Long-Range Orders in Models of Itinerant Electrons Interacting with Heavy Quantum Fields

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Received November 3, 2000; revised July 15, 2001

The Falicov-Kimball model consists of itinerant lattice fermions interacting with Ising spins by an on-site potential of strength U. Kennedy and Lieb proved that at half filling there is a low temperature phase with chessboard long range order on \mathbb{Z}^d , $d \ge 2$, for all non-zero values of U. Here we investigate the stability of this phase when small quantum fluctuations of the "Ising spins" are introduced in two different ways. The first one corresponds to replace the classical spins by quantum two level systems attached to each site of the lattice. In the second one we interpret the spins as occupation numbers of localized f-electrons or heavy ions which have a small kinetic energy. This leads to the so-called asymmetric Hubbard model. For both models we prove that for all non-zero values of U the long range order of the original Falicov-Kimball model remains stable if the additional quantum fluctuations are small enough. This result is proved by non-perturbative methods based on a chessboard estimate and the principle of exponential localisation. In order to derive the chessboard estimate the phase factors in the kinetic energy of fermions must have a flux equal to π . We also investigate the models where the fermions are replaced by hard-core bosons and prove the same result for large U. For hard core bosons the kinetic term is the conventional one with zero phase factors. For small U and hard-core bosons we find that there is an off-diagonal long range order for low enough temperature and any strength of the additional quantum fluctuations. Open problems are discussed.

KEY WORDS: Long-range order; Falicov–Kimball model; quantum fluctuations; off-diagonal long-range order; reflection positivity; chessboard estimates.

1. INTRODUCTION

A large class of models relevant for the understanding of phase diagrams in condensed matter physics involves itinerant electrons on a lattice interacting

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with other degrees of freedom, for example ions, phonons, impurity spins. Much work has been devoted to the case where these degrees of freedom are treated as a classical field and the electrons quantum mechanically. According to the physical situation, the classical field may be a discrete Ising spin $s_x = \pm 1$, a scalar field $q_x \in \mathbb{R}$ or also a vector field $\phi_x \in \mathbb{R}^3$, $\|\phi_x\|$ = 1. In transition metal oxides or rare earth compounds the f-electrons are in localized orbitals, so that it is reasonable to treat them as classical particles described by occupation numbers or equivalently by Ising spins taking values $s_x = \pm 1$. A popular model to describe this situation is the so called Falicov-Kimball model.⁽¹⁾ In order to describe a phonon branch, neglecting the quantum fluctuations of the elastic field, one can attach to each site of the lattice a scalar variable $q_x \in \mathbb{R}$ which is coupled linearly to the electron density and add an appropriate elastic energy to the Hamiltonian. One then obtains the (static) Holstein model originally introduced in the context of molecular crystals.⁽²⁾ A third interesting situation is the one where the classical field is vectorial $\phi_x \in \mathbb{R}^3$ with $\|\phi_x\| = 1$, and describes the magnetic moment of impurities. The model obtained is the static version of the Kondo model. The ground states and phase diagrams of these "semiquantum models" have been the object of many investigations. The most studied case is that of the Falicov-Kimball model for which there is a very rich structure in all dimensions. We refer to refs. 3 and 14 for reviews on the subject.

An important question is to study the effects of adding small quantum fluctuations to the classical field. In this contribution, we address this question in the simplest and best understood context of the Falicov-Kimball model at half-filling. On a lattice $\Lambda \subset \mathbb{Z}^d$ the hamiltonian of the usual Falicov-Kimball model is

$$H_{\Lambda} = \sum_{x, y \in \Lambda} t_{xy} c_x^+ c_y + U \sum_{x \in \Lambda} s_x (c_x^+ c_x - 1/2)$$
(1.1)

where $s_x = \pm 1$ is a classical Ising spin, c_x^+ , c_x the creation and annihilation operators of itinerant spinless electrons obeying the canonical anticommutation relations. The coupling constant U between the classical spin and the electron density at site x can be positive or negative according to the physical interpretation. We choose a hopping matrix of the form $t_{xy} = te^{i\theta_{xy}}$, |x-y| = 1 and $t_{xy} = 0$ otherwise, where t > 0 and θ_{xy} are for the moment arbitrary phases. The phase factors may be interpreted² as the orbital coupling of a magnetic field to the electrons and the magnetic flux through a square elementary plaquette p is the gauge invariant sum of the phases around p, $\Phi_p = \sum_{\langle x, y \rangle \in p} \theta_{xy} \mod 2\pi$. Any choice of phases is permissible

² Other interpretations are possible, see refs. 10, 19, and 18.

and corresponds to some magnetic flux. But for non planar lattices it is not true in general that any magnetic flux corresponds to some set of phases. In fact we will consider only situations with $\Phi_p = \pi$ or $\Phi_p = 0$ for all plaquettes p of \mathbb{Z}^d , where there always exists a set of corresponding phases. We will often use the notation $\langle x, y \rangle$ for nearest neighbor pairs of sites.

Let $\langle - \rangle_A$ denote the finite volume Gibbs state associated to (1.1), with periodic boundary conditions and inverse temperature β . The electron-hole and spin flip symmetries imply that $\langle s_x \rangle_A = 0$ and $\langle c_x^+ c_x \rangle_A = 1/2$ indicating that we are in a half-filled band. Kennedy and Lieb⁽⁴⁾ proved that for the half-filled band there is a low temperature phase $\beta > \beta_1(U) > 0$ where long-range order is present for all $U \neq 0$ and $d \ge 2$, namely $(-1)^{|x|+|y|} \langle s_x s_y \rangle_A \ge c > 0$ and a high temperature phase $\beta < \beta_2(U) < \beta_1(U)$ where the correlations are exponentially clustering (with periodic boundary conditions and c independent of x, y and |A|).

In this work, we investigate the stability of the low temperature phase at half filling for all values of $U \neq 0$, when small quantum fluctuations of the spins are introduced. There are at least two meaningful ways to incorporate quantum fluctuations at the level of the Ising spins depending on the interpretation that one has in mind.

The first one is to replace the Ising spin $s_x = \pm 1$ by a quantum twolevel system $|\downarrow\rangle$, $|\uparrow\rangle$ attached at each site $x \in \Lambda$. A standard description is in term of Pauli matrices $(\sigma_x^{(1)}, \sigma_x^{(2)}, \sigma_x^{(3)})$, such that $\sigma_x^{(3)} |\uparrow\rangle = |\uparrow\rangle$, $\sigma_x^{(3)} |\downarrow\rangle =$ $-|\downarrow\rangle$. We consider the hamiltonian

$$H_{\Lambda} = \sum_{x, y \in \Lambda} t_{xy} c_x^+ c_y + U \sum_{x \in \Lambda} \sigma_x^{(3)} (c_x^+ c_x - 1/2) + \alpha \sum_{x \in \Lambda} \sigma_x^{(1)}$$
(1.2)

where α controls the transition rate between the two states $\sigma_x^{(1)} |\uparrow\rangle = |\downarrow\rangle$ and $\sigma_x^{(1)} |\downarrow\rangle = |\uparrow\rangle$. This model describes itinerant electrons interacting with a lattice of two-level systems. One may interpret the two-level systems as a caricature of Einstein oscillators in which case (1.2) can be viewed as a simplification of the so-called Holstein model. This later electron-phonon system corresponds to $\sigma_x^{(3)} \rightarrow q_x \in \mathbb{R}$ and $\alpha \sigma_x^{(1)} \rightarrow p_x^2/2m$ with $[q_x, p_x] = i\hbar$.

A second natural way to introduce quantum fluctuations comes from the interpretation of $s_x = \pm 1$ as occupation numbers $w_x = (s_x + 1)/2$ of classical particles (for example localized f-electrons or ions). If one endows these particles with a small kinetic term described by a hopping matrix, the model obtained is the so-called asymmetric Hubbard model. More precisely renaming the original itinerant electrons as "spin up electrons" $c_x^+ \rightarrow c_{x\uparrow}^+$ and the f-electrons as "spin down electrons" $c_{x\downarrow}^+$ with $w_x \rightarrow c_{x\downarrow}^+ c_{x\downarrow}$ we have

$$H_{A} = \sum_{x, y \in A} t_{xy}^{\downarrow} c_{x\downarrow}^{+} c_{y\downarrow} + \sum_{x, y \in A} t_{xy} c_{x\uparrow}^{+} c_{y\uparrow}$$
$$+ U \sum_{x \in A} (c_{x\downarrow}^{+} c_{x\downarrow} - 1/2) (c_{x\uparrow}^{+} c_{x\uparrow} - 1/2)$$
(1.3)

where $t_{xy}^{\downarrow} = t^{\downarrow} e^{i\theta_{xy}}, t^{\downarrow} > 0$ with $t^{\downarrow} \ll t$.

We choose periodic boundary conditions in order to retain the same symmetries than in the original Falicov–Kimball model. For the hamiltonian (1.2) the transformations $\sigma_x^{(3)} \to -\sigma_x^{(3)}$ (spin space rotation of angle π around the 1 axis) and $c_x^+ \to (-1)^{|x|} c_x$ (electron-hole transformation) map H_A onto its complex conjugate \bar{H}_A and imply $\langle \sigma_x^{(3)} \rangle_A = 0$ and $\langle c_x^+ c_x \rangle_A = \frac{1}{2}$. We also note that a spin space rotation of angle π around the 1 (respectively 3) axis is equivalent to a change of sign of U (respectively α). Thus without loss of generality we may restrict ourselves to $U \ge 0$ and $\alpha \ge 0$. For the hamiltonian (1.3) one can use an electron-hole transformation on both electron species to show that $\langle c_{x\uparrow}^+ c_{x\uparrow} \rangle_A = \langle c_{x\downarrow}^+ c_{x\downarrow} \rangle_A = \frac{1}{2}$. Moreover an electron-hole transformation on spin up particles only is equivalent to a change of sign for U so we may restrict ourselves to $U \ge 0$.

For models (1.2) and (1.3) we prove that the long-range order of antiferromagnetic type remains stable for all values of $U \neq 0$. We always take periodic boundary conditions and in each direction Λ has an even number of sites.

Theorem 1. Long-Range Order in Model (1.2). Assume $\Phi_p = \pi$ and $d \ge 2$. For all $U \ne 0$ there exist $\beta_c(U) > 0$ and $\alpha_c(U) > 0$ such that for $\beta > \beta_c(U)$, and $|\alpha| < \alpha_c(U)$, we have

$$(-1)^{|x|+|y|} \left\langle \sigma_x^{(3)} \sigma_y^{(3)} \right\rangle_A \ge \epsilon > 0 \tag{1.4}$$

for some ϵ independent of x, y and Λ .

The qualitative behavior of $\beta_c(U)$ and $\alpha_c(U)^{-1}$ for $U \to 0$ and $U \to \infty$ is indicated on Figs. 4 and 5 in Section 3. For large U (1.4) is expected and the asymptotic behaviors of $\beta_c(U)$ and $\alpha_c(U)^{-1}$ are linear in U. This is optimal since if one integrates over electrons, one finds to leading order an effective Hamiltonian for the two-level systems corresponding to the Ising model with coupling t^2/U and transverse field α . For small U, this intuition is not valid and it is remarkable that sufficiently small quantum fluctuations do not destroy the order even when $U \to 0$. It is not clear if (in the small U region) the curve for $\alpha_c(U)$ is qualitatively correct at zero temperature. More generally it is an open problem to determine whether the whole region above it corresponds to a single disordered phase when $d \ge 2$. In this

connection we mention that for the one dimensional Holstein model it has been shown rigorously⁽¹⁷⁾ that at sufficiently small electron-phonon coupling the quantum fluctuations (analog to the α term) lead to a disordered zero temperature phase. In particular there is no Peierls instability (i.e., no LRO) but rather Luttinger liquid behavior of correlation functions. We expect that the same property holds in the present model for d = 1.

Theorem 2. Long-Range Order in Model (1.3). Assume $\Phi_p = \pi$ and $d \ge 2$. For all $U \ne 0$ there exist $\beta_c(U) > 0$ and $t_c^{\downarrow}(U) > 0$ such that for $\beta > \beta_c(U)$, and $0 \le t < t_c^{\downarrow}(U)$, we have

$$(-1)^{|x|+|y|} \langle (c_{x\perp}^+ c_{x\perp} - 1/2) (c_{y\perp}^+ c_{y\perp} - 1/2) \rangle_A \ge \epsilon > 0$$

$$(1.5)$$

for some ϵ independent of x, y and Λ .

In Section 3 we give details about the asymptotic behaviour for $U \to 0$ and $U \to \infty$, see Figs. 4 and 5. In the large U limit, we obtain that $\beta_c(U)$ and $t_c^{\downarrow}(U)^{-1}$ are linear in U. In this limit, the effective Hamiltonian is given by the anisotropic Heisenberg model with coupling constants $(t^2+t^{\downarrow 2})/U$ for the Ising part and tt^{\downarrow}/U for the XY part so that one should expect (1.5) to be true for $tt^{\downarrow} \ll t^2 + t^{\downarrow 2}$ which is independent of U. Thus our result is certainly not optimal in the large U limit. At zero temperature we expect that there should be LRO for any value of $t^{\downarrow} \leqslant t$ and $U \neq 0$. Indeed this is the case for $t^{\downarrow} = 0$ (Falicov–Kimball model) and generally believed to be the case for $t^{\downarrow} = t$ (Hubbard model on a square lattice). In fact as Fig. 5 shows we are unable to prove this even for $t^{\downarrow} \ll t$.

The low temperature phase of Kennedy-Lieb for the usual Falicov-Kimball model is now recovered for all $U \neq 0$ as a special case when we set $\alpha = t^{\downarrow} = 0$. Their proof does not make any use of the phase condition $\Phi_p = \pi$ so in this respect it is more general but their technique is based on the fact that for each fixed spin configuration the itinerant particles are noninteracting fermions and thus can be "explicitly integrated out," reducing the problem to one of classical statistical mechanics with a complicated effective hamiltonian. When α and t^{\downarrow} are non zero this step cannot be performed explicitly and we have to rely on other methods. We use chessboard estimates and the principle of exponential localization as developed by Fröhlich and Lieb⁽⁵⁾ in their treatment of anisotropic Heisenberg antiferromagnets. The principal advantage of this technique over perturbative methods (in the spirit of refs. 12 and 13) is that it permits us to obtain information in the non-perturbative region of small U. However in order to prove the chessboard estimates, the hamiltonian has to satisfy the reflection positivity condition. Usually fermions fail to satisfy this condition, but it was observed recently that on \mathbb{Z}^d it is fulfilled when $\Phi_p = \pi$ through all elementary square plaquettes p. This fact underlies the proof of Lieb⁽⁶⁾ of the flux phase conjecture for the Hubbard model, and was put into a more systematic form in ref. 7. Unfortunately we do not know how to perform the proofs of our results if this special condition is not satisfied but we think that the results should be independent of the choice of the phase. This claim is supported by the large U case where one may use perturbative cluster expansions.^(12, 13)

It turns out that our method is also able to deal with the case where the itinerant particles are hard-core bosons provided $\Phi_p = 0$ (i.e., one can choose $\theta_{xy} = 0$). Hard-core bosons may be realized from the following algebra of creation and annihilation operators

$$[c_x, c_y^+] = [c_x^+, c_y^+] = [c_x, c_y] = 0, \qquad x \neq y$$

$$\{c_x, c_x^+\} = 1, \qquad (c_x^+)^2 = (c_x)^2 = 0.$$

(1.6)

Physically this corresponds to usual bosons interacting with an infinite twobody on-site repulsion which prevents two of them to occupy the same site. For model (1.3) each spin index satisfies (1.6) and operators with different spin indices commute. For the quantum statistics (1.6) we prove that the long-range orders (1.4) and (1.5) occur for large enough U.

Theorem 3. Long-Range Order for the Hard-Core Bosons. Assume $\Phi_p = 0$ and $d \ge 2$. There exist U_c , $\beta_c(U)$, $\alpha_c(U)$, $\mu_c(U)$ (all strictly positive) such that for $U > U_c$, $\beta > \beta_c(U)$, $|\alpha| < \alpha_c(U)$ or $0 \le t^{\downarrow} < t_c^{\downarrow}(U)$ the long-range orders (1.4), (1.5) occur.

Interestingly the hard-core condition for bosons which is an on-site repulsion in direct space suffices to create long-range order. This is not a priori evident since long-range order of type (1.4), (1.5) does not exist for ordinary non-interacting bosons. Indeed Kennedy and Lieb have shown⁽⁴⁾ that for the Falicov–Kimball model (1.2) if itinerant particles are bosons then the classical spins segregate into a large droplet of $s_x = +1$.

It is interesting to investigate what happens when U is small for hardcore bosons. We have not proved or disproved (1.4) and (1.5) but we have shown, using infrared bounds, that there is an off-diagonal long-range order. Let c_k^{\dagger} , c_k denote the Fourier transform defined by

$$c_k^{\dagger} = \frac{1}{\sqrt{|A|}} \sum_{x \in A} e^{ik.x} c_x^{\dagger}$$
(1.7)

where k runs over the Brillouin zone B associated to Λ , and let k_{π} be the wave vector with all components equal to π .

Theorem 4. Off-Diagonal Long Range Order. Assume $\Phi_p = 0$ and $d \ge 3$. There exist $U_c \ne 0$, $\beta_c(U) > 0$ such that for $|U| < U_c$, $\beta > \beta_c(U)$ and any α , t^{\downarrow}

$$\frac{1}{|\Lambda|} \langle c_{k_{\pi}}^{+} c_{k_{\pi}} \rangle_{\Lambda} \ge \epsilon > 0$$
(1.8)

and

$$\frac{1}{|\Lambda|} \langle c_{k_{\pi}\sigma}^{+} c_{k_{\pi}\sigma} \rangle_{\Lambda} \ge \epsilon > 0, \qquad \sigma = \uparrow, \downarrow$$
(1.9)

for some ϵ independent of Λ .

Note that (1.8) and (1.9) are not affected by the strength of the quantum fluctuations α and t^{\downarrow} as lons as U is small enough. When $U = \alpha = t^{\downarrow} = 0$ the situation is identical to that of the quantum XY model where the above result is known for $d \ge 3^{(9)}$ and also for d = 2 and $\beta = \infty$.⁽¹¹⁾ In fact Theorem 4 can also be extended to the case d = 2 and $\beta = \infty$ using the improvements of ref. 11.

An interesting open problem is to understand if the "magnetic" and "charge density wave" LRO (1.4) and (1.5) can or cannot coexist with "superfluid" ODLRO (1.8) and (1.9) for small $U \neq 0$. For large U, one may argue using perturbative methods that $\langle c_x^+ c_y \rangle_A$ and $\langle c_{x\sigma}^+ c_{y\sigma} \rangle_A$ decay exponentially fast so that the ODLRO is destroyed. At this point we would like to draw the attention of the reader to the simpler case $\alpha = t^{\downarrow} = 0$ of the Falicov-Kimball model with hard core bosons. When $\Phi_n = 0$ it is easy to show, using standard reflection positivity methods, that for all U there is at least one ground state of chessboard type $s_x^{CB} = (-1)^x$ (here ground state means the spin configuration minimising the energy of the bosons, see refs. 16 and 14). An open question is whether the bosonic density $\langle c_x^+ c_x \rangle_A$ has the same periodicity than s_x^{CB} for all $U \neq 0$. For small enough U, by the same proof than that of Theorem 4 one may show that there is an ODLRO in the chessboard configuration of spins for $\beta = \infty$ and $d \ge 2$. For large enough U using the formalism of ref. 15 one can show that the bosonic density has period two (i.e., it follows the spin configuration) and at the same time there is no ODLRO (the corresponding one point function decays exponentially fast). So the issue is to decide if a periodic modulation of the bosonic density can coexist with the ODLRO in the chessboard configuration of the spins. For fermions since one can reduce the problem to a single particle one, it is easy to observe that the fermionic density has period two for all $U \neq 0$, and there is no ODLRO (for all values of the flux).

The paper is organised as follows. In Section 2 we briefly review basic facts about reflection positivity and apply them to our specific problem to derive the chessboard estimate and the Peierls argument. Section 3 contains the application of the principle of exponential localisation and the completion of the proof of Theorems 1–3. Finally the proof of Theorem 4 is outlined in Section 4.

2. CHESSBOARD ESTIMATE

The proof of Theorems 1–3 rely on a Peierls argument where the weight of a contour is estimated with the help of a chessboard estimate. To keep the discussion simpler we set d = 2 but every step can be performed in arbitrary dimension. The derivation of this estimate is based on reflection positivity about which we recall the basic facts. Let us consider a Hilbert space of the form $\mathcal{H}_L \otimes \mathcal{H}_R$ where \mathcal{H}_L and \mathcal{H}_R are two copies of a *n*-dimensional Hilbert space (*L* stands for left and *R* for right). For any $n \times n$ matrix *O*, we define O_L and O_R acting on $\mathcal{H}_L \otimes \mathcal{H}_R$ by

$$O_L = O \otimes \mathbb{1}, \qquad O_R = \mathbb{1} \otimes O \tag{2.1}$$

where 1 is the $n \times n$ identity matrix. In the following, we denote by \overline{O} the matrix obtained by complex conjugation of all the elements of O. Let A be a hermitian $n \times n$ matrix and $C^{(i)}$, i = 1, ..., l be real $n \times n$ matrices. We say that a Hamiltonian H^{RP} is reflection positive if it has the form

$$H^{RP} = A_L + \bar{A}_R + \sum_{i=1}^{l} (C_L^{(i)} - C_R^{(i)})^2$$
(2.2)

with $\sum_{i=1}^{l} (C_L^{(i)} - C_R^{(i)})^2$ symmetric. Note that the plus sign in front of the sum of squares is necessary. Such Hamiltonians have two interesting properties.

Lemma 5. Reflection Positivity 1.⁽⁹⁾ Let H^{RP} be a reflection positive Hamiltonian and h_i , i = 1, ..., l be real numbers. We define

$$H^{RP}(\{h_i\}) = A_L + \bar{A}_R + \sum_{i=1}^{l} (C_L^{(i)} - C_R^{(i)} - h_i)^2.$$
(2.3)

Then we have the following inequality

$$\Gamma r e^{-\beta H^{RP}(\{h_i\})} \leq T r e^{-\beta H^{RP}(\{0\})}.$$
(2.4)

Lemma 6. Reflection Positivity 2.⁽⁹⁾ Let H^{RP} be a reflection positive Hamiltonian and O, Q be two $n \times n$ matrices. Then we have

$$|\mathrm{Tr} \, O_L \bar{Q}_R \, \mathrm{e}^{-\beta H}| \leq (\mathrm{Tr} \, O_L \bar{O}_R \, \mathrm{e}^{-\beta H^{R^P}})^{1/2} \, (\mathrm{Tr} \, Q_L \bar{Q}_R \, \mathrm{e}^{-\beta H^{R^P}})^{1/2}$$
(2.5)

In order to use these lemmas one has to transform the Hamiltonians (1.2) and (1.3) into the reflection positive form. For hard core bosons with $\Phi_p = 0$ the situation is similar to antiferromagnetic Heisenberg models.⁽⁹⁾ For fermions with $\Phi_p = \pi$ this transformation can be conveniently done by the method introduced in ref. 7.

Case of Fermions

We need three transformations to bring the hamiltonians into a reflection positive form. Here, we perform them successively in (a), (b) and (c) for the first model (1.2) (the discussion for the second model is similar). Since Λ is a torus with an even number of sites in each direction, there exist planes of symmetry P dividing it in two equal parts L and R. Given such a plane, we can decompose our Hamiltonian as follows

$$H_{A} = \sum_{x \in L, y \in L} t_{xy}c_{x}^{+}c_{y} + \sum_{x \in R, y \in R} t_{xy}c_{x}^{+}c_{y} + \sum_{x \in L, y \in R} t_{xy}c_{x}^{+}c_{y} + \sum_{x \in R, y \in L} t_{xy}c_{x}^{+}c_{y}$$
$$+ U \sum_{x \in L} \sigma_{x}^{(3)}(n_{x} - 1/2) + U \sum_{x \in R} \sigma_{x}^{(3)}(n_{x} - 1/2) + \alpha \sum_{x \in L} \sigma_{x}^{(1)}$$
$$+ \alpha \sum_{x \in R} \sigma_{x}^{(1)}.$$
(2.6)

(a) Gauge transformation. We note that there exists a gauge transformation bringing (2.6) into the following Hamiltonian

$$H'_{A} = \sum_{x \in L, y \in L} t_{xy} c_{x}^{+} c_{y} - \sum_{x \in R, y \in R} t_{r(x)r(y)} c_{x}^{+} c_{y} - \sum_{x \in L, y \in R} |t_{xy}| c_{x}^{+} c_{y}$$
$$- \sum_{x \in R, y \in L} |t_{xy}| c_{x}^{+} c_{y} + U \sum_{x \in L} \sigma_{x}^{(3)} (n_{x} - 1/2) + U \sum_{x \in R} \sigma_{x}^{(3)} (n_{x} - 1/2)$$
$$+ \alpha \sum_{x \in L} \sigma_{x}^{(1)} + \alpha \sum_{x \in R} \sigma_{x}^{(1)}$$
(2.7)

where r(x) is the image of the site x through the plane P. To prove that such a gauge transformation exists, it is sufficient to show that the fluxes

defined by (2.7) are also π across each plaquette p.⁽¹⁰⁾ For the new hoppings $t'_{xy} = te^{i\theta'_{xy}}$ of H'_A we have

$$\begin{aligned} \theta'_{xy} &= \theta_{xy}, & x \in L, \quad y \in L \\ \theta'_{xy} &= \theta_{r(x)\,r(y)} + \pi, & x \in R, \quad y \in R \\ \theta'_{xy} &= \pi, & x \in L, \quad y \in R \quad \text{or} \quad x \in R, \quad y \in L. \end{aligned}$$
(2.8)

Let us now examine the flux Φ'_p defined by θ'_{xy} for the three different types of plaquettes. For a plaquette *p* entirely contained in *L*, we clearly have $\Phi'_p = \pi$ since the phases of H'_A in *L* are the same as the ones of H_A . For a plaquette *p* defined by *x*, *y*, *z*, *t* as in Fig. 1 entirely contained in *R*, we have (mod 2π)

$$\Phi'_{p} = \theta'_{xy} + \theta'_{yz} + \theta'_{zt} + \theta'_{tx} = \theta_{r(x)r(y)} + \theta_{r(y)r(z)} + \theta_{r(z)r(t)} + \theta_{r(t)r(x)} + 4\pi = \pi$$
(2.9)

The four first terms in the right-hand side of the last equation correspond to sum the phases of H_A on an anticlockwise circuit in L and give a flux $-\pi$. Finally, for a plaquette x, y, r(y), r(x) cut by the plane P, we have (mod 2π)

$$\Phi'_{p} = \theta'_{xy} + \theta'_{yr(y)} + \theta'_{r(y)r(x)} + \theta'_{r(x)x} = (\theta_{r(x)r(y)} + \pi) + \pi + \theta_{r(y)r(x)} + \pi = \pi$$
(2.10)

In the last equality, we used that $\theta_{r(x)r(y)} = -\theta_{r(y)r(x)}$.



Fig. 1. Plaquettes reflected through the symmetry plane P.

(b) Klein transformation for the electrons. The hamiltonian acts on the antisymmetric Fock space associated to Λ which does not have the form of a tensor product $\mathscr{H}_L \otimes \mathscr{H}_R$. However we introduce new operators d_x^+ and d_x for all $x \in \Lambda$

$$d_x^+ = c_x^+ (-1)^{N_L}, \qquad d_x = (-1)^{N_L} c_x$$
 (2.11)

where $N_L = \sum_{x \in L} c_x^+ c_x$ is the total number of fermions in the left part of the lattice. It is easy to verify that the operators for two sites in the two separate parts L and R are commuting

$$[d_x^+, d_y^+] = [d_x, d_y] = [d_x^+, d_y] = 0, \qquad x \in L, \quad y \in R.$$
(2.12)

whereas for two sites in the same part of the lattice they satisfy the canonical anticommutation relations

$$\{d_x, d_y^+\} = \delta_{xy}, \qquad \{d_x^+, d_y^+\} = 0, \qquad \{d_x, d_y\} = 0, x \in L, \quad y \in L \quad \text{or} \quad x \in R, \quad y \in R.$$
 (2.13)

In terms of the new operators the hamiltonian H'_{A} is transformed into

$$H_{A}^{"'} = \sum_{x \in L, y \in L} t_{xy} d_{x}^{+} d_{y} - \sum_{x \in R, y \in R} t_{r(x) r(y)} d_{x}^{+} d_{y} - \sum_{x \in L, y \in R} |t_{xy}| d_{x}^{+} d_{y}$$
$$- \sum_{x \in R, y \in L} |t_{xy}| d_{x}^{+} d_{y} + U \sum_{x \in L} \sigma_{x}^{(3)} (d_{x}^{+} d_{x} - 1/2)$$
$$+ U \sum_{x \in R} \sigma_{x}^{(3)} (d_{x}^{+} d_{x} - 1/2) + \alpha \sum_{x \in L} \sigma_{x}^{(1)} + \alpha \sum_{x \in R} \sigma_{x}^{(1)}.$$
(2.14)

which naturally acts on $\mathscr{H}_L \otimes \mathscr{H}_R$ where \mathscr{H}_L and \mathscr{H}_R are the Fock spaces associated to L and R.

(c) Particle-hole transformation on the right. Here, we perform a particle-hole transformation, but only on the right part of the lattice $d_x^+ \rightarrow d_x$, $\sigma_x^{(1)} \rightarrow \sigma_x^{(1)}$, $\sigma_x^{(2)} \rightarrow -\sigma_x^{(2)}$, $\sigma_x^{(3)} \rightarrow -\sigma_x^{(3)}$, for $x \in R$. It leaves the relations (2.12) and (2.13) and the commutation relations for the Pauli matrices unchanged. Through this transformation the following terms in (2.14) change

$$-\sum_{x \in R, y \in R} t_{r(x)r(y)} d_x^+ d_y \to +\sum_{x \in R, y \in R} \overline{t}_{r(x)r(y)} d_x^+ d_y$$
(2.15)

$$-\sum_{x \in L, y \in R} |t_{xy}| d_x^+ d_y - \sum_{x \in R, y \in L} |t_{xy}| d_x^+ d_y$$

$$\rightarrow -\sum_{x \in L, y \in R} |t_{xy}| d_x^+ d_y^+ - \sum_{x \in R, y \in L} |t_{xy}| d_x d_y$$

$$= \frac{1}{2} \sum_{x \in L} |t_{xr(x)}| (d_x^+ - d_{r(x)}^+)^2 + \frac{1}{2} \sum_{x \in L} |t_{xr(x)}| (d_x - d_{r(x)})^2 \quad (2.16)$$

where we used the relations (2.12) and (2.13) and the hermicity of t_{xy} . We have obtained a Hamiltonian H_A^{RP} that is reflection positive

$$H_{A}^{RP} = A_{L} + \bar{A}_{R} + \sum_{i=1}^{l} (C_{L}^{(i)} - C_{R}^{(i)})^{2}$$
(2.17)

with

$$A_{L} = \sum_{x \in L, y \in L} t_{xy} d_{x}^{+} d_{y} + U \sum_{x \in L} \sigma_{x}^{3} (d_{x}^{+} d_{x} - \frac{1}{2}) + \alpha \sum_{x \in L} \sigma_{x}^{(1)}$$

$$\sum_{i=1}^{l} (C_{L}^{(i)} - C_{R}^{(i)})^{2} = \frac{1}{2} \sum_{x \in L} |t_{xr(x)}| (d_{x}^{+} - d_{r(x)}^{+})^{2} + \frac{1}{2} \sum_{x \in L} |t_{xr(x)}| (d_{x} - d_{r(x)})^{2}.$$
(2.18)

Case of Hard-Core Bosons

In this case the operators associated to the *L* and *R* parts of the lattice commute and the flux is zero $(t_{xy} \ge 0)$. Thus we only need to perform the following particle-hole transformation on the right $c_x^+ \to c_x$, $\sigma_x^{(1)} \to \sigma_x^{(1)}$, $\sigma_x^{(2)} \to -\sigma_x^{(2)}$, $\sigma_x^{(3)} \to -\sigma_x^{(3)}$, for $x \in R$. This transformation leaves the relations (1.6) unchanged and the hamiltonian (1.2) becomes of the form (2.17) with

$$A_{L} = \sum_{x \in L, y \in L} |t_{xy}| c_{x}^{+} c_{y} + U \sum_{x \in L} \sigma_{x}^{(3)} (n_{x} - \frac{1}{2}) + \alpha \sum_{x \in L} \sigma_{x}^{(1)}$$
(2.19)

$$\sum_{i=1}^{l} (C_{L}^{(i)} - C_{R}^{(i)})^{2} = \frac{1}{2} \sum_{x \in L} |t_{xr(x)}| (c_{x}^{+} - c_{r(x)}^{+})^{2} + \frac{1}{2} \sum_{x \in L} |t_{xr(x)}| (c_{x} - c_{r(x)})^{2}$$
(2.20)

where we used the commutation relation (1.6) to rewrite the hopping terms across the plane.

In the rest of this section we derive the chessboard estimate. It is convenient to introduce new variables defined as $m_x = (-1)^{|x|} \sigma_x^{(3)}$ for model (1.2) and $m_x = (-1)^{|x|} (c_{x\downarrow}^+ c_{x\downarrow} - 1/2)$ for model (1.3). In these new variables,

the long-range order we want to prove is expressed as $\langle m_x m_y \rangle_A \ge c > 0$. At each site, we define two orthogonal projectors P_x^+ and P_x^- that project onto the states with $m_x = +1$ and $m_x = -1$. We have the trivial equality $P_x^+ + P_x^- = 1$. By the particle-hole symmetry, P_x^+ is transformed into P_x^- . Since the hamiltonian is invariant under this symmetry, we have $\langle P_x^+ \rangle_A =$ $\langle P_x^- \rangle_A = 1/2$ and in general the expectation value of any product of P's is invariant under the interchange of P_x^+ and P_x^- . We have

$$\langle m_x m_y \rangle_A = \langle m_x (P_x^+ + P_x^-) m_y (P_y^+ + P_y^-) \rangle_A$$

$$= \langle P_x^+ P_y^+ \rangle_A + \langle P_x^- P_y^- \rangle_A - \langle P_x^+ P_y^- \rangle_A - \langle P_x^- P_y^+ \rangle_A$$

$$= \langle P_x^+ (1 - P_y^-) \rangle_A + \langle P_x^- (1 - P_y^+) \rangle_A - \langle P_x^+ P_y^- \rangle_A - \langle P_x^- P_y^+ \rangle_A$$

$$= 1 - 4 \langle P_x^+ P_y^- \rangle_A.$$

$$(2.21)$$

A proof of long-range order will be achieved if we are able to prove that the terms $\langle P_x^+ P_y^- \rangle_A$ are small enough. Following Fröhlich and Lieb,⁽⁵⁾ we define contours γ as the sets of pairs of nearest neighbors $\gamma = \{\langle i_1, j_1 \rangle, \langle i_2, j_2 \rangle, ..., \langle i_n, j_n \rangle\}$ that decompose Λ in exactly two disjoint and connected subsets Λ_x and Λ_y , i.e., $\Lambda_x \cup \Lambda_y = \Lambda$ such that $\{x, i_1, i_2, ..., i_n\} \subset \Lambda_x$ and $\{y, j_1, j_2, ..., j_n\} \subset \Lambda_y$. It is clear that n can only take the values n = 4, 6, 8, ... Any bond xy is either horizontal or vertical. If xy is horizontal (vertical), let $x \land y$ be the smallest horizontal (vertical) coordinate of the two sites x and y. Given a contour γ , we decompose it in the following way $\gamma = \gamma_{h,e} \cup \gamma_{h,o} \cup \gamma_{v,e} \cup \gamma_{v,o}$ where $\gamma_{h,e} = \{\langle x, y \rangle$ horizontal and $x \land y$ even}, $\gamma_{h,o} = \{\langle x, y \rangle$ horizontal and $x \land y$ odd}, $\gamma_{v,e} = \{\langle x, y \rangle$ vertical and $x \land y$ even}, $\gamma_{v,o} = \{\langle x, y \rangle$ vertical and $x \land y$ odd}. The following estimate holds⁽⁵⁾

$$\langle P_x^+ P_y^- \rangle_A \leq \sum_{\gamma} \prod_{\alpha,\beta} \left\langle \prod_{\langle z, z' \rangle \in \gamma_{\alpha,\beta}} P_z^+ P_{z'}^- \right\rangle_A$$
 (2.22)

The final step consists in using lemma 6 to estimate each term in (2.22). For simplicity we give the details in the simplest case where $\gamma_{\alpha,\beta}$ consists of one bond $\langle z_1, z_2 \rangle$. We need to perform the transformations (a), (b), (c) on H_A and the projectors P_x^{\pm} . These are transformed in the same way for fermions and hard-core bosons, since in both cases, we have that m_x goes into $-m_x$ for $x \in R$. At this point, we have to be careful since these transformations were expressed in terms of the $\sigma_x^{(3)}$ or $(c_{x\downarrow}^+ c_{x\downarrow} - \frac{1}{2})$ variables and the projector we are working with are for the m_x variables. For this reason, let us come back for a moment to the original variables. The projector $P_{z_1}^+ P_{z_2}^$ projects onto the state $s_{z_1} = m_{z_1} = +$ and $s_{z_2} = -m_{z_2} = +$ (on Fig. 2 we have



Fig. 2. Construction of the Fröhlich-Lieb configuration for m-variables.

written the configuration for the m_x). If we denote by \tilde{P}_x^{\pm} the projectors for the $s_x = (-1)^{|x|} m_x$ variables, we can write

$$\langle P_{z_1}^+ P_{z_2}^- \rangle_A = \langle \tilde{P}_{z_1}^+ \tilde{P}_{z_2}^+ \rangle_A = \frac{1}{Z_A} \operatorname{Tr} \left(\tilde{P}_{z_1}^+ \tilde{P}_{z_2}^+ e^{-\beta H_A} \right).$$
(2.23)

We now introduce the symmetry plane P_1 that defines the two parts of the lattice and do the transformations (a), (b), (c) to get

$$\langle \tilde{P}_{z_1}^+ \tilde{P}_{z_2}^+ \rangle_A = \frac{1}{Z_A} \operatorname{Tr} \left(\tilde{P}_{z_1}^+ \tilde{P}_{z_2}^+ e^{-\beta H_A^{RP}} \right)$$
(2.24)

since, as z_1 and z_2 are on the left, $\tilde{P}_{z_1}^+$ and $\tilde{P}_{z_2}^+$ are not affected by these transformations. We can now apply Lemma 6 with $O_L = \tilde{P}_{z_1}^+ \tilde{P}_{z_2}^+$ and $\bar{Q}_R = 1$

$$\operatorname{Tr}(\tilde{P}_{z_{1}}^{+}\tilde{P}_{z_{2}}^{+}e^{-\beta H_{A}^{RP}}) \leq \{\operatorname{Tr}(\tilde{P}_{z_{1}}^{+}\tilde{P}_{z_{2}}^{+}\tilde{P}_{z_{3}}^{+}\tilde{P}_{z_{4}}^{+}e^{-\beta H_{A}^{RP}})\}^{1/2} \{\operatorname{Tr}(1e^{-\beta H_{A}^{RP}})\}^{1/2}$$

$$= \{\operatorname{Tr}(\tilde{P}_{z_{1}}^{+}\tilde{P}_{z_{2}}^{+}\tilde{P}_{z_{3}}^{-}\tilde{P}_{z_{4}}^{-}e^{-\beta H_{A}})\}^{1/2} Z_{A}^{1/2}$$

$$= \langle \tilde{P}_{z_{1}}^{+}\tilde{P}_{z_{2}}^{+}\tilde{P}_{z_{3}}^{-}\tilde{P}_{z_{4}}^{-}\rangle_{A}^{1/2} Z_{A} = \langle P_{z_{1}}^{+}P_{z_{2}}^{-}P_{z_{3}}^{-}P_{z_{4}}^{+}\rangle_{A}^{1/2} Z_{A}. \quad (2.25)$$

In conclusion

$$\langle P_{z_1}^+ P_{z_2}^- \rangle_A \leq \langle P_{z_1}^+ P_{z_2}^- P_{z_3}^- P_{z_4}^+ \rangle_A^{1/2}.$$
 (2.26)

+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	+	+	-	-

Fig. 3. The Fröhlich-Lieb configuration for m-variables.

Here, we see that, once reflected through a plane, P_z^+ becomes $P_{r(z)}^+$. This fact is general. Now we can go on and introduce a second plane P_2 to obtain

$$\langle P_{z_1}^+ P_{z_2}^- \rangle_A \leqslant \langle P_{z_1}^+ P_{z_2}^- P_{z_3}^- P_{z_4}^+ P_{z_5}^+ P_{z_6}^- P_{z_7}^- P_{z_8}^+ \rangle_A^{1/4}.$$
 (2.27)

It is clear that, applying this procedure repeatedly, we obtain

$$\langle P_{z_1}^+ P_{z_2}^- \rangle_A \leqslant \langle P_{FL} \rangle_A^{2/|A|} \tag{2.28}$$

where P_{FL} projects on the Fröhlich–Lieb configuration defined in Fig. 3.

Such a procedure can be extended to the case where there are many bonds in $\gamma_{\alpha,\beta}$ if the size *L* of the lattice is a multiple of 4 (simply because the Fröhlich-Lieb configuration is defined only for such lattices). In this case, the situation is more complicated but it is sufficient to follow the combinatorial machinery developed in ref. 5. The final result is

$$\left\langle \prod_{\langle z, z'\rangle \in \gamma_{\alpha,\beta}} P_z^+ P_{z'}^- \right\rangle_A \leqslant \left\langle P_{FL} \right\rangle_A^{\frac{2|\gamma_{\alpha,\beta}|}{|A|}}$$
(2.29)

where $|\gamma_{\alpha,\beta}|$ is the length of the contour $\gamma_{\alpha,\beta}$. If we introduce (2.29) into (2.22), we finally obtain the chessboard estimate

$$\langle P_x^+ P_y^- \rangle_A \leqslant \sum_{\gamma} \langle P_{FL} \rangle_A^{\frac{|\gamma|}{2|A|}}.$$
 (2.30)

We now perform the sum over the contours in (2.30). As already mentioned, all contours have an even length $|\gamma| = 2l$, l = 2, 3,... If we denote by n(l) the number of contours of length 2l, we can write

$$\sum_{\gamma} \langle P_{FL} \rangle_{\Lambda}^{\frac{|\gamma|}{2|\mathcal{A}|}} = \sum_{l=2}^{\infty} n(l) \langle P_{FL} \rangle_{\Lambda}^{\frac{l}{|\mathcal{A}|}}.$$
(2.31)

A contour must have length 2l and surround x or y. First we estimate the number of contours surrounding x. We draw a vertical line starting from x and we begin to construct the contour from a site on this line going to the right. We have at most l-1 possibilities to start. Having chosen one of them, we have at each step three possibilities to go on in the construction except for the last step since the contour has to be closed. This gives at most 3^{2l-2} different contours. We can perform the same discussion for the contours surrounding y and we finally get $n(l) \leq 2(l-1) 3^{2l-2}$. From (2.21), (2.30), and (2.31) we see that to complete the proof of long-range order it remains to show that

$$\langle P_{FL} \rangle_{\mathcal{A}}^{\frac{1}{|\mathcal{A}|}} \leqslant x_0 \tag{2.32}$$

where x_0 is a sufficiently small positive number. This is the object of the next section.

3. EXPONENTIAL LOCALIZATION AND PROOF OF LONG-RANGE ORDER

Let E_0, \ldots, E_i, \ldots be the eigenvalues of the Hamiltonian (1.2) or (1.3). We can introduce the corresponding basis of normalized eigenvectors $|\phi_0\rangle, \ldots, |\phi_i\rangle, \ldots$ to write

$$\langle P_{FL} \rangle = \frac{\sum_{i} e^{-\beta E_{i}} \langle \phi_{i} | P_{FL} | \phi_{i} \rangle}{\sum_{i} e^{-\beta E_{i}}}.$$
(3.1)

For large values of E_i , the factor $e^{-\beta E_i} \langle \phi_i | P_{FL} | \phi_i \rangle$ is small due to the weight $e^{-\beta E_i}$ of highly excited levels. However, for low energies E_i , the small term is the matrix element $\langle \phi_i | P_{FL} | \phi_i \rangle$ if the quantum fluctuations are weak. The reason is that the Fröhlich–Lieb projector projects the small energy vector $|\phi_i\rangle$ onto a high energy part of the Hilbert space. The idea is thus to divide the sum in the numerator of (3.1) in two parts depending whether E_i is small or large

$$\langle P_{FL} \rangle = R_{-}(\varDelta) + R_{+}(\varDelta)$$
 (3.2)

with

$$R_{-}(\varDelta) = \sum_{E_0 \leqslant E_i \leqslant E_0 + \varDelta |\varDelta|} e^{-\beta E_i} \langle \phi_i | P_{FL} | \phi_i \rangle / \sum_i e^{-\beta E_i}$$
(3.3)

$$R_{+}(\varDelta) = \sum_{E_{i} \ge E_{0} + \varDelta | \varDelta |} e^{-\beta E_{i}} \langle \phi_{i} | P_{FL} | \phi_{i} \rangle \Big/ \sum_{i} e^{-\beta E_{i}}$$
(3.4)

where Δ is a parameter that will be determined later on. The term $R_+(\Delta)$ corresponding to high energies is easy to estimate

$$R_{+}(\varDelta) \leq \sum_{E_{i} \geq E_{0}+\varDelta |\varDelta|} e^{-\beta(E_{0}+\varDelta |\varDelta|)} \langle \phi_{i} | P_{FL} | \phi_{i} \rangle / e^{-\beta E_{0}}$$
$$\leq \sum_{E_{i} \geq E_{0}+\varDelta |\varDelta|} e^{-\beta \varDelta |\varDelta|} \leq \sum_{i} e^{-\beta \varDelta |\varDelta|} \leq 4^{|\varDelta|} e^{-\beta \varDelta |\varDelta|}$$
(3.5)

where we used the fact that $\langle \phi_i | P_{FL} | \phi_i \rangle \leq 1$ and that the dimension of the Hilbert space is $4^{|\Delta|}$. Clearly if β is large enough this last bound is small. For $R_{-}(\Delta)$ we have

$$R_{-}(\varDelta) \leq \max_{E_{0} \leq E_{i} \leq E_{0} + \varDelta |\varDelta|} \langle \phi_{i} | P_{FL} | \phi_{i} \rangle$$
(3.6)

To prove that these matrix elements are small we need the following theorem

Theorem 7. Exponential Localization.⁽⁵⁾ Let *A* and *B* be bounded selfadjoint operators on a Hilbert space \mathscr{H} such that: (i) $A \ge 0$, (ii) there exists $0 < \epsilon < 1$ such that $\pm B \le \epsilon A$. Let $|\phi\rangle$ be a normalized eigenvector of A+B, i.e., $(A+B) |\phi\rangle = \lambda |\phi\rangle$, $\langle \phi | \phi \rangle = 1$. Let us choose $\rho > \lambda \ge 0$ such that $\sigma = \epsilon \rho (\rho - \lambda)^{-1} < 1$. Let P_{ρ} be the spectral projection of *A* corresponding to $[\rho, \infty)$ and $M_{\rho} = P_{\rho} \mathscr{H}$. Let $N \subset M_{\rho}$ be a subspace of M_{ρ} such that for each $|\Psi\rangle \in N$ we have: (iii) $\{B(A-\lambda)^{-1}\}^j |\Psi\rangle \in M_{\rho}$ for j = 0, ..., d-1 with $d \ge 1$. Let finally *P* be the projector onto *N*. Then $\langle \phi | P | \phi \rangle \leq \sigma^{2d}$.

We now apply Theorem 7 to our hamiltonians. Let us first give the details for model (1.2). Once this case understood, we will simply indicate the result for (1.3). In order to fulfill (i) and (ii) we need to shift (1.2) by some constant. Let α_0 be some real positive constant to be determined later on and consider the new hamiltonian

$$\tilde{H}(\alpha) = \sum_{x, y \in A} t_{xy} c_x^+ c_y + U \sum_{x \in A} \sigma_x^{(3)}(n_x - 1/2) + \alpha \sum_{x \in A} \sigma_x^{(1)} - E_0(\alpha = \alpha_0) \quad (3.7)$$

where $E_0(\alpha = \alpha_0)$ is the ground state energy of

$$\sum_{x, y \in A} t_{xy} c_x^+ c_y + U \sum_{x \in A} \sigma_x^{(3)}(n_x - 1/2) + \alpha_0 \sum_{x \in A} \sigma_x^{(1)}.$$
 (3.8)

The hamiltonian $\tilde{H}(\alpha)$ is simply (1.2) shifted by some constant so its eigenvectors are $|\phi_i\rangle$ and the corresponding eigenvalues are $\tilde{E}_i = E_i - E_0(\alpha = \alpha_0)$. To apply the theorem, we decompose $\tilde{H}(\alpha) = A + B$ with

$$A = \sum_{x, y \in A} t_{xy} c_x^+ c_y + U \sum_{x \in A} \sigma_x^{(3)}(n_x - 1/2) - E_0(\alpha = \alpha_0)$$
(3.9)

$$B = \alpha \sum_{x \in \Lambda} \sigma_x^{(1)}.$$
 (3.10)

The eigenvectors of A have the form $|\{s_x\}\rangle \otimes |\phi_i^A(\{s_x\})\rangle$ with eigenvalues $e_i^A(\{s_x\})$ where $\{s_x\}$ is a spin configuration and $|\phi_i^A(\{s_x\})\rangle$ are the eigenvectors of A restricted to the subspace defined by the configuration $\{s_x\}$. We know that the minimizers of $e_i^A(\{s_x\})$ are the two chessboard configurations,⁽⁴⁾ i.e., the ground states have the form $|\{s_x^{CB}\}\rangle \otimes |\phi_0^A(\{s_x^{CB}\})\rangle = |\phi_{GS}^A\rangle$ where $s_x^{CB} = \pm (-1)^{|x|}$.

We note that $\tilde{H}(\alpha = \alpha_0) \ge 0$ by definition. Since $\langle \phi_{GS}^A | \sigma_x^{(1)} | \phi_{GS}^A \rangle = 0$ we have

$$\langle \phi_{GS}^{A} | A | \phi_{GS}^{A} \rangle = \langle \phi_{GS}^{A} | \tilde{H}(\alpha = \alpha_{0}) | \phi_{GS}^{A} \rangle \ge 0$$
(3.11)

so (i) is satisfied. Moreover $\tilde{H}(\alpha = \alpha_0) = A + \alpha_0 \alpha^{-1}B$ therefore $\epsilon A + B \ge 0$ with $\epsilon = \alpha/\alpha_0$ and $\alpha < \alpha_0$. We also have that $\epsilon A - B \ge 0$ since we can transform *B* into -B through a spin space rotation of angle π around the 3 axis. So (ii) is also satisfied. We now take $P = P_{FL}$, *N* the image of P_{FL} and $|\phi\rangle$ an eigenvector of $\tilde{H}(\alpha)$ with eigenvalue λ satisfying $\tilde{E}_0 \le \lambda \le \tilde{E}_0 + \Delta |A|$. Any vector $|\Psi\rangle$ in the Hilbert space can be decomposed in terms of the eigenvectors of *A* as

$$|\Psi\rangle = \sum_{\{s_x\}} \sum_i c_i(\{s_x\}) |\{s_x\}\rangle \otimes |\phi_i^A(\{s_x\})\rangle$$
(3.12)

where the $c_i(\{s_x\})$ are the Fourier coefficients of the decomposition. Since $P_{FL} |\{s_x\}\rangle = 0$ if $\{s_x\} \neq \{s_x^{FL}\}$ and $P_{FL} |\{s_x^{FL}\}\rangle = |\{s_x^{FL}\}\rangle$, we have

$$P_{FL} |\Psi\rangle = \sum_{i} c_i(\{s_x^{FL}\}) |\{s_x^{FL}\}\rangle \otimes |\phi_i^A(\{s_x^{FL}\})\rangle$$
(3.13)

Thus the subspace N is described by all the linear combinations of the form appearing in the preceding equation and $N \subset M_{e_0^A(\{s_x^{FL}\})}$. Let us now apply

the operator $B(A-\lambda)^{-1}$ on a vector belonging to N. Evidently the vector $(A-\lambda)^{-1} P_{FL} |\Psi\rangle$ remains in N. Let us now apply B on a vector in N. If we introduce the notation $\{s_x\}_y$ for the configuration where we flip $s_y \to -s_y$ and leave the other s_x ($x \neq y$) unchanged, we have

$$\sigma_y^1 | \{s_x\} \rangle = | \{s_x\}_y \rangle. \tag{3.14}$$

This yields

$$BP_{FL} |\Psi\rangle = \sum_{y \in A} \sum_{i} c_i(\{s_x^{FL}\}) |\{s_x^{FL}\}_y\rangle \otimes |\phi_i^A(\{s_x^{FL}\})\rangle$$
(3.15)

The vectors in the right-hand side of (3.15) are not eigenvectors of A, however we can write

$$|\phi_i^A(\{s_x^{FL}\})\rangle = \sum_j \tilde{c}_j |\phi_i^A(\{s_x^{FL}\}_y)\rangle$$
(3.16)

and insert it into (3.15) to find

$$BP_{FL} |\Psi\rangle = \sum_{y \in A} \sum_{i,j} c_i(\{s_x^{FL}\}) \tilde{c}_j |\{s_x^{FL}\}_y\rangle \otimes |\phi_i^A(\{s_x^{FL}\}_y)\rangle.$$
(3.17)

The vector $BP_{FL} | \Psi \rangle$ is now decomposed in terms of eigenvectors of A with eigenvalues $e_i^A (\{s_x^{FL}\}_y)$. If we set

$$\gamma^{FL} = \max_{y \in A} |e_0^A(\{s_x^{FL}\}) - e_0^A(\{s_x^{FL}\}_y)|.$$
(3.18)

we have that

$$BP_{FL} |\Psi\rangle \in M_{e_0^A(\{s_x^{FL}\}) - \gamma^{FL}}.$$
(3.19)

In summary, applying once the operator $B(A-\lambda)^{-1}$ on a vector belonging to N, we obtain a vector belonging to $M_{e_0^A(\{s_x^{FL}\}-\gamma^{FL}\}}$. If we apply it a second time, we need again to estimate the loss in A-energy. This loss cannot be greater than

$$\gamma = \max_{y \in A} \max_{\{s_x\}} |e_0^A(\{s_x\}) - e_0^A(\{s_x\}_y)|$$
(3.20)

In order to determine the *d* appearing in hypothesis (iii) of Theorem 7, we have to know how many times we can apply the operator $B(A-\lambda)^{-1}$ without leaving the subspace M_{ρ} . If we apply it *d* times, we get a vector belonging to $M_{\epsilon_0^A(\{s_x^{FL}\})-d\gamma}$ that must be contained in M_{ρ} . Thus we can choose $d = (e_0^A(\{s_x^{FL}\})-\rho) \gamma^{-1}$. We set $\rho = \tilde{E}_0 + n\Delta |A|$ with *n* a positive number to be

determined later on. Since $|\phi_{GS}^A\rangle = |\{s_x^{CB}\}\rangle \otimes |\phi_0^A(\{s_x^{CB}\})\rangle$ is the ground state of A, the variational principle implies $\tilde{E}_0 \leq \langle \phi_{GS}^A | \tilde{H}(\alpha) | \phi_{GS}^A \rangle = e_0^A(\{s_x^{CB}\})$. Therefore we find

$$d = \frac{e_0^A(\{s_x^{FL}\}) - \tilde{E}_0 - n\Delta |\Delta|}{\gamma} \ge \frac{e_0^A(\{s_x^{FL}\}) - e_0^A(\{s_x^{CB}\}) - n\Delta |\Delta|}{\gamma} = \frac{g |\Delta|}{2\gamma}$$
(3.21)

For σ we have

$$\sigma \leq \frac{\alpha}{\alpha_0} \frac{\rho}{\rho - \tilde{E}_0 - \Delta |\Lambda|} = \frac{\alpha}{\alpha_0} \frac{\tilde{E}_0 + n\Delta |\Lambda|}{(n-1)\Delta |\Lambda|} \leq \frac{\alpha}{\alpha_0} \frac{(\alpha_0 - \alpha) + n\Delta |\Lambda|}{(n-1)\Delta |\Lambda|}$$
(3.22)

In the first inequality we used that $\lambda < \tilde{E}_0 + \Delta |\Lambda|$ and in the second we applied the variational principle in the form

$$\widetilde{E}_{0} \leq \langle \phi_{0}(\alpha = \alpha_{0}) | \widetilde{H}(\alpha) | \phi_{0}(\alpha = \alpha_{0}) \rangle
= \langle \phi_{0}(\alpha = \alpha_{0}) | (\alpha - \alpha_{0}) \sum_{x \in A} \sigma_{x}^{(1)} | \phi_{0}(\alpha = \alpha_{0}) \rangle
\leq (\alpha_{0} - \alpha) |A|.$$
(3.23)

We have now to determine α_0 , *n* and Δ . The natural quantity entering the discussion is the *A*-energy difference *g* between the Fröhlich–Lieb and chessboard configurations given by

$$g = \frac{e_0^A(\{s_x^{FL}\}) - e_0^A(\{s_x^{CB}\})}{|\Lambda|}$$
(3.24)

We choose n = 2, $\Delta = g/4$, $\alpha_0 = \frac{g}{2}$, which leads to $d \ge \frac{g|A|}{2\gamma}$ and $\sigma = 8\alpha/g$. Theorem 7 states that $\langle \phi | P_{FL} | \phi \rangle \le \sigma^{2d}$ for any eigenvector $| \phi \rangle$ of A with eigenvalue $\tilde{E}_0 \le \lambda \le \tilde{E}_0 + \Delta |A|$. We can now insert this last inequality into (3.6) and use (3.5) and (3.2) to obtain

$$\langle P_{FL} \rangle_{\Lambda}^{\frac{1}{|A|}} \leq \left(e^{-\beta \Delta |A|} 4^{|A|} + \left(\frac{8\alpha}{g} \right)^{\frac{g|A|}{\gamma}} \right)^{\frac{1}{|A|}}.$$
 (3.25)

Using the inequality $(a+b)^s \le a^s + b^s$ for 0 < s < 1, we get

$$\langle P_{FL} \rangle_{\Lambda}^{\frac{1}{|\Lambda|}} \leq 4 \mathrm{e}^{-\beta g/4} + \left(\frac{8\alpha}{g}\right)^{\frac{8}{\gamma}}.$$
 (3.26)

If we combine the bound (3.26) with the Peierls argument, we obtain that there is long-range order (1.4) for hamiltonian (1.2) if the following condition is satisfied

$$4\mathrm{e}^{-\beta g/4} + \left(\frac{8\alpha}{g}\right)^{\frac{g}{\gamma}} \leq x_0 \tag{3.27}$$

It remains to compute γ and g as functions of U, two quantities that are related to the static Falicov–Kimball model (1.1). We can find an upper bound for γ as follows

$$A(\{s_x\}_y) = A(\{s_x\}) - 2Us_y(n_y - 1/2).$$
(3.28)

so by the variational principle

$$e_{0}^{A}(\{s_{x}\}_{y}) - e_{0}^{A}(\{s_{x}\}) \leq \langle \phi_{0}^{A}(\{s_{x}\}) | A(\{s_{x}\}_{y}) | \phi_{0}^{A}(\{s_{x}\}) \rangle - \langle \phi_{0}^{A}(\{s_{x}\}) | A(\{s_{x}\}) | \phi_{0}^{A}(\{s_{x}\}) \rangle = -2U \langle \phi_{0}^{A}(\{s_{x}\}) | s_{y}(n_{y} - 1/2) | \phi_{0}^{A}(\{s_{x}\}) \rangle \leq U. \quad (3.29)$$

Similarly

$$e_{0}^{A}(\{s_{x}\}) - e_{0}^{A}(\{s_{x}\}_{y}) \leq \langle \phi_{0}^{A}(\{s_{x}\}_{y}) | A(\{s_{x}\}) | \phi_{0}^{A}(\{s_{x}\}_{y}) \rangle$$

- $\langle \phi_{0}^{A}(\{s_{x}\}_{y}) | A(\{s_{x}\}_{y}) | \phi_{0}^{A}(\{s_{x}\}_{y}) \rangle$
= $2U \langle \phi_{0}^{A}(\{s_{x}\}_{y}) | s_{y}(n_{y} - 1/2) | \phi_{0}^{A}(\{s_{x}\}_{y}) \rangle \leq U.$ (3.30)

These estimates imply the general bound $\gamma \leq U$ valid for all U. For the particular case where $U \rightarrow \infty$ we can use a t/U expansion⁽⁸⁾ to obtain $\gamma \sim t^2/U$.

For g we need a lower bound. Here we discuss explicitly the case d = 2 but the conclusions hold for any $d \ge 2$. In the limit of large volume and for Fermi statistics

$$g = \frac{e_0^A(\{s_x^{FL}\}) - e_0^A(\{s_x^{CB}\})}{|A|} = \frac{1}{4\pi^2} \int_0^{\pi} dk_x \int_0^{2\pi} dk_y$$
$$\times (-\sqrt{2+4\cos^2 k_y + U^2 + 2\sqrt{\cos^2(2k_x) + U^2}})$$
$$-\sqrt{2+4\cos^2 k_y + U^2 - 2\sqrt{\cos^2(2k_x) + U^2}}$$
$$+ 2\sqrt{4(\cos^2 k_x + \cos^2 k_y) + U^2}). \tag{3.31}$$



Fig. 4. Bound on $\beta_c(U)^{-1}$ for fixed α and t^{\downarrow} and for fermions.

From this formula one can check that g is always strictly positive for any $U \neq 0$. For the hard-core bosons we are not able to compute g for all values of U but we can use the expansion in t/U,⁽⁸⁾ to get $g \sim t^2/U$.

Using these results on γ and g we get $\beta_c^{-1} \sim g$ (see Fig. 4 for d = 2) and $\alpha_c \sim g e^{-\frac{\gamma}{g} |\log x_0|}$. We have shown that $\gamma \leq U$. When $U \to 0$, one can check that $\gamma/g \leq U/g$ goes to infinity and thus the upper bound on α goes to zero exponentially fast. When $U \to \infty$, both g and γ behave like t^2/U , thus $\alpha_c(U) \sim t^2/U$. We have indicated in Fig. 5 the qualitative behavior of the critical α as a function of U.

For the asymmetric Hubbard model (1.3) all the above estimates can be performed in a similar way and we find that there is long-range order if the following condition is satisfied

$$4\mathrm{e}^{-\beta g/4} + \left(\frac{32t^{\downarrow}}{g}\right)^{\frac{g}{\gamma}} \leq x_0 \tag{3.32}$$

We note that this is the same condition than (3.27) with α replaced by t^{\downarrow} .



Fig. 5. Bound on $\alpha_c(U)$ or $t_c^{\downarrow}(U)$ for fixed β and for fermions.

Concerning the hard-core bosons, all the discussion presented in this section is valid except that it is not possible to compute the function g for all U. Using the asymptotic behavior $g \equiv t^2/U$ of ref. 8 we conclude that there is long-range order for large U.

4. OFF-DIAGONAL LONG RANGE ORDER FOR HARD CORE BOSONS

We prove that there exists ϵ independent of Λ such that

$$\frac{1}{|\Lambda|} \langle c_{k_{\pi}}^{+} c_{k_{\pi}} \rangle_{\Lambda} = \frac{1}{|\Lambda|^{2}} \sum_{x, y \in \Lambda} (-1)^{|x|+|y|} \langle c_{x}^{+} c_{y} \rangle_{\Lambda} \ge \epsilon > 0$$

$$(4.1)$$

for sufficiently large Λ and low temperatures for the two models (1.2) and (1.3) in dimension $d \ge 3$. A similar result may be obtained for d = 2 at zero temperature following⁽¹¹⁾ but the derivation is more lengthy so that we will omit it. The proof uses Lemma 5 to derive infrared bounds.

Let us first discuss the model (1.2). The starting point is the sum rule

$$\sum_{k \in B} \langle c_k^+ c_k \rangle_A = \frac{1}{|\mathcal{A}|} \sum_{k \in B} \sum_{x, y \in A} e^{ik \cdot (y-x)} \langle c_y^+ c_x \rangle_A = \sum_{x \in A} \langle c_x^+ c_x \rangle_A = |\mathcal{A}|/2.$$
(4.2)

which implies

$$\frac{1}{|\Lambda|} \langle c_{k_{\pi}}^{+} c_{k_{\pi}} \rangle_{\Lambda} = \frac{1}{2} - \frac{1}{|\Lambda|} \sum_{\substack{k \in B \\ k \neq k_{\pi}}} \langle c_{k}^{+} c_{k} \rangle_{\Lambda}.$$

$$(4.3)$$

The proof of off-diagonal long-range order will be achieved if we are able to show that the two-point correlation functions $\langle c_k^+ c_k \rangle_A$ are small enough for $k \neq k_{\pi}$. We introduce in the Hamiltonian external fields $\{h_{xy}\}$

$$H_{A}(\{h_{xy}\}) = \frac{1}{2} \sum_{x, y \in A} t_{xy} (c_{x}^{+} + c_{y} - h_{xy})^{2} + U \sum_{x \in A} \sigma_{x}^{(3)} (n_{x} - \frac{1}{2}) + \alpha \sum_{x \in A} \sigma_{x}^{(1)}$$
(4.4)

where h_{xy} is real and symmetric, $h_{xy} = h_{yx}$. In the case where all the h_{xy} are zero, $H_A(\{h_{xy}\})$ is exactly the original Hamiltonian. By the usual electron-hole transformation the Hamiltonian (4.4) can be rewritten in a reflection positive form and a standard application of Lemma 5 (see ref. 9) leads to

$$Z_{A}(\{h_{xy}\}) \leq Z_{A}(\{0\}).$$
 (4.5)

Expanding to second order in powers of the fields h_{xv} , one gets:

$$\sum_{\substack{\langle x, y \rangle \\ \langle x', y' \rangle}} h_{xy} h_{x'y'} (c_x^+ + c_x, c_{x'}^+ + c_{x'})_A \leq \frac{1}{\beta t} \sum_{\langle x, y \rangle} h_{xy}^2.$$
(4.6)

Up to now, we have considered only real fields h_{xy} , but (4.6) may be extended to complex ones

$$\sum_{\substack{\langle x, y \rangle \\ \langle x', y' \rangle}} \bar{h}_{xy} h_{x'y'} (c_x^+ + c_x, c_{x'}^+ + c_{x'})_A \leqslant \frac{1}{\beta t} \sum_{\langle x, y \rangle} |h_{xy}|^2.$$
(4.7)

We now choose a specific form for the fields h_{xy} . For k a fixed wave vector, we take

$$h_{xy} = \frac{1}{\sqrt{|A|}} \left(e^{-ik \cdot x} + e^{-ik \cdot y} \right).$$
(4.8)

Inserting this form into inequality (4.7), we obtain the following infrared bound

$$(c_k^+ + c_{-k}, c_{-k}^+ + c_k)_A \leq \frac{1}{\beta t (d + \sum_{i=1}^d \cos k_i)}.$$
(4.9)

The number of bosons is conserved by Hamiltonian (1.2) so that $(c_k^+, c_{-k}^+)_A = (c_k, c_{-k})_A = 0$. Moreover $(c_k^+, c_k)_A = (c_{-k}, c_{-k}^+)_A$. Finally

$$(c_k^+, c_k)_A \leq \frac{1}{2\beta t (d + \sum_{i=1}^d \cos k_i)} = \frac{B_k}{\beta t}.$$
 (4.10)

We now transfer the information contained in (4.10) onto the (symmetrized) two-point correlation function through the upper bound⁽⁹⁾

$$\frac{1}{2} \langle c_k^+ c_k + c_k c_k^+ \rangle_A \leqslant \frac{1}{2} \sqrt{\frac{B_k C_k}{t}} \operatorname{coth} \sqrt{\frac{\beta^2 t C_k}{4B_k}}$$
(4.11)

where C_k is an upper bound on the expectation value of double commutator $C_k = \langle [c_k^+, [H_A, c_k]] \rangle_A$. The symmetrized two-point correlation function can be expressed as

$$\frac{1}{2} \langle c_k c_k^+ + c_k^+ c_k \rangle_A = \frac{1}{2 |A|} \sum_{\substack{x, y \in A \\ x \neq y}} e^{ik \cdot (y-x)} \langle c_x c_y^+ + c_y^+ c_x \rangle_A$$
$$= \frac{1}{|A|} \sum_{\substack{x, y \in A \\ x \neq y}} e^{ik \cdot (y-x)} \langle c_y^+ c_x \rangle_A + \frac{1}{2 |A|} \sum_{\substack{x \in A \\ x \in A}} 1$$
$$= \frac{1}{|A|} \sum_{\substack{x, y \in A \\ x, y \in A}} e^{ik \cdot (y-x)} \langle c_y^+ c_x \rangle_A = \langle c_k^+ c_k \rangle_A$$
(4.12)

where we used the commutation relations (1.3) for the hard-core bosons and the fact that $\langle c_x^+ c_x \rangle_A = 1/2$. Inserting (4.11) into the sum rule (4.2), we get

$$\frac{1}{|\Lambda|} \langle c_{k_{\pi}}^{+} c_{k_{\pi}} \rangle_{\Lambda} \geq \frac{1}{2} - \frac{1}{|\Lambda|} \sum_{\substack{k \in B \\ k \neq k_{0}}} \frac{1}{2} \sqrt{\frac{B_{k}C_{k}}{t}} \coth \sqrt{\frac{\beta^{2}tC_{k}}{4B_{k}}}.$$
(4.13)

In the limit of large Λ , we obtain

$$\frac{1}{|A|} \langle c_{k_{\pi}}^{+} c_{k_{\pi}} \rangle_{A} \geq \frac{1}{2} - \frac{1}{(2\pi)^{d}} \int_{B} \mathrm{d}^{d} k \, \frac{1}{2} \sqrt{\frac{B_{k} C_{k}}{t}} \coth \sqrt{\frac{\beta^{2} t C_{k}}{4B_{k}}}.$$
(4.14)

This last integral is convergent at finite temperature for $d \ge 3$. To have long-range order at finite temperatures in three dimensions, it is sufficient to have

$$1 - \frac{1}{(2\pi)^d} \int_B d^d k \sqrt{\frac{B_k C_k}{t}} > 0$$
 (4.15)

since, if (4.15) is true (4.14) will also be true for large but finite values of β , because the integrand in (4.14) is continuous in β . Below we check that this condition is fulfilled for t/U small enough and $d \ge 3$. By the Cauchy–Schwarz inequality (note that $C_k \ge 0$):

$$\frac{1}{(2\pi)^d} \int_B \mathrm{d}^d k \sqrt{B_k C_k} \leqslant \sqrt{\frac{1}{(2\pi)^3}} \int_B \mathrm{d}^3 k B_k \sqrt{\frac{1}{(2\pi)^3}} \int_B \mathrm{d}^3 k C_k \,. \tag{4.16}$$

The double commutator is

$$[c_{k}^{+}, [H_{A}, c_{k}]] = -\frac{2}{|A|} \sum_{x, y \in A} t_{xy} c_{x}^{+} c_{y} + \frac{1}{|A|} \sum_{x, y \in A} t_{xy} \cos[k \cdot (x - y)] \times (2n_{x} - 1)(2n_{y} - 1) - \frac{U}{|A|} \sum_{x \in A} \sigma_{x}^{(3)}(2n_{x} - 1).$$
(4.17)

The first term can be identified to the XY model through $c_x^+ = S_x^1 + iS_x^2$ and $c_x = S_x^1 - iS_x^2$ and we can use a bound of ref. 9 to show that its expectation value is smaller than $t\sqrt{d(d+1)}$. The second one gives zero when integrated over k in (4.16), and the expectation value of the third one is obviously less than U. Thus

$$\frac{1}{(2\pi)^d} \int_B \mathrm{d}^d k \ C_k \leqslant t \ \sqrt{d(d+1)} + U \tag{4.18}$$

From (4.18), (4.16) and (4.15 we get the condition

$$\frac{U}{t} + \frac{\sqrt{d(d+1)}}{(2\pi)^d} \int_B \mathrm{d}^d k \; B_k < 1 \tag{4.19}$$

One may check numerically that the second term in (4.19) is strictly less than 1 for all $d \ge 3$, so that there is ODLRO if U is small enough.

Finally, a similar discussion holds for model (1.3) both for the spin up and spin down particles. One simply introduces h_{xy} fields coupling either with the spins up or with the spins down and uses the sum rule

$$\sum_{k \in B} \langle c_{k\sigma}^+ c_{k\sigma} \rangle_A = \sum_{x \in A} \langle c_{x\sigma}^+ c_{x\sigma} \rangle_A = \frac{|A|}{2}.$$
(4.20)

ACKNOWLEDGMENTS

C.-A. Piguet acknowledges support from the Swiss National Science Foundation.

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