \\ \sum_{j=|\Lambda|+1}^{|\Omega|} \delta_j &\leqslant (U+4d)\, 2^d \eta(U)|\partial(\Omega\setminus\Lambda)| + \frac{8d^2}{U-2d}|\partial\Lambda|. \end{aligned} \tag{6.24}$$

Notice that the last term can be written with $|\partial\Lambda|$ instead of $|\partial(\Omega\setminus\Lambda)|$, as can be seen from (4.8). We use $\partial(\Omega\setminus\Lambda)| \leqslant 2d|\partial\Lambda|$, and we finally obtain

$$\sum_{j=1}^{|\Omega|} \delta_j \leqslant (2dU + 4d + 8d^2)\, 2^d \eta(U)|\partial\Lambda| + \frac{(4d)^2}{U-2d}|\partial\Lambda|. \tag{6.25}$$

□

6.3. **Upper bound.** We turn to the upper bound for the electronic free energy. We first notice that the free energy is raised when one decorrelates the domain occupied by the classical particles, from the empty domain. The following proposition applies to all finite subsets of $\mathbb{Z}^d$, and it also applies when Ω is a finite d-dimensional torus.

Proposition 6.3. *We have the upper bounds*

- $F^U_{\Omega,\Lambda}(\beta,\mu) \leqslant F_\Lambda(\beta,\mu) + F_{\Omega\setminus\Lambda}(\beta,\mu-U)$.
- $F_\Lambda(\beta,\mu) \leqslant |\Lambda| f(\beta,\mu) + \frac{1}{1+\mathrm{e}^{-\beta\mu}}\big(\frac{4\pi\sqrt{d}}{|S_d|^{1/d}}|\Lambda|^{\frac{d-1}{d}} + 2d|\partial\Lambda|\big)$.

Notice that the isoperimetric inequality implies that for all finite $\Lambda \subset \mathbb{Z}^d$, $|\Lambda|^{\frac{d-1}{d}} \leqslant |\partial\Lambda|$. This does not hold, however, when Λ is e.g. a box with periodic boundary conditions.

Proof. The Peierls inequality allows to write

$$\operatorname{Tr} \mathrm{e}^{-\beta(H^U_{\Omega,\Lambda} - \mu N_\Omega)} \geqslant \sum_j \mathrm{e}^{-\beta(\psi_j, [H^U_{\Omega,\Lambda} - \mu N_\Omega]\psi_j)}, \tag{6.26}$$

for any set of orthonormal functions $\{\psi_j\}$ (in the Fock space of antisymmetric wave functions on Ω). We can choose the ψ_j to be eigenfunctions of H_Λ and $H_{\Omega\setminus\Lambda}$ — decorrelating Λ and $\Omega\setminus\Lambda$. In $\Omega\setminus\Lambda$, the free electrons experience a uniform potential U; the energy levels are given by the spectrum of $h_{\Omega\setminus\Lambda}$ plus U. This only shifts the chemical potential, so that we obtain the first claim of the proposition.

Now we estimate $F_\Lambda(\beta,\mu)$. Let us introduce

$$\tilde e_j = \big(1 - \tfrac{|\partial\Lambda|}{|\Lambda|}\big)e^*_j + 2d\tfrac{|\partial\Lambda|}{|\Lambda|} = \int \mathrm{d}\mu_j(k)\big[\varepsilon_k + (2d - \varepsilon_k)\tfrac{|\partial\Lambda|}{|\Lambda|}\big]; \tag{6.27}$$

then $\tilde e_j \leqslant \tilde e_{j+1}$, $\sum_{j=1}^{|\Lambda|} \tilde e_j = \sum_{j=1}^{|\Lambda|} e^*_j$, and the upper bound for the ground state energy can be cast in the form

$$\sum_{j=1}^N e_j \leqslant \sum_{j=1}^N \tilde e_j. \tag{6.28}$$

This allows to summon again the Hardy, Littlewood, Pólya inequality, and we get

$$F_\Lambda(\beta,\mu) \leqslant \sum_{j=1}^{|\Lambda|} g\Big(\int \mathrm{d}\mu_j(k)\big[\varepsilon_k + (2d-\varepsilon_k)\tfrac{|\partial\Lambda|}{|\Lambda|}\big]\Big). \tag{6.29}$$

The derivative of $g(e)$ satisfies

$$0 < g'(e) \leqslant \frac{1}{1+\mathrm{e}^{-\beta\mu}} \tag{6.30}$$

(recall that $e \geqslant 0$). Since the measure μ_j is concentrated on those k where ε_k lies between $\varepsilon_{\mathrm{F}}(\frac{j-1}{|\Lambda|})$ and $\varepsilon_{\mathrm{F}}(\frac{j}{|\Lambda|})$, we can bound (6.29) by

$$F_\Lambda(\beta,\mu) \leqslant \frac{|\Lambda|}{(2\pi)^d}\int_{[-\pi,\pi]^d} \mathrm{d}k\, g(\varepsilon_k) + \frac{1}{1+\mathrm{e}^{-\beta\mu}}\Big(\sum_{j=1}^{|\Lambda|}\big[\varepsilon_{\mathrm{F}}(\tfrac{j}{|\Lambda|}) - \varepsilon_{\mathrm{F}}(\tfrac{j-1}{|\Lambda|})\big] + 2d|\partial\Lambda|\Big). \tag{6.31}$$

We need a bound for $\varepsilon_{\mathrm{F}}(\frac{j}{|\Lambda|}) - \varepsilon_{\mathrm{F}}(\frac{j-1}{|\Lambda|})$; since $\nabla\varepsilon_k = 2(\sin k_1,\dots,\sin k_d)$, we have $\|\nabla\varepsilon_k\| \leqslant 2\sqrt{d}$. Let us take k such that $\varepsilon_k = \varepsilon_{\mathrm{F}}(\frac{j-1}{|\Lambda|})$, and $\delta k \parallel k$ such that $\varepsilon_{k+\delta k} = \varepsilon_{\mathrm{F}}(\frac{j}{|\Lambda|})$. Then

$$\varepsilon_{\mathrm{F}}(\tfrac{j}{|\Lambda|}) - \varepsilon_{\mathrm{F}}(\tfrac{j-1}{|\Lambda|}) \leqslant 2\sqrt{d}\,\|\delta k\|. \tag{6.32}$$

If $\delta k_{\min}$ is chosen so as to minimize the norm of such δk, we have

$$\frac{1}{|\Lambda|} = \frac{1}{(2\pi)^d}\int_{\varepsilon_{\mathrm{F}}(\frac{j-1}{|\Lambda|})<\varepsilon_k<\varepsilon_{\mathrm{F}}(\frac{j}{|\Lambda|})} \mathrm{d}k \geqslant \frac{1}{(2\pi)^d}\|\delta_{\min}\|^d |S_d|. \tag{6.33}$$

Combining this inequality with (6.32), we get

$$\varepsilon_{\mathrm{F}}(\tfrac{j}{|\Lambda|}) - \varepsilon_{\mathrm{F}}(\tfrac{j-1}{|\Lambda|}) \leqslant \frac{4\pi\sqrt{d}}{|S_d|^{1/d}}|\Lambda|^{-1/d}. \tag{6.34}$$

This leads to the upper bound of Proposition 6.3. □

6.4. Proofs of the corollaries.

Proof of Corollary 1.3. Let $e^- = -d+h$ and $e^+ = -d-h$ be the energies per site of the all $-$ and all $+$ Ising configurations. A configuration can be specified by the set Λ of $-$ spins. Let $\mathcal{B}(\Lambda)$ be the set of bonds connecting Λ and $\Omega\setminus\Lambda$. Notice that $\frac{1}{2d}|\mathcal{B}(\Lambda)| \leqslant |\partial\Lambda| \leqslant |\mathcal{B}(\Lambda)|$. The partition function of the Ising model can be written as

$$Z_{\mathrm{I},\Omega} = \sum_{\Lambda\subset\Omega} \mathrm{e}^{-\beta[|\Lambda|e^- + |\Omega\setminus\Lambda|e^+]}\,\mathrm{e}^{-2\beta|\mathcal{B}(\Lambda)|}. \tag{6.35}$$

Now the upper bound for $F^U_{\Omega,\Lambda}(\beta,\mu)$ implies that the partition function of the Falicov-Kimball model is bounded below by

$$Z_\Omega \geqslant \sum_{\Lambda\subset\Omega} \mathrm{e}^{-\beta[|\Lambda|f(\beta,\mu)+|\Omega\setminus\Lambda|f(\beta,\mu-U)]}\,\mathrm{e}^{-\beta C_{d,\mu}|\partial\Lambda|}\,\mathrm{e}^{-\beta C'_{d,\mu}|\Omega|^{\frac{d-1}{d}}}. \tag{6.36}$$

The last factor vanishes in the thermodynamic limit. One then makes the connection with Ising by multiplying Z_Ω by

$$\exp\Big\{\beta|\Omega|\Big(\tfrac{d}{2}C_{d,\mu} + \tfrac12\big[f(\beta,\mu)+f(\beta,\mu-U)\big]\Big)\Big\},$$

and by choosing the temperature to be $\frac{1}{2}C_{d,\mu}\beta$, and the magnetic field to be

$$h = \frac{1}{C_{d,\mu}}[f(\beta,\mu) - f(\beta,\mu-U)] \tag{6.37}$$

(the magnetic field is negative). The other bound is similar, simply replace $C_{d,\mu}$ by $\bar{\alpha}/2d$. □

Proof of Corollary 1.4. Because Ω was assigned periodic boundary conditions, we have

$$\langle \delta_{w_x,w_y} \rangle_\Omega = \frac{1}{|\Omega|} \Big\langle \sum_{z\in\Omega} \delta_{w_{x+z},w_{y+z}} \Big\rangle_\Omega. \tag{6.38}$$

It is not hard to check that for any configuration w specified by $\Lambda \subset \Omega$, one has

$$\sum_{z\in\Omega} \delta_{w_{x+z},w_{y+z}} \;\geqslant\; |\Omega| - |\partial\Lambda|\,|x-y|_1. \tag{6.39}$$

Then

$$\langle \delta_{w_x,w_y} \rangle_\Omega \;\geqslant\; 1 - |x-y|_1 \Big\langle \frac{|\partial\Lambda|}{|\Omega|} \Big\rangle_\Omega. \tag{6.40}$$

We need a bound for the last term. The fact is that typical configurations of classical particles cannot have too much boundary: $\frac{|\partial\Lambda|}{|\Omega|}$ is smaller than $r = \frac{2\log 2}{\beta\bar{\alpha}(\beta,\mu)}$. Indeed,

$$\begin{aligned}
&\frac{\sum_{\Lambda\subset\Omega} \chi\big[|\partial\Lambda| > r|\Omega|\big]\, \mathrm{e}^{-\beta F^U_{\Omega,\Lambda}(\beta,\mu)}}{\sum_{\Lambda\subset\Omega} \mathrm{e}^{-\beta F^U_{\Omega,\Lambda}(\beta,\mu)}} \\
&\qquad \leqslant \frac{2^{|\Omega|}\, \mathrm{e}^{-\beta|\Lambda| f(\beta,\mu) - \beta(|\Omega|-|\Lambda|) f(\beta,\mu-U)}\, \mathrm{e}^{-(2\log 2)|\Omega|}}{\mathrm{e}^{-\beta|\Lambda| f(\beta,\mu) - \beta(|\Omega|-|\Lambda|) f(\beta,\mu-U)}\, \mathrm{e}^{-\beta C_{d,\mu}(n_c|\Omega|)^{\frac{d-1}{d}}}\, \mathrm{e}^{-\beta C'_{d,\mu}|\Omega|^{\frac{d-1}{d}}}} \\
&\qquad \leqslant 2^{-|\Omega|}\, \mathrm{e}^{\beta(C_{d,\mu}+C'_{d,\mu})|\Omega|^{\frac{d-1}{d}}}.
\end{aligned} \tag{6.41}$$

Therefore

$$\langle \delta_{w_x,w_y} \rangle_\Omega \;\geqslant\; 1 - \frac{2\log 2}{\beta\bar{\alpha}(\beta,\mu)} |x-y|_1 - 2^{-|\Omega|}\, \mathrm{e}^{\beta(C_{d,\mu}+C'_{d,\mu})|\Omega|^{\frac{d-1}{d}}}. \tag{6.42}$$

The last term vanishes in the limit $\Omega \nearrow \mathbb{Z}^d$, and the term involving $|x-y|_1$ vanishes when $\beta \to \infty$. □

7. Conclusion

Our analysis of the Falicov-Kimball model away from half-filling allows some extrapolations. We expect segregation to survive at small temperature, when both the classical particles and the electrons are described by the grand-canonical ensemble, at inverse temperature β and with chemical potentials μ_c and μ_e. Segregation is a manifestation of coexistence between a phase with many classical particles and few electrons, and a phase with many electrons and few classical particles. It is therefore natural to conjecture the following, for $d \geqslant 2$:

> *A first order phase transition occurs at low temperature, when varying the chemical potentials.*

The transition from the chessboard state at half-filling (and large U) to the segregated state is still not clear. A heuristical analysis suggests that these states should coexist, hence there should be another first-order phase transition.

One interest of the Falicov-Kimball model is its possible relevance in understanding the Hubbard model, a notoriously difficult task. See e.g. [Lieb2] and [Tas2] for reviews of rigorous results. The relationship between the Falicov-Kimball model and the Hubbard model is somehow like the one between Ising and Heisenberg. The former does not possess the continuous symmetry of the latter, and therefore the approximation is a crude one. Still, the two models share many similarities; for instance, the Falicov-Kimball model displays long-range order of the chessboard type at half-filling and at low temperature [KL], and the ground state of the Hubbard model is a spin singlet [Lieb].

Ferromagnetism in the Hubbard model depends on the dimension and on the filling, and also on the geometry: it has been shown to occur on special lattices such as 'line-graphs' [MT, Tas, Mie, Tas2]. Does ferromagnetism take place in the Hubbard model on $\mathbb{Z}^3$, for large repulsions and away from half-filling?

Returning to Falicov-Kimball, let us walk on the road that leads to Hubbard. We consider the *asymmetric Hubbard model* that describes spin $\frac{1}{2}$ electrons with hoppings depending on the spins (this interpretation is more convenient than physical). Its Hamiltonian is

$$H_t = -\sum_{x,y:|x-y|=1} c^\dagger_{x\uparrow} c_{y\uparrow} - t \sum_{x,y:|x-y|=1} c^\dagger_{x\downarrow} c_{y\downarrow} + U \sum_x n_{x\uparrow} n_{x\downarrow}. \tag{7.1}$$

Notice that H_0 is the Falicov-Kimball model, while H_1 is the usual Hubbard model. Although we did not prove it, it is rather clear that segregation still takes place for very small t. Furthermore, the density of the phase with classical particles, in the ground state, should still be exactly 1 — indeed, the electrons exert a sort of 'pressure' that packs the classical particles together, and the tendency of the latter to delocalize is not strong enough to overcome this pressure. This is summarized in the following conjecture:

> *For $t \leqslant t_0$, segregation occurs in the ground state, at large U and away from half-filling, in the form of a coexistence between a phase of classical particles with density 1, and a phase of electrons with smaller density.*

This should also hold at positive temperature, although the density of the phase of the classical particles will be reduced, due to the presence of some holes.

If we increase t, assuming that segregation remains, we should reach a critical value $t_c < 1$ where the region of classical particles starts to grow. The density of the phase of particles with smaller hoppings is now strictly less than 1. A major question is whether segregation survives all the way when t reaches 1 — this would imply the existence of a ferromagnetic phase in the Hubbard model. We note, however, that while it is conceivable that there is a segregated (i.e., ferromagnetic) ground state at $t = 1$, it cannot be true that *every* ground state (for equal number of up and down spins) is segregated. This follows from the SU(2) symmetry. If Ψ is a totally ferromagnetic ground state with $2N$ up electrons, we can construct $\Phi = (S_-)^N \Psi$, which is also a ground state, with N up and N down electrons. However, Φ has the up and down electrons inextricably mixed, which is the opposite of a segregated state.

The Hubbard model is a rich and complicated model that poses difficult challenges. The Falicov-Kimball model can be of some help, for instance in checking scenarios that should apply to both models. This discussion of ferromagnetism illustrates however that the links between them are subtle.

Appendix A.

We derive in the sequel various expressions that are too intricate to appear in the main body of this paper.

Lemma A.1.

(a) $\frac{1}{(2\pi)^d}\int \mathrm{d}k|\varepsilon_k-\varepsilon_{\rm F}|^{-1/4} < 2.$

(b) *Assume that* $\alpha^2 \leqslant \frac{16\sqrt{2}\pi d}{|S_d|^{1/d}} n^{1/d}$*; then for all* k *such that* $\varepsilon_k=\varepsilon_{\rm F}$,

$$\int_{\varepsilon_{k'}<\varepsilon_{\rm F}} \mathrm{d}k'\ \chi\big[|k'-k|<\alpha\big] \ \geqslant\ |S_d|\big(\frac{\alpha^2}{8\pi d}\big)^d.$$

(c) $e(n) \geqslant 12(\frac{9}{10})^d n^{1+\frac{2}{d}}/|S_d|^{\frac{2}{d}}.$

(d) $\|\nabla\frac{\|b_k\|^2}{|\partial\Lambda|}\| \leqslant 8d^{5/2}.$

(e) $\|\nabla\frac{\|(h_\Lambda-\varepsilon)b_k\|^2}{|\partial\Lambda|}\| \leqslant 2^9 d^{11/2}.$

(f) $\|\nabla\frac{(b_k,h_\Lambda b_k)}{|\partial\Lambda|}\| \leqslant 32d^{7/2}.$

(g) *Assume that* $\|b_k\|^2/|\partial\Lambda| \geqslant \eta$*. Then if* $\eta\leqslant 1$, $\|\nabla\frac{(b_k,h_\Lambda b_k)}{\|b_k\|^2}\| \leqslant \eta^{-2}2^8 d^{11/2}.$

Proof of Lemma A.1 (a). Setting $Y=2d-\varepsilon_{\rm F}-2\sum_{i=2}^d\cos k_i$, and making the change of variables $\xi=\cos k_1$, one gets

$$\begin{aligned}\int \mathrm{d}k|\varepsilon_k-\varepsilon_{\rm F}|^{-1/4} &= 2\int_{[-\pi,\pi]^{d-1}}\mathrm{d}k_2\dots\mathrm{d}k_d\int_0^\pi \mathrm{d}k_1\frac{1}{|Y-2\cos k_1|^{1/4}}\\ &= 2\int_{[-\pi,\pi]^{d-1}}\mathrm{d}k_2\dots\mathrm{d}k_d\int_{-1}^1\mathrm{d}\xi\frac{1}{\sqrt{1-\xi^2}}\frac{1}{|Y-2\xi|^{1/4}}\\ &\leqslant 2\int_{[-\pi,\pi]^{d-1}}\mathrm{d}k_2\dots\mathrm{d}k_d\Big(2\int_0^1\mathrm{d}\xi\frac{1}{(1-\xi^2)^{3/4}}\Big)^{2/3}\Big(\int_{-1}^1\mathrm{d}\xi|Y-2\xi|^{-3/4}\Big)^{1/3}\\ &\leqslant 2\int_{[-\pi,\pi]^{d-1}}\mathrm{d}k_2\dots\mathrm{d}k_d\Big(2\int_0^1\mathrm{d}\zeta\frac{1}{\sqrt{\zeta}(1-\zeta)^{3/4}}\Big)^{2/3}\Big(2^{-3/4}\int_{-1}^1\mathrm{d}\xi|\xi|^{-3/4}\Big)^{1/3}\end{aligned}$$

The integral over ζ can be split into one running from 0 to $\frac12$, and one running from $\frac12$ to 1. For the first part we bound $\frac{1}{\sqrt{\zeta}(1-\zeta)^{3/4}} \leqslant 2^{3/4}\frac{1}{\sqrt{\zeta}}$, while the bound for the second part can be chosen to be $\sqrt{2}\frac{1}{(1-\zeta)^{3/4}}$. Everything can now be computed explicitly, and we find $2^{31/12}3^{2/3}(2\pi)^{d-1} < 2(2\pi)^d$. □

Proof of Lemma A.1 (b). Let us introduce a map $\gamma(\xi)$ such that $1-\frac12\gamma^2(\xi)=\cos\xi$; precisely,

$$\gamma(\xi)=\begin{cases}\sqrt{2(1-\cos\xi)} & \text{if } \xi\in[0,\pi]\\ -\sqrt{2(1-\cos\xi)} & \text{if } \xi\in[-\pi,0].\end{cases} \tag{A.1}$$

The condition $\varepsilon_k<\varepsilon_{\rm F}$ becomes $\sum_{i=1}^d|\gamma(k_i)|^2<\varepsilon_{\rm F}$. The derivative of γ is

$$\frac{\mathrm{d}\gamma}{\mathrm{d}\xi}=\frac{|\sin\xi|}{\sqrt{2(1-\cos\xi)}}. \tag{A.2}$$

We check now that $|\gamma(\xi')-\gamma(\xi)| > |\xi'-\xi|^2/4\pi$. Let us assume that $\gamma(\xi') > \gamma(\xi)$. Then

$$\gamma(\xi')-\gamma(\xi) = \int_\xi^{\xi'} \mathrm{d}\lambda \frac{|\sin\lambda|}{\sqrt{2(1-\cos\lambda)}} \geqslant \frac{1}{2}\int_\xi^{\xi'} \mathrm{d}\lambda |\sin\lambda| \tag{A.3}$$

$$\geqslant \frac{1}{\pi}\int_\xi^{\xi'} \mathrm{d}\lambda |\lambda| \geqslant |\xi'-\xi|^2/4\pi. \tag{A.4}$$

Then we can write

$$\int_{\varepsilon_{k'}<\varepsilon_{\mathrm{F}}} \mathrm{d}k' \, \chi\left[|k'-k|<\alpha\right] \geqslant \int_{\varepsilon_{k'}<\varepsilon_{\mathrm{F}}} \mathrm{d}k' \, \chi\left[|k'_i-k_i| < \tfrac{\alpha}{\sqrt{d}} \, \forall i\right]$$

$$\geqslant \int \mathrm{d}\gamma'_1 \ldots \mathrm{d}\gamma'_d \, \chi\left[\sum_{i=1}^d |\gamma'_i|^2 < \varepsilon_{\mathrm{F}}\right] \chi\left[|\gamma'_i-\gamma_i| < \tfrac{\alpha^2}{4\pi d}\right]$$

One gets a lower bound by replacing the last characteristic function by the condition $\sum_{i=1}^d |\gamma'_i-\gamma_i|^2 < \frac{\alpha^2}{4\pi d}$. Recall that $\varepsilon_{\mathrm{F}} \geqslant \frac{32}{|S_d|^{2/d}} n^{2/d}$; the assumption of the lemma implies that $\sqrt{\varepsilon_{\mathrm{F}}} > \frac{\alpha^2}{4\pi d}$; as a consequence, a lower bound is the volume of the sphere of radius $\frac{\alpha^2}{8\pi d}$. □

Proof of Lemma A.1 (c). By (3.15),

$$e(n) \geqslant \frac{8}{\pi^2(2\pi)^d}\int_{|k|^2<\varepsilon_{\mathrm{F}}} \mathrm{d}k |k|^2 = \frac{8d|S_d|}{\pi^2(2\pi)^d(d+2)} \varepsilon_{\mathrm{F}}^{\frac{d}{2}+1}. \tag{A.5}$$

The lower bound then follows from

$$\varepsilon_{\mathrm{F}} \geqslant \frac{32}{|S_d|^{2/d}} n^{2/d}. \tag{A.6}$$

□

Proof of Lemma A.1 (d)–(g). Since

$$\|b_k\| = \sum_{x\in\partial\Lambda} \sum_{\substack{e:x+e\notin\Lambda \\ e':x+e'\notin\Lambda}} \mathrm{e}^{\mathrm{i}k(e-e')}, \tag{A.7}$$

we have

$$\Bigl(\nabla\frac{\|b_k\|}{|\partial\Lambda|}\Bigr)_j = \frac{1}{|\partial\Lambda|}\sum_{x\in\partial\Lambda}\sum_{e,e'} \mathrm{i}(e_j-e'_j)\,\mathrm{e}^{\mathrm{i}k(e-e')}. \tag{A.8}$$

This is less than $2(2d)^2$, and we obtain the bound (d).

We consider now $\|(h_\Lambda-\varepsilon)b_k\|^2$.

$$\mathrm{e}^{ikx}\left[(h_\Lambda-\varepsilon)b_k\right](x) = (2d-\varepsilon)\sum_{e':x+e'\notin\Lambda} \mathrm{e}^{-\mathrm{i}ke'} - \sum_{\substack{e:x+e\in\partial\Lambda \\ e':x+e+e'\notin\Lambda}} \mathrm{e}^{-\mathrm{i}k(e+e')}$$

$$= \sum_{\substack{e:x+e\in\partial\Lambda,|e|=0,1 \\ e':x+e+e'\notin\Lambda}} \mathrm{e}^{-\mathrm{i}k(e+e')}\Bigl((2d-\varepsilon)\,\chi\left[|e|=0\right] - \chi\left[|e|=1\right]\Bigr). \tag{A.9}$$

In the last line, e is allowed to be 0. Let $\xi(e) = \Bigl((2d-\varepsilon)\,\chi\left[|e|=0\right] - \chi\left[|e|=1\right]\Bigr)$. Then

$$\Bigl|\bigl[(h_\Lambda-\varepsilon)b_k\bigr](x)\Bigr|^2 = \sum_{\substack{e:x+e\in\partial\Lambda,|e|=0,1 \\ e':x+e+e'\notin\Lambda}} \sum_{\substack{e'':x+e''\in\partial\Lambda,|e''|=0,1 \\ e''':x+e''+e'''\notin\Lambda}} \mathrm{e}^{\mathrm{i}k(e+e'-e''-e''')}\,\xi(e)\xi(e''). \tag{A.10}$$

One computes now the j-th component of the gradient; it involves a term $e_j + e'_j - e''_j - e'''_j$ that is smaller than 4; there are sums over e', e''', with less than $(2d)^2$ terms; the sum $\sum_e |\xi(e)|$ is bounded by $4d$; finally, the number of sites where $(h_\Lambda - \varepsilon)b_k$ differs from 0 is bounded by $2d|\partial\Lambda|$. As a result, the j-th component of the gradient is bounded by $\frac{1}{2}(4d)^5$, and we obtain (e).

We estimate now the gradient of $(b_k, h_\Lambda b_k)$. One easily checks that

$$(b_k, h_\Lambda b_k) = \|b_k\|^2 - \sum_{x\in\partial\Lambda} \sum_{e:x+e\notin\Lambda} \sum_{e':x+e'\in\partial\Lambda} \sum_{e'':x+e'+e''\notin\Lambda} \mathrm{e}^{\mathrm{i}k(e-e'-e'')}. \tag{A.11}$$

We can use the bound (d) for the gradient of $\|b_k\|^2$. The gradient of the last term is less than $3(2d)^3|\partial\Lambda|$, so we can write

$$\Big\|\nabla \frac{(b_k, h_\Lambda b_k)}{|\partial\Lambda|}\Big\| \leqslant 8d^{5/2} + 24d^{7/2} \leqslant 32d^{7/2}. \tag{A.12}$$

Finally, one easily checks that

$$\Big\|\nabla \frac{(b_k, h_\Lambda b_k)}{\|b_k\|^2}\Big\|^2 \leqslant 2\Big(\frac{|\partial\Lambda|}{\|b_k\|^2}\Big)^2 \Big\|\nabla \frac{(b_k, h_\Lambda b_k)}{|\partial\Lambda|}\Big\|^2 + 2\Big(\frac{(b_k, h_\Lambda b_k)}{|\partial\Lambda|}\Big)^2 \Big(\frac{|\partial\Lambda|}{\|b_k\|^2}\Big)^4 \Big\|\nabla \frac{\|b_k\|^2}{|\partial\Lambda|}\Big\|^2. \tag{A.13}$$

Using (d) and (f), as well as $(b_k, h_\Lambda b_k)/|\partial\Lambda| \leqslant 2(2d)^3$, one gets (g). $\square$

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