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Some rigorous results on the ground states of the Falicov-Kimball model

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Dedicated to Elliott Lieb on the occasion of his sixtieth birthday

Abstract:

The Falicov-Kimball model consists of nuclei which are not allowed to hop and spinless electrons which can hop between nearest neighbor sites. There is an on-site interaction between electrons and nuclei. We consider the model in two dimensions with a large attractive potential. For the neutral model with densities between 1/4 and 1/2 we prove that the configuration of the nuclei in the ground state must consist of parallel lines of lattice sites which are either completely occupied by nuclei or completely free of nuclei. (The angle of the lines with respect to the lattice depends on the density. Some mild assumptions on the ground state are needed for this result.) For densities 1/3, 1/4 and 1/5 we prove that the ground state configuration of the nuclei is indeed that which had been conjectured [8]. For the nonneutral model we show that if the model is close to neutrality in the sense that both the electron and nuclear densities are close to 1/2, 1/3, 1/4 or 1/5 then the configuration of the nuclei in the ground state is close to the nuclear ground state for the neutral model with density 1/2, 1/3, 1/4 or 1/5.

1. Introduction

The Hubbard model is one of the simplest models of interacting fermions. In this model the interacting fermions are usually thought of as electrons, and they can hop between nearest neighbor sites. The only interaction between the electrons is on-site. It costs energy U to put two electrons on the same site. Otherwise there is no interaction between them. It is important to observe that there is no explicit spin-spin interaction in this model. If the spins are in an ordered state, it must arise through a subtle interplay between the kinetic and potential energy terms in the Hamiltonian. Unfortunately, the Hubbard model has not been very amenable to rigorous results. Two notable exceptions to this statement are the following. In one dimension the model was solved exactly by Lieb and Wu [14]. In any number of dimensions Lieb showed that on a bipartite lattice the ground state of the Hubbard model has total spin zero in the attractive case and total spin $\frac{1}{2}||A|-|B||$ in the replusive case where $|A|$ and $|B|$ are the number of sites in the two sublattices [13].

Another model of interacting fermions that has been more receptive to rigorous treatment is the Falicov-Kimball model. It consists of spinless electrons and classical particles, which we refer to as nuclei. The electrons can hop between nearest neighbor sites and there is an on-site interaction between electrons and nuclei. At most one nuclei is allowed at each lattice site. The Hamiltonian is

$$H = \sum_{x,y:|x-y|=1} c_x^\dagger c_y - 2U \sum_x c_x^\dagger c_x W(x) \tag{1.1}$$

where $c_x^\dagger$ and c_x are creation and annihilation operators for the electrons. $W(x) = 1$ if there is a nucleus at x and $W(x) = 0$ if there is not. The sum over x, y is over nearest neighbor bonds in a hypercubic lattice. (One can consider the model on other lattices or with a more general form of the hopping, but our results will be for this particular model.) As in the Hubbard model the only interaction term in the model is on site. If the nuclei exhibit long range order it must come about because the electrons produce an effective interaction between the nuclei.

The above description is only one of several interpretations of the Hamiltonian (1.1). Falicov and Kimball used the model to study the metal-insulator transition in transition-metal oxides [4]. In this interpretation the $c_x^\dagger$ and c_x are creation and annihilation operators for mobile d-electrons while $W(x)$ specifies the locations of localized f-electrons. Another interpretation of the model is as an approximation to the Hubbard model in which the spin up electrons are taken to be infinitely massive [11]. Since we have put a minus sign in front of the interaction term, for the interpretation of the model as nuclei and electrons we should take $U > 0$. For the other interpretations $U < 0$ is more appropriate. We will consider both cases although we will use the language of the nuclei-electron interpretation.

What makes the Falicov-Kimball model simpler to study than the Hubbard model is that the former may be reduced to a single particle Hamiltonian. There are no interactions between the electrons, so the Hamiltonian is just the second quantized form of the single electron Hamiltonian $T - 2UW$, where T is the operator with matrix elements t_{xy} with $t_{xy} = 1$ if $|x - y| = 1$ and $t_{xy} = 0$ otherwise. W is the diagonal operator with entries

$W(x)$. The Falicov-Kimball model is not trivial because we consider all possibilities for the locations of the nuclei, i.e., all binary potentials W. For example, to find the ground state for a particular density of electrons and nuclei we must consider all W with the desired nuclear density. It is convenient to let $2W(x) = s_x + 1$, so $s_x = 1$ when there is a nucleus at x and $s_x = -1$ when there is not. We then take

$$H = \sum_{x,y:|x-y|=1} c_x^\dagger c_y - U \sum_x c_x^\dagger c_x s_x$$

This differs from the original Hamiltonian by a term proportional to $\sum_x s_x$, but we will only consider problems in which the number of nuclei is fixed, so such a term is constant.

In the Hubbard model in the half filled band (the number of electrons is equal to the number of lattice sites) with large U there is a perturbative argument that predicts antiferromagnetic long range order [1]. Large U essentially forces there to be one electron at each site. The second order pertubation theory then yields an effective interaction between the spins of neighboring electrons that is given by the Heisenberg antiferromagnetic Hamiltonian. If one does the corresponding perturbation theory for the Falicov-Kimball model with the number of electrons and number of nuclei both equal to half the number of lattice sites then the resulting effective interaction for the s_x's is the Ising antiferromagnet.

Two different hole-particle symmetries imply that the model with interaction strength U, nuclear density ρ_n and electron density ρ_e is equivalent to the models with parameters $(-U, 1-\rho_n, \rho_e)$, $(-U, \rho_n, 1-\rho_e)$ and $(U, 1-\rho_n, 1-\rho_e)$. Thus statements about the attractive model in the neutral case ($\rho_n = \rho_e$) may be translated into statements about the repulsive model in the half-filled case ($\rho_n + \rho_e = 1$) and about the attractive model in the neutral case with the density ρ replaced by $1 - \rho$. For the sake of simplicity we state our results only for the attractive model with the nuclear density in $[0, 1/2]$, and leave the applications of the symmetries to the reader.

Throughout this paper we shall only be concerned with the case of large U. Rigorous and nonrigorous results suggest two general principles for the large U model. The segregation principle [5] says that if the nuclear and electron densities are not equal, i.e., the model is not neutral, then the ground state configuration for the nuclei is to clump the nuclei together. (Remember that the nuclei must occupy different sites.) In one dimension this has been proved by Lemberger [12]. We should emphasize that how large U must be can depend on how far the model is from neutrality. As we will see later, results in this paper show that as the nuclear density and electron density approach each other the U at which this segregation holds may go to infinity. Freericks and Falicov gave a simple physical argument for this segregation. Suppose that the number of electrons is less than the number of nuclei. For large U the electrons spend most of their time at sites occupied by nuclei. If we clump the nuclei together in a single large "box", then the electrons moving in this box will have lower kinetic energy than they would if we spread out the nuclei and formed a bunch of small boxes for the electrons to move in.

The second general principle concerns the neutral model. When the number of nuclei and the number of electrons are both equal to half the number of lattice sites, then for all dimensions and all nonzero U the ground state for the nuclei has been proven to be the checkerboard configuration in which the nuclei occupy one of the two sublattices

[3,11]. Thus in this case the nuclei like to spread out as much as possible into the most homogeneous configuration. (Rigorous results with a chemical potential included have also been obtained [7].) In one dimension Lemberger [12] gave a precise definition of "most homogeneous" for any density and proved that for the neutral model if U is large enough (depending on the density) then the ground state for the nuclei is the most homogeneous one. (Partial results in this direction had been obtained previously [2,6]. There is a strengthening of the result for low densities [9,10].) In dimensions greater than one there is no corresponding theorem; in fact it is not clear what the definition of most homogeneous should be. There are some nonrigorous results in two dimensions. Gruber, Jedrzejewski and Lemberger [8] studied the neutral model in two dimensions nonrigorously by doing perturbation theory in $1/U$. They determined the ground state for densities $1/3$, $1/4$ and $1/5$. (See figure 1.) The configurations in figure 1 appear to be the most homogenous configuration for the given densities.

In this paper we obtain rigorous results for the two dimensional model with large U for both the neutral and nonneutral cases. Since complete statements of the results will follow, we will state some special cases here to try to explain what the results say. Consider the neutral model with density between $1/3$ and $1/2$. With some assumptions on the nature of the ground state configuration of the nuclei, we will prove in theorem 2.1 that the nuclear ground state configuration has the following property. There is a choice of $m = 1$ or -1 such that every line of lattices sites with slope m is either completely occupied by nuclei or completely empty of nuclei. (Clearly the checkerboard configuration has this property as does the conjectured ground state for density $1/3$.) This property does not determine the ground state, but it does reduce the search for the ground state from a two dimensional to a one dimensional problem. We will also argue that it implies that the ground state is not always the most homogeneous one, at least for a reasonable definition of "most homogenous". (See remark 2 following theorem 2.1.) For the neutral model with densities $1/3$,$1/4$ and $1/5$ we prove in theorem 2.2 that the ground state is indeed that conjectured in [8].

For the nonneutral model we prove a result which is very different from the segregation principle. Take U large but fixed. We show that if the nuclear and electron densities are both close to $1/2$ then the ground state configuration of the nuclei is close (in a sense made precise in theorem 3.1) to a checkerboard configuration. These does not violate the segregation principle. It says that if we fix these densities and then increase U the ground state configuration will eventually segregate.

We conclude the introduction with some speculation and open questions. Our results on the neutral model are for densities between $1/4$ and $1/3$ and between $1/3$ and $1/2$. (Only the second case was discussed above.) It would be interesting to find analogous results for densities less than $1/4$. This will require studying higher order terms in the perturbation theory. A more interesting question is whether or not there are three dimensional analogs of these results.

The segregation principle and our theorems suggest the following picture. Consider the plane of nuclear density vs. electron density. On the diagonal (the neutral model) we expect a periodic arrangement of the nuclei in the ground state. For slightly nonneutral models the ground state arrangement will be close to a periodic arrangement and far from segregated. If the difference between the nuclear and electron densities is large enough, the nuclear ground state will be segregated. As U increases the size of the region where there is segregation grows, eventually encompassing all of the phase diagram except the neutral line. The only part of this picture with any rigorous support in two dimensions is the existence of regions where the nuclear ground state configuration is far from segregation. An important open problem is to show that segregation does indeed occur in dimensions greater than one.

2. The neutral case

Throughout this section the number of electrons is equal to the number of nuclei, the number of dimensions is two, and U is positive and large. Gruber, Jedrzejewski and Lemberger [8] studied this situation nonrigously by doing perturbation theory in $1/U$. They showed that if one computes the first two nontrivial orders in the perturbation series and ignores the higher orders, then for nuclear densities of $1/3$ and $1/5$ the ground state configuration for the nuclei is the configuration shown in figure 1. For nuclear density $1/4$ they conjectured that the ground state is the configuration shown in figure 1. In this section we will prove that for these three nuclear densities the ground state configurations are indeed those shown in figure 1 even when one does not ignore the higher order terms. However, the more interesting result in this section concerns rational densities in $(1/3, 1/2)$ and $(1/4, 1/3)$. If we assume that the nuclear ground state configuration is periodic and independent of U for sufficiently large U, then we can show that for large U the configuration must have period $(1, 1)$ or $(1, -1)$ if the density is in $(1/3, 1/2)$ and period $(1, 2)$, $(1, -2)$, $(2, 1)$ or $(2, -1)$ if the density is in $(1/4, 1/3)$. We say that s has period (p_1, p_2) if it is invariant under translation by (p_1, p_2), i.e., $s_x = s_{x+(np_1,np_2)}$ for all sites x and all integers n. We should emphasize that "period (p_1, p_2)" is only periodicity in one lattice direction. It does not imply that the ground state is determined by the configuration at a finite number of sites. However, it does reduce the search for the nuclear ground state from a two dimensional to a one dimensional problem.

Theorem 2.1: Fix a rational density ρ. Suppose there exists $U_0 > 0$ and a configuration s with density ρ such that for all $U \geq U_0$, s is a nuclear ground state configuration for the neutral model. Suppose also that s is periodic in the sense that there is a positive integer l such that $s_x = s_{x+(nl,ml)}$ for all sites x and all integers n and m. If the density $\rho \in [1/3, 1/2]$ then s has period $(1, 1)$ or period $(1, -1)$, i.e., $s_x = s_{x+(n,n)}$ for all sites x and all integers n or $s_x = s_{x+(n,-n)}$ for all sites x and all integers n. Moreover, on every horizontal line and every vertical line, each pair of consecutive nuclei is separated by either one or two empty sites. If the density $\rho \in [1/4, 1/3]$ then s has period $(1, 2)$,$(2, 1)$,$(1, -2)$ or $(2, -1)$. Moreover, in the case of period $(1, 2)$ or $(1, -2)$, on every vertical line each pair of consecutive nuclei is separated by either two or three empty sites, and in the case of period $(2, 1)$ or $(2, -1)$, on every horizontal line each pair of consecutive nuclei is separated by either two or three empty sites.

Remarks:

1. It is possible to prove a slightly stronger statement. There is a constant c such that the following is true. Let s be a ground state configuration for the nuclei in the sector with nuclear density ρ. Suppose that there is an integer l such that s has period l in each coordinate direction and $U \geq cl$. Then the conclusions of the theorem hold. The statement of the theorem requires that s be a ground state for all sufficiently large U. The above only requires that s be a ground state for some large U, but how large U must be depends on the period of s.

2. Although we cannot be certain the hypotheses of the theorem are ever satisfied, we can use the theorem to prove that certain s are not the ground state for a particular density. For example, consider a density that is less than but very close to $1/2$. A natural candidate for the ground state s for large U would be to take the checkerboard configuration and remove nuclei in a periodic way so that the sites from which nuclei are removed are as widely separated as possible. The theorem says that this is not the nuclear ground state.

3. It is possible for s to have more than one of the periods mentioned. For example the checkerboard configuration has both period $(1,1)$ and $(1,-1)$. The ground states for density $1/3$ have one of the periods $(1,1)$ or $(1,-1)$ as well as one of the periods $(1,2)$,$(2,1)$,$(1,-2)$,or $(2,-1)$.

Theorem 2.2: If the density is $1/5, 1/4$ or $1/3$ and U is sufficiently large then the nuclear ground state for the neutral model in a square with periodic boundary conditions is given (up to symmetries of the lattice) by figure 1. (We assume that the size of the square is commensurate with the configuration in figure 1.)

The proofs of both theorems are based on perturbation theory in $1/U$, so we begin by reviewing this perturbation theory, following the treatment by Gruber, Jedrzejewski and Lemberger [8]. A somewhat different derivation may be found in [12]. Let $H(s)$ be the ground state energy for the nuclear configuration s with the number of electrons equal to the number of nuclei. We will expand $H(s)$ in powers of $1/U$. Each term in the expansion will be a function of the configuration s.

If $U > 2d$ then the number of negative eigenvalues of $T - US$ is equal to the number of sites with $s_x = 1$, i.e., the number of nuclei. Thus when the number of electrons equals the number of nuclei, we have

$$H(s) = \sum_{\lambda_i < 0} \lambda_i = \frac{1}{2}[Tr(T - US) - Tr(|T - US|)] \tag{2.1}$$

Now $Tr(T) = 0$, and if we keep the number of nuclei fixed then $Tr(S)$ is a constant. So we might as well redefine $H(s) = -\frac{1}{2}Tr(|T - US|)$. Continuing to follow [8], we have

$$Tr(|T - US|) = Tr([(T - US)^2]^{\frac{1}{2}}) = UTr(1 + \Delta)^{\frac{1}{2}}$$

with

$$\Delta = -U^{-1}(TS + ST) + U^{-2}T^2$$

We have used the fact that $S^2 = 1$.

If U is sufficiently large, then $||\Delta|| < 1$ and we may expand $(1+\Delta)^{\frac{1}{2}}$ in a power series in Δ. Grouping together terms with the same power of $1/U$, we have

$$H(s) = U \sum_{n=0}^{\infty} U^{-n} \sum_{p_1,\cdots,p_k:n} c(p_1,p_2,\cdots,p_k)\, Tr(T^{p_1} S T^{p_2} S \cdots T^{p_k} S) \tag{2.2}$$

where the notation $p_1,\cdots,p_k : n$ means that the sum over $p_1,p_2,\cdots p_k$ is over all finite sequences of positive integers which sum to n. So k ranges from 1 to n. We also include the case of $k=0$ and interpret the operator in the trace to be T^n in this case. It is not hard to show that we have the following bound

$$\sum_{p_1,\cdots,p_k:n} |c(p_1,p_2,\cdots,p_k)| \leq c^n \tag{2.3}$$

for some constant c. The trace vanishes unless the number of T's is even, i.e,. unless n is even. Furthermore, the operator inside the trace is built up from TS,ST and T^2, so we see that the number of S's must also be even, i.e., k must be even.

Keeping in mind that T is just a nearest neighbor hopping,

$$Tr(T^{p_1} S T^{p_2} S \cdots T^{p_k} S) = \sum_{\omega} s_{\omega(t_1)} s_{\omega(t_2)} \cdots s_{\omega(t_k)} \tag{2.4}$$

where the sum is over all closed walks ω. $\omega(t)$ is the location of the walk after t steps with $t_j = \sum_{i=1}^{j} p_i$. The walks can start at any site. We now group together walks that start at the same site by letting

$$H_{n,x}(s) = \sum_{p_1,\cdots,p_k:n} \sum_{\omega:\omega(0)=x} c(p_1,p_2,\cdots,p_k) s_{\omega(t_1)} s_{\omega(t_2)} \cdots s_{\omega(t_k)} \tag{2.5}$$

We now have

$$H(s) = U \sum_{n=0}^{\infty} U^{-n} H_{n,x}(s)$$

As we noted before, only the terms with n even are nonzero.

The $n=2$ and $n=4$ terms in this perturbation theory were computed in [8]. We will denote the sum of the $n=2$ and $n=4$ terms by $H_0(s)$. They found that

$$\begin{aligned} H_0(s) = [\frac{1}{4}U^{-1} - \frac{9}{16}U^{-3}] \sum_{<xy>:|x-y|=1} s_x s_y + \frac{3}{16}U^{-3} \sum_{<xy>:|x-y|=\sqrt{2}} s_x s_y \\ + \frac{1}{8}U^{-3} \sum_{<xy>:|x-y|=2} s_x s_y + \frac{5}{16}U^{-3} \sum_{P} s(P) \end{aligned} \tag{2.6}$$

The sum over P is over all unit squares in the lattice. $s(P)$ is the product of s_x as x ranges over the four corners of the square. The sums over $< xy >$ are over bonds of length 1, $\sqrt{2}$

and 2. Note that we only count each bond once in the sums, whereas in [8] each bond is counted twice in their sums. This is why there is a relative factor of 2 between the above constants and those in [8] for the two body terms.

We rewrite this Hamiltonian as a sum over three by three blocks. Each square is contained in 4 different such blocks. Each bond $< xy >$ with $|x-y| = 1, \sqrt{2}$ or 2, is contained in 6,4 or 3 such blocks respectively. To avoid fractions with large denominators here and especially in the appendix, we will consider $5760 H_0(s)$. For a three by three block B we define

$$\begin{aligned} H_B = [240U^{-1} - 540U^{-3}] \sum_{<xy>\subset B:|x-y|=1} s_x s_y + 270U^{-3} \sum_{<xy>\subset B:|x-y|=\sqrt{2}} s_x s_y \\ + 240U^{-3} \sum_{<xy>\subset B:|x-y|=2} s_x s_y + 450U^{-3} \sum_{P\subset B} s(P) \end{aligned} \tag{2.7}$$

(The notation $< xy >\subset B$ means that both endpoints x and y of the bond are in B.) Then we have

$$5760 H_0(s) = \sum_B H_B$$

Note that H_B depends only on the spins in the three by three block B.

If there is a configuration for which the value of each individual H_B is equal to its minimum, then this configuration is obviously a ground state. It is usually not possible to find such a configuration. However, it may be possible to find another decomposition of the Hamiltonian so that this can be done. This was how [8] proved that certain configurations were the ground state of $H_0(s)$ for densities 1/3 and 1/5. The idea is the following. Suppose K_B is another Hamiltonian that depends only on the spins in block B and such that

$$\sum_B K_B = 0 \tag{2.8}$$

Then obviously adding K_B to H_B does not change the total Hamiltonian. Since we are always looking for the ground state with the nuclear density fixed, instead of requiring that the sum of the K_B be zero, it is enough that their sum be proportional to the total number of nuclei. The game now is to try and choose the K_B so that it is possible to find a configuration for which the value of $H_B + K_B$ is equal to its minimum for every three by three block B. H_B is invariant under rotations and reflections of the block B. K_B will also have this invariance. In figure 2 we show all possibile configurations for a three by three block up to rotations and reflections of the block.

Lemma 2.3 There are K_B^i for $i = 1, 2, \cdots, 7$, such that for each i, $\sum_B K_B^i$ is equal to a multiple of the total density plus a constant. For each three by three block B, the ground states of $H_B + K_B^i$ are as follows. (The numbering that follows refers to figure 2).
$i = 1$: 1,2,3,4,8,9
$i = 2$: 2,8
$i = 3$: 2,5,8,11

$i=4$: 2,5,11
$i=5$: 2,5,6,11,12,13
$i=6$: 12,13
$i=7$: 12,13,17,19,20
Let $I_1=[0,1/5]$, $I_2=\{1/5\}$, $I_3=[1/5,1/4]$, $I_4=\{1/4\}$, $I_5=[1/4,1/3]$, $I_6=\{1/3\}$, $I_7=[1/3,1/2]$. For $i=1,2,\cdots,7$, for every rational density in I_i it is possible to construct a configuration with that given density such that every three by three block in the configuration is one of those listed above. Moreover, if $\rho=p/q$ with p and q integers then we may choose this configuration so that it has period q in each of the two lattice directions.

The lemma for $i=2$ and 6 (densities 1/5 and 1/3) was proved in [8], although not in the above form. The proof of the lemma consists of defining the K_B^i and then doing a lot of computation to show that the ground states of H_B+K_B are as given. The details are in the appendix. For theorem 2.1 the relevant cases of the lemma are $i=5$ and 7. For theorem 2.2 the relevant cases are $i=2,4$ and 6. Cases $i=1$ and 3 are not needed for any of our results. They are included for the sake of completeness. For densities in these two intervals the first two orders in the perturbation theory put some constraints on the ground states, but not enough to yield a result like theorem 2.1.

Proof of theorem 2.1:

Recall that we are assuming that s is periodic. Let $e(U)$ be the energy per site for the configuration s. It has an expansion in powers of $1/U$.

$$e(U)=e_1U^{-1}+e_3U^{-3}+\cdots$$

Let $\bar{s}$ be the configuration given by the second half of the lemma. Let $\bar{e}(U)$ be its energy per site. It also has an expansion.

$$\bar{e}(U)=\bar{e}_1U^{-1}+\bar{e}_3U^{-3}+\cdots$$

Since s is a ground state for $U\geq U_0$, we must have $e(U)\leq\bar{e}(U)$ for $U\geq U_0$. This implies that $e_1\leq\bar{e}_1$ and $e_3\leq\bar{e}_3$. But this can only happen if the value of H_B+K_B on s is equal to its minimum for every three by three block B. If the density is in $[1/3,1/2]$ then the lemma with $i=7$ now implies that every three by three block in s must be one of 12,13,17,19 or 20, as labelled in figure 2. If the density is in $[1/4,1/3]$ then the lemma with $i=5$ implies that every three by three block in s must be one of 2,5,6,11,12 or 13, as labelled in figure 2. The theorem now follows from the following two lemmas. ∎

Lemma 2.4: Let s be a periodic configuration such that every three by three block is one of 12,13,17,19 or 20 in figure 2. Then s has period $(1,1)$ or period $(1,-1)$. Moreover, on every horizontal line and every vertical line, each pair of consecutive nuclei is separated by either one or two empty sites.

Proof:

Recall that when we say that every three by three block is one of 12,13,17,19 or 20 we mean that it is equal to one of these or can be mapped into one by lattice symmetries, i.e., 90 degree rotations and reflections. For this proof it is convenient to write out all the three by three configurations that are equivalent to one of 12,13,17,19 or 20. They are shown in figure 3. We use this figure throughout the proof.

Since the configuration is periodic, to prove that it has period $(1,1)$ it suffices to prove that whenever there is a nuclei at x then there is a nuclei at $x+(1,1)$. A similar statement holds for $(1,-1)$. We claim that if configuration D never appears then we have period $(1,1)$. Assume D never appears and let x be a site at which s has a nuclei. Consider the 3 by 3 block whose lower left corner is x. Since D does not occur, this block must be either A, G, I, K, or L. But all of these blocks have a nuclei in the center, and so there is a nuclei at $x+(1,1)$. Thus s has period $(1,1)$.

A similar argument shows that if C nevers occurs then we have period $(1,-1)$. Thus the proof of the lemma reduces to showing that C and D cannot both appear in the same configuration. Suppose the block centered at x is C. Consider the block at $x+(1,0)$. It shares 6 sites with the block at x, so the possibilities for the block at $x+(1,0)$ are constrained by the block at x being D. Examining the list of allowable blocks, we find that the only possibility for the block at $x+(1,0)$ is E. This in turn implies that the only possibility for the block at $x+(1,1)$ is C. Thus C at x implies C at $x+(1,1)$. By the periodicity this implies C at $x+(n,n)$ for all integers n. Similarly, if the block at y is D, then the block at $y+(-1,0)$ must be F, and this implies that the block at $y+(-1,1)$ must be D. So we have D at $y+(-m,m)$ for all integers m. We now have a contradiction since $x+(n,n)=y+(-m,m)$ for some n and m. Thus at most one of C and D occur. ∎

Lemma 2.5: Let s be a periodic configuration such that every three by three block is one of 2,5,6,11,12 or 13 in figure 2. Then s has period $(1,2)$,$(2,1)$,$(1,-2)$,or $(2,-1)$. Moreover, in the case of period $(1,2)$ or $(1,-2)$, on every vertical line each pair of consecutive nuclei is separated by either two or three empty sites, and in the case of period $(2,1)$ or $(2,-1)$, on every horizontal line each pair of consecutive nuclei is separated by either two or three empty sites.

The idea of the proof of this lemma is the same as the proof of the previous lemma, but the proof is now much longer and so is hidden in the appendix.

We now turn to the proof of theorem 2.2. If we did not have to worry about the higher order terms in the perturbation theory then the theorem would follow immediately from lemma 2.3. Unlike theorem 2.1, we now assume nothing about the ground state, so controlling the higher terms in the perturbation theory requires some work. The idea is the following. Suppose we take one of the purported ground states (figure 1) and change it a little. By lemma 2.3 this will cost us some energy of order U^{-3} from the first two orders in the perturbation series. The question is whether we might gain enough energy from the higher orders so that the total energy actually decreases. The higher order terms are smaller by factors of $1/U$, but the number of terms which change grows as we go to higher and higher orders since the range of terms in the Hamiltonian grows as the order grows. We must play off the number of factors of $1/U$ against the number of terms in the Hamiltonian that change. We will do this for a general Hamiltonians for Ising type spins and then show that the Hamiltonian we have in theorem 2.2 fulfills the hypotheses of the general theorem. The general theorem is valid in any number of dimensions.

Theorem 2.6: We consider a Hamiltonian of the form

$$H(s) = \sum_{n=0}^{\infty} \epsilon^n \sum_x H_{n,x}(s) \tag{2.9}$$

$H_{n,x}$ is equal to the translation of $H_{n,0}$ by x. We require the following four hypotheses.
H1: There are constants a and c such that the support of $H_{n,x}$ is contained in a ball of radius an about x and $||H_{n,x}||_\infty \leq c^n$.
H2: If we apply a lattice rotation or reflection to $H_{n,x}$, then the result is simply a translate of $H_{n,x}$.
H3: There is a nonnegative integer m, a finite set of sites Y, a Hamiltonian h_0 supported on Y, a periodic configuration s_{gs}, and a constant $\delta > 0$ such that the following two properties hold. The first property is that

$$\sum_{n=0}^{m} \epsilon^n \sum_x H_{n,x} = \sum_x h_x \tag{2.10}$$

(h_x is the translation of h_0 by x). Let $s^1_{gs}, s^2_{gs}, \cdots, s^l_{gs}$ be all the configurations which can be obtained from s_{gs} by lattice rotations, reflections and translations. (There are a finite number of them since s_{gs} is periodic.) Let e denote the ground state energy of h_0, i.e., $e = \min_s h_0(s)$. The second property is that $h_0(s) = e$ whenever the restriction of s to Y is equal to some s^i_{gs} and $h_0(s) \geq e + \delta\epsilon^m$ whenever it is not.
H4: Let X be a set of sites which is nearest neighbor connected. Define $V_X = \cup_{y \in X}(Y + y)$ where $Y + y$ denotes the translate of Y by y. Suppose that s is a configuration such that for each $y \in X$, there is an i such that s and s^i_{gs} agree on $Y + y$. Then there exits a single s^i_{gs} which is equal to s on all of V_X.
We consider periodic boxes with sides of length L where for each coordinate direction, L is a multiple of the period of s_{gs} in that direction. Given H1, H2, H3, and H4, there is an $\epsilon_0 > 0$ (which depends on the various constants and sets in the hypotheses) such that $0 < \epsilon < \epsilon_0$ implies that a configuration s is a ground state if and only if it is one of s^i_{gs}.

Remark:

Some comments on these hypotheses are in order. $H(s)$ may be infinite range, but H1 says that the the terms in the Hamiltonian are exponentially small in the diameter of their range. H2 says that $H(s)$ is invariant under lattice rotations and reflections, and it also says that the decomposition in H1 respects this invariance in a natural way. H3 says that for the lower order part of the Hamiltonian it is possible to find a decomposition of the Hamiltonian which is "unfrustated" in the sense that there is a configuration in which each term in the decomposition attains its minimum energy. H4 says that there is sufficient overlap between adjacent translates of Y so that in a connected region in which the configuration on each block agrees with some ground state, the configuration on the entire connected region must agree with a single ground state.

Proof:

Fix a configuration s. Define X by

$$X = \{x : h_x(s) > e\}$$

Obviously, if s is some s^i_{gs}, then $X = \emptyset$. Conversely, if $X = \emptyset$ then by H3 for each y, the restriction of s to $Y + y$ is equal to some s^i_{gs}. H4 then implies that s is equal to a single s^i_{gs} on all of the lattice. Thus our goal is to show that s is a ground state if and only if $X = \emptyset$. The definition of X and H3 imply

$$\sum_{n=0}^{m} \epsilon^n \sum_x [H_{n,x}(s) - H_{n,x}(s_{gs})] \geq \delta \epsilon^m |X| \tag{2.11}$$

where $|X|$ denotes the number of sites in X. We will complete the proof by showing that a similar bound holds when we include the higher order terms in the Hamiltonian.

At each order the Hamiltonian is invariant with respect to lattice rotations, reflections and translations, but this does not imply that $H_{n,x}(s^i_{gs}) = H_{n,x}(s^j_{gs})$ for $i \neq j$. By a slight reorganization of the Hamiltonian we can insure that this equality does hold. Since s_{gs} is periodic, we can choose a positive integer l such that translation of s_{gs} in any lattice direction by l leaves it unchanged. Let $P = \{x : 1 \leq x_i \leq l, i = 1, 2, \cdots, d\}$. Now define

$$\tilde{H}_{n,x} = l^{-d} \sum_{z \in P} H_{n,x+z} \tag{2.12}$$

Then it is easy to see that $\tilde{H}_{n,x}(s) = \tilde{H}_{n,x}(s_{gs})$ whenever s is equal to some s^i_{gs} on the support of $\tilde{H}_{n,x}$. Of course $\sum_x H_{n,x} = \sum_x \tilde{H}_{n,x}$.

Thanks to H1, if we choose r large enough depending on Y and l, then $dist(x, X) > r + an$ implies that

$$(Y + y) \cap supp(\tilde{H}_{n,x}) = \emptyset$$

for all $y \in X$. By H3 and H4 this implies that on the support of $\tilde{H}_{n,x}$, s is equal to some s^i_{gs}. Hence

$$\tilde{H}_{n,x}(s) = \tilde{H}_{n,x}(s_{gs})$$

The number of sites x with $dist(x, X) \leq r + an$ is bounded by $M(r + an)^d\,|X|$ for some constant M. Thus

$$|\sum_x [\tilde{H}_{n,x}(s) - \tilde{H}_{n,x}(s_{gs})]| \leq M(r + an)^d |X|\, 2\, ||\tilde{H}_{n,x}||_\infty \leq M(r + an)^d |X|\, 2\, c^n \tag{2.13}$$

Summing the above over orders $n > m$ and using (2.11) for orders $n \leq m$, we have

$$H(s) - H(s_{gs}) \geq |X| \delta \epsilon^m - |X| 2M \sum_{n=m+1}^{\infty} (r + an)^d \epsilon^n c^n \geq |X| \delta \epsilon^m / 2 \tag{2.14}$$

The last inequality follows by taking ϵ small enough that

$$2M \sum_{n=m+1}^{\infty} (r+an)^d \epsilon^n c^n \leq \delta \epsilon^m /2$$

Thus s is a ground state if and only if X is empty. ■

Proof of theorem 2.2:

We simply need to show that the hypotheses of theorem 2.6 are satisfied. H1 and H2 follow from the definition of $H_{n,x}$, eq. (2.5), and the bound (2.3). H3 follows from cases $i = 2, 4$ and 6 of lemma 2.3. The finite set of sites Y is a three by three block. H4 is verified in the same way that lemmas 2.4 and 2.5 were proved. Suppose that the configuration agrees with s^i_{gs} in the three by three block centered at x and with s^j_{gs} in the three by three block centered at y where x and y are nearest neighbors. Then these two three by three blocks share six sites. By checking cases it is straightforward although a little tedious to show that this can only happen if $i = j$. ■

3. The nonneutral case

When the density of nuclei and the density of electrons are both equal to 1/2, then the ground state configuration for the nuclei is the checkerboard configuration. In one dimension Lemberger [12] has proved that in the nonneutral model if U is large enough then the ground state configuration for the nuclei is obtained by putting them all together. How large U must be can depend on how nonneutral the model is. In this section we consider the following question. Let U be large but fixed. What happens as the nuclear and electron densities approach 1/2? We will show that the ground state approaches the checkerboard configuration. A similar result holds when the densities both approach one of 1/3,1/4 or 1/5. Thus if we take U large but fixed, there will be open regions in the density-density plane in which the nuclei are spread out in the ground state configuration rather than clumped together.

Theorem 3.1 Let ρ_0 be $1/2, 1/3, 1/4$ or $1/5$. Consider a square with periodic boundary conditions and sides of length L where L is a multiple of $1/\rho_0$. For a configuration s let $f(s)$ be the number of three by three blocks for which the configuration s is not equal to one of the blocks that may be found in a nuclear ground state for the neutral model with density ρ_0 (figure 1) divided by the total number of three by three blocks. (So $f(s)$ is a fraction between 0 and 1.) There are positive constants c and U_0 such that if $U \geq U_0$ and s_{gs} is a nuclear ground state for nuclear density ρ_n and electron density ρ_e then

$$f(s_{gs}) \leq c[|\rho_n - \rho_0| + |\rho_e - \rho_0|]U^p \tag{3.1}$$

where $p = 2$ for $\rho_0 = 1/2$ and $p = 4$ in the other three cases.

Remarks:

1. The density f is a measure of how close the configuration s is to a ground state configuration for the neutral model with density ρ_0. Recall from section two (see the proof of theorem 2.2) that if there is a connected region in which the configuration on every three by three block is equal to some ground state of the neutral ρ_0 model, then the configuration on the entire region is equal to a single ground state for the neutral density ρ_0 model. (For $\rho_0 = 1/2$ we could have defined f to be the density of nearest neighbor bonds $< xy >$ such that $s_x = s_y$. In a connected region with $s_x = -s_y$ it is easy to see that the configuration is one of the checkerboard configurations.) The theorem says that if the two densities are close to ρ_0 then f is close to zero, i.e., s is close to a neutral density ρ_0 ground state in a certain sense. Note that even if f is tiny, s can still contain a domain wall with respect to the ρ_0 configuration. For example s might agree with one checkerboard configuration in one half of the lattice and with the other checkerboard configuration in the other half. So f being small does not imply the strict long range order that is present in the neutral model.

2. For the case of $\rho_0 = 1/2$ the theorem is valid in any number of dimensions and in place of the hypotheses that U is large we need only require that $U > 0$. In this case the upper bound on f is

$$f(s_{gs}) \leq c\frac{(2d+U)^3}{U^2}[4U|\rho_n - \frac{1}{2}| + (2U+4d)|\rho_e - \frac{1}{2}|] \tag{3.2}$$

where d is the number of dimensions and c is a constant that depends only on the number of dimensions.

Proof:

We will let $E(s, \rho_e)$ denote the ground state energy for the nuclear configuration s with the electron density equal to ρ_e. Then $E(s, \rho_e) \geq E(s_{gs}, \rho_e)$ for any configuration s with nuclear density ρ_n.

Each eigenvalue of the single particle operator associated with s_{gs} has absolute value no bigger than $U + 2d$. Hence

$$E(s_{gs}, \rho_e) \geq E(s_{gs}, \rho_0) - (U+2d)|\rho_e - \rho_0|L^2 \tag{3.3}$$

Let s' be a nuclear configuration which is obtained from s_{gs} by changing s_{gs} at $|\rho_n - \rho_0|L^2$ sites in such a way that s' has nuclear density ρ_0. Then the change in the second quantized operator H when we replace s_{gs} by s' has norm at most $2U|\rho_n - \rho_0|L^2$, so we have

$$E(s_{gs}, \rho_0) \geq E(s', \rho_0) - 2U|\rho_n - \rho_0|L^2 \tag{3.4}$$

Let s_0 be the nuclear ground state for the neutral model with density ρ_0 (figure 1). Theorem 2.2 says that $E(s', \rho_0) \geq E(s_0, \rho_0)$, but the proof actually shows much more: There is a constant $\gamma > 0$ such that

$$E(s', \rho_0) \geq E(s_0, \rho_0) + \gamma f(s')L^2U^{-p+1} \tag{3.5}$$

By the construction of s', $f(s') \geq f(s_{gs}) - 9|\rho_n - \rho_0|$.

Let $\tilde{s}$ be a configuration which is obtained from s_0 by changing $|\rho_0 - \rho_n| L^2$ sites so that $\tilde{s}$ has density ρ_n. Then by the same arguments we used above,

$$\begin{aligned} E(s_0, \rho_0) &\geq E(\tilde{s}, \rho_0) - 2U \, |\rho_n - \rho_0| \, L^2 \\ &\geq E(\tilde{s}, \rho_e) - (U + 2d) \, |\rho_e - \rho_0| \, L^2 - 2U \, |\rho_n - \rho_0| \, L^2 \end{aligned} \tag{3.6}$$

But we must have $E(\tilde{s}, \rho_e) \geq E(s_{gs}, \rho_e)$. Combining all our inequalities we find

$$\gamma f(s_{gs}) U^{-p+1} \leq 9\gamma \, |\rho_n - \rho_0| \, U^{-p+1} + 4U \, |\rho_n - \rho_0| + 2(U + 2d) \, |\rho_e - \rho_0| \tag{3.7}$$

The inequality in the theorem follows.

To prove the statement in remark 2, we use a result from [11]. It follows from eq. (2.21) of [11] that there is a constant γ that depends only on the number of dimensions such that for $U > 0$

$$E(s', \rho_0) \geq E(s_0, \rho_0) + \gamma f(s') L^d \frac{U^2}{(2d + U)^3} \tag{3.8}$$

Inequality (3.2) follows. ∎

If we fix the nuclear density to be 1/2 and let the electron density approach 1/2, then the previous theorem says that the nuclear ground state converges to the checkerboard configuration in the sense that the fraction of the square in which the configuration is not checkerboard goes to zero. In fact it must go to zero at least linearly in the difference between the electron density and 1/2. The following theorem gives a bound in the other direction. It says that the fraction of the square in which the configuration is not the checkerboard configuration is at least linear in the difference between the electron density and 1/2.

Theorem 3.2: Consider a periodic box with sides of length L where L is even and the number of dimensions d is arbitrary. Fix the density of the nuclei equal to 1/2. Let s be a nuclear ground state for electron density ρ_e. Define $f(s)$ as in theorem 3.1, or simply define it to be the density of nearest neighbor bonds $< xy >$ such that $s_x = s_y$, i.e., the number of such bonds divided by the total number of bonds. (So $f(s) = 0$ if and only if s is a checkerboard configuration.) There are positive constants c, U_0 and $\epsilon > 0$ such that for $U \geq U_0$ and $|\rho_e - 1/2| < \epsilon$

$$f(s) \geq c|\rho_e - \frac{1}{2}| \tag{3.9}$$

for L sufficiently large (depending on U and ρ_e).

Remarks:
1. We have taken the nuclear density to be exactly 1/2 in the theorem. If the nuclear density ρ_n is not equal to 1/2 then obviously s cannot be one of the checkerboard configurations, and it is trivial to prove a bound of the form $f(s) \geq c|\rho_n - 1/2|$.

2. In two dimensions it may be possible to extend this theorem to densities 1/3,1/4 and 1/5 instead of just 1/2. The proof for the case of 1/2 is already rather long since it involves a fair amount of explicit computation for the checkerboard configuration.

Proof:

The idea of the proof of inequality (3.9) is the following. For the checkerboard configuration one may explicitly compute the energy for $\rho_e L^d$ electrons. One can then construct a "trial" nuclear configuration $\tilde{s}$ whose energy for $\rho_e L^d$ electrons is lower. If s were too close to the checkerboard configuration then its energy would be close to that of the checkerboard configuration and so would be greater than the energy of the trial nuclear configuration, contradicting the fact that s is a ground state. We consider first the case of $\rho_e < 1/2$.

The nuclear configuration $\tilde{s}$ is defined as follows. Let l be a positive integer which will be chosen later. For x with $1 \leq x_1 \leq L-2l$ we set $\tilde{s}_x = s^{cb}_x$. For $L-2l+1 \leq x_1 \leq L-l$ we set $\tilde{s}_x = -1$, and for $L-l+1 \leq x_1 \leq L$ we set $\tilde{s}_x = 1$. So the configuration consists of three regions: a checkerboard region of size $(L-2l) \times L^{d-1}$, a region with no nuclei of size $l \times L^{d-1}$ and a region fully occupied by nuclei of size $l \times L^{d-1}$. Let H be the second quantized Hamiltonian for $\tilde{s}$, i.e.,

$$H = \sum_{x,y:|x-y|=1} c^\dagger_x c_y - U \sum_x c^\dagger_x c_x \tilde{s}_x$$

Let H' be the Hamiltonian obtained from H by deleting the hopping terms which go between two of the three regions and adding the hopping terms needed to have periodic boundary conditions on each of these three regions individually. Explicitly,

$$H' = \sum_{|x-y|=1}{}^{'} c^\dagger_x c_y + \sum_z [c^\dagger_{(1,z)} c_{(L-2l,z)} + c^\dagger_{(L-2l+1,z)} c_{(L-l,z)} + c^\dagger_{(L-l+1,z)} c_{(L-1,z)} + h.c.] \quad (3.10)$$

$$-U \sum_x c^\dagger_x c_x \tilde{s}_x$$

where the $'$ on the first sum means that we only sum over x, y with x and y in the same region. Here z is summed over $\{1, 2, \ldots, L\}^{d-1}$. Since $||c^\dagger_x c_y + c^\dagger_y c_x|| \leq 1$, and we deleted $3L^{d-1}$ bonds while adding the same number,

$$||H - H'|| \leq 6L^{d-1}$$

The reason we approximated H by H' is that the eigenvalues of H' are more easily calculated. We will put $\frac{1}{2}(L-2l)L^{d-1}$ electrons in the checkerboard region (so it is neutral) and no electrons in the region with no nuclei. The total number of electrons is $\rho_e L^d$, so this leaves $(\rho_e L - \frac{1}{2}L + l)L^{d-1}$ for the region fully occupied by nuclei. Thus the density of electrons in the fully occupied region is $(\rho_e L - \frac{1}{2}L + l)/l$. We choose l to be the closest integer to $2(\frac{1}{2} - \rho)L$ so that this electron density is $\frac{1}{2} + O(\frac{1}{L})$. (We will use $O(\frac{1}{L})$ to denote a quantity that is $\leq c/L$ for some constant c that may depend on U and ρ.)

Let $\epsilon(k) = 2\sum_{i=1}^d cos(k_i)$. In the checkerboard region the electron energies are given by $\pm\sqrt{U^2 + \epsilon(k)^2}$. k should range over the Brillouin zone for the lattice with spacing

$\sqrt{2}$. Equivalently we can let it range over the Brillouin zone for the unit lattice and note that this simply counts each eigenvalue twice. The electron density is 1/2, so the ground state is obtained by filling all the negative energy levels. The sum over k when suitably normalized is a Riemann sum approximation to an integral. The difference between the integral and the Riemann sum is $O(\frac{1}{L})$. This error is multiplied by $(L-2l)L^{d-1}$, and so the energy from the checkerboard region is

$$-\frac{1}{2}(L-2l)L^{d-1}e_{cb}+O(L^{d-1})$$

where

$$e_{cb}=\frac{1}{(2\pi)^d}\int_{[0,2\pi]^d}\sqrt{U^2+\epsilon(k)^2}d^dk \tag{3.11}$$

The electron energies in the region fully occupied by nuclei are $-U+\epsilon(k)$. $\epsilon(k)$ ranges from $-2d$ to $2d$. The density of electrons here is $\frac{1}{2}$, so we fill up these levels until $-U+\epsilon(k)=-U$. Thus the energy in this region can be bounded above by $(-U-\gamma)\frac{1}{2}lL^{d-1}+O(L^{d-1})$ where γ is a constant that depends only on the number of dimensions. So the ground state energy for H' with $\rho_e L^d$ electrons is no bigger than

$$-\frac{1}{2}(L-2l)L^{d-1}e_{cb}-(U+\gamma)\frac{1}{2}lL^{d-1}+O(L^{d-1})$$

Since H and H' differ in norm by $O(L^{d-1})$, the above is also an upper bound for the ground state energy of H. Thus we have constructed an $\tilde{s}$ with nuclear density 1/2 for which the ground state energy for $\rho_e L^d$ electrons, which we denote by $\tilde{E}$, satisfies

$$\tilde{E}\le-\frac{1}{2}(L-2l)L^{d-1}e_{cb}-(U+\gamma)\frac{1}{2}lL^{d-1}+O(L^{d-1}) \tag{3.12}$$

Now let s be a ground state nuclear configuration. We want to bound the difference between the ground state energies for s and s^{cb} in terms of fL^d. Let H and H_{cb} denote the second quantized Hamiltonian for s and s^{cb}. We will show that by deleting some of the hopping terms from H and H_{cb} we can obtain two Hamiltonians which are unitarily equivalent. The number of bonds we need to delete will be proportional to fL^d.

Recall that s^{cb} denotes one of the two checkerboard configurations. (Although the following construction depends on which one we choose, either one will do.) Decompose the lattice into the two sets

$$P=\{x:s_x=s_x^{cb}\}$$

$$M=\{x:s_x=-s_x^{cb}\}$$

The unitary operator we will use will come from simply permuting the lattice sites. We would like to leave the sites in P fixed and shift those in M by one lattice unit. We take the shift to be in the 1-direction, i.e., $x\to x+\hat{e}_1$ where $\hat{e}_1$ is a unit vector in the 1-direction. Some of the sites in M will be shifted out of M, and some sites not in M will be shifted into M. So we make the following definitions.

$$M_l=\{x\in M:x+\hat{e}_1\in M\}$$

$$M_r = \{x \in M : x - \hat{e}_1 \in M\}$$

Thus M_l consists of the sites in M whose shift is still in M, while M_r consists of the sites in M whose preimage under the shift is in M. Define

$$\phi : P \cup M_l \to P \cup M_r$$

by

$$\phi(x) = \begin{cases} x & \text{if } x \in P \\ x + \hat{e}_1 & \text{if } x \in M_l \end{cases}$$

So ϕ is one to one and onto.

Clearly $s_x = s^{cb}_{\phi(x)}$ for $x \in P \cup M_l$. In particular, the number of sites in $P \cup M_l$ with $s_x = 1$ is equal to the number of sites in $P \cup M_r$ with $s^{cb}_x = 1$. Since each of s and s^{cb} have $\frac{1}{2}L^d$ sites in the entire lattice where they equal $+1$, the number of sites not in $P \cup M_l$ with $s_x = 1$ must equal the number of sites not in $P \cup M_r$ with $s^{cb}_x = 1$. Thus we may extend the definition of ϕ from $P \cup M_l$ to the entire lattice in such a way that $s_x = s^{cb}_\phi(x)$ for all x.

We let H' be the Hamiltonian obtained from H by deleting the hopping term $c^\dagger_x c_y$ for the following two classes of bonds : (1) bonds $< xy >$ with $s_x = s_y$, (2) bonds $< xy >$ with at least one of x or y not in $P \cup M_l$. The number of bonds in (1) is fL^d. If a site x is not in $P \cup M_l$ then $s_x = s_{x+\hat{e}_1}$ So there are at most fL^d such sites. Thus the number of bonds in (2) is at most $2dfL^d$. Hence

$$||H - H'|| \leq (2d+1)fL^d \tag{3.13}$$

We let H'_{cb} denote the Hamiltonian obtained from H_{cb} by deleting the hopping terms for bonds in the following two classes of bonds : (1) as above, $(2')$ bonds $< xy >$ with at least one of x or y not in $P \cup M_r$. As above

$$||H_{cb} - H'_{cb}|| \leq (2d+1)fL^d \tag{3.14}$$

Note that H' does not contain any hopping terms that involve sites not in $P \cup M_l$ and H'_{cb} does not contain any hopping terms that involve sites not in $P \cup M_r$. Thus H' and H'_{cb} are unitarily equivalent under the unitary corresponding to the permutation ϕ.

The energy levels for H_{cb} are $\pm\sqrt{U^2 + \epsilon(k)^2}$. Since $\rho_e < 1/2$ we fill only some of the negative levels. The sum of the lowest $\frac{1}{2}L^d$ levels is

$$-\frac{1}{2}L^d e_{cb} + O(L^{d-1})$$

We must subtract $(1/2 - \rho_e)L^d$ levels from this sum. Since $\sqrt{U^2 + \epsilon(k)^2} \geq U$, the levels we must subtract are bounded above by $-U$. Thus the energy for H_{cb} with $\rho_e L^d$ electrons is at least

$$-\frac{1}{2}L^d e_{cb} + (\frac{1}{2} - \rho_e)L^d U + O(L^{d-1})$$

This fact and (3.13) and (3.14) imply that the ground state energy E of H with $\rho_e L^d$ electrons satisfies

$$E \geq -\frac{1}{2}L^d e_{cb} + (\frac{1}{2} - \rho_e)L^d U - 2(2d+1)fL^d + O(L^{d-1})$$

If s is a ground state nuclear configuration, then we must have $E \leq \tilde{E}$, so by (3.12)

$$-\frac{1}{2}(L-2l)L^{d-1}e_{cb} - (U+\gamma)\frac{1}{2}lL^{d-1} + O(L^{d-1}) \geq -\tfrac{1}{2}L^d e_{cb} + (\tfrac{1}{2} - \rho_e)L^d U - 2(2d+1)fL^d$$

Recall that l was chosen so that $l/L = 2(1/2 - \rho_e) + O(\frac{1}{L})$. Dividing the above by L^d we obtain

$$2(2d+1)f \geq (\frac{1}{2} - \rho_e)[\gamma + 2U - 2e_{cb}] + O(\frac{1}{L}) \tag{3.15}$$

As $U \to \infty$, $e_{cb} - U \to 0$. Thus the above implies (3.9).

The proof for $\rho_e > 1/2$ is similar; we briefly discuss the differences. We use the same configuration for $\tilde{s}$. For this configuration we take the electron density to be 1/2 in the checkerboard region, 1 in the region fully occupied by nuclei and 1/2 in the region with no nuclei. l is taken to be the integer nearest to $2(\rho_e - \frac{1}{2})L$. The energy in the checkerboard region is as before. In the fully occupied region it is $-lL^d U$. In the region with no nuclei it is $\leq \frac{1}{2}lL^{d-1}(U-\gamma)$ Thus eq. (3.12) is replaced by

$$\tilde{E} \leq -\frac{1}{2}(L-2l)L^{d-1}e_{cb} - lL^{d-1}U + \frac{1}{2}lL^{d-1}(U-\gamma) + O(L^{d-1}) \tag{3.16}$$

The second difference comes when we consider the ground state energy E_{cb} of H_{cb} with $\rho_e L^d$ electrons. The positive eigenvalues of H_{cb} are $\geq U$, so

$$E_{cb} \geq -\frac{1}{2}L^d e_{cb} + (\rho_e - \frac{1}{2})L^d U + O(L^{d-1})$$

Proceeding as before we obtain

$$2(2d+1)f \geq (\rho_e - \frac{1}{2})[\gamma + 2e_{cb} - 2U] + O(\frac{1}{L})$$

Inequality (3.9) follows. ∎

Appendix

In this appendix we prove two lemmas used in section 2.

Proof of Lemma 2.3:

Each K_B^i will be a linear combination of the following functions. We give their definition when B is the three by three block centered at $(1,1)$. For other blocks B we simply translate appropriately. Let

$$\begin{aligned}
k_B^1 &= s_{(0,1)} + s_{(1,0)} + s_{(1,2)} + s_{(2,1)} - 4s_{(1,1)} \\
k_B^2 &= s_{(0,0)} + s_{(2,0)} + s_{(0,2)} + s_{(2,2)} - 4s_{(1,1)} \\
k_B^3 &= -s_{(0,0)}s_{(2,0)} + 2s_{(0,1)}s_{(2,1)} - s_{(0,2)}s_{(2,2)} - s_{(0,0)}s_{(0,2)} + 2s_{(1,0)}s_{(1,2)} - s_{(2,0)}s_{(2,2)} \\
k_B^4 &= -s_{(0,0)}s_{(1,0)} - s_{(1,0)}s_{(2,0)} + 2s_{(0,1)}s_{(1,1)} + 2s_{(1,1)}s_{(2,1)} - s_{(0,2)}s_{(1,2)} - s_{(1,2)}s_{(2,2)} \\
&\quad - s_{(0,0)}s_{(0,1)} - s_{(0,1)}s_{(0,2)} + 2s_{(1,0)}s_{(1,1)} + 2s_{(1,1)}s_{(1,2)} - s_{(2,0)}s_{(2,1)} - s_{(2,1)}s_{(2,2)} \\
k_B^5 &= -s_{(1,0)}s_{(2,1)} - s_{(1,0)}s_{(0,1)} - s_{(2,1)}s_{(1,2)} - s_{(0,1)}s_{(1,2)} \\
&\quad + s_{(0,0)}s_{(1,1)} + s_{(1,1)}s_{(2,2)} + s_{(2,0)}s_{(1,1)} + s_{(1,1)}s_{(0,2)} \\
k_B^6 &= -\delta(-s_{(0,0)})\,\delta(s_{(1,0)})\,\delta(-s_{(2,0)}) + 2\delta(-s_{(0,1)})\,\delta(s_{(1,1)})\,\delta(-s_{(2,1)}) \\
&\quad - \delta(-s_{(0,2)})\,\delta(s_{(1,2)})\,\delta(-s_{(2,2)}) - \delta(-s_{(0,0)})\,\delta(s_{(0,1)})\,\delta(-s_{(0,2)}) \\
&\quad + 2\delta(-s_{(1,0)})\,\delta(s_{(1,1)})\,\delta(-s_{(1,2)}) - \delta(-s_{(2,0)})\,\delta(s_{(2,1)})\,\delta(-s_{(2,2)}) \\
k_B^7 &= s_{(0,0)} + s_{(0,1)} + s_{(0,2)} + s_{(1,0)} + s_{(1,1)} + s_{(1,2)} + s_{(2,0)} + s_{(2,1)} + s_{(2,2)}
\end{aligned}$$

Here $\delta(s_x)$ is 1 if $s_x = 1$ and 0 if $s_x = -1$. Clearly $\sum_B k_B^i$ vanishes for $i = 1, 2, \cdots, 6$, while this sum equals a multiple of the total number of nuclei plus a constant when $i = 7$.

The coefficients in the linear combinations are given by table 1. It is now just a matter of computation to find the energy of $H_B + K_B^i$ for each of the configurations in figure 2 and each choice of i and check that the conclusions in the lemma hold. This proves the first half of the lemma.

The construction of a configuration with the desired properties is as follows. For $i = 2, 4$ and 6 the configurations are given by figure 1. Now consider the case of $i = 5$. So the density is between 1/4 and 1/3. Choose an arrangement of nuclei along a horizontal line so that the density of nuclei on the line is equal to the desired density and so that consecutive nuclei are separated by two or three empty sites. Now extend this configuration so that it has period $(2, 1)$. It is straightforward although somewhat tedious to check that all three by three blocks in the resulting configuration are among those given in case $i = 5$ of the lemma. The construction for $i = 7$ is similar except that one arranges the nuclei on the line so that adjacent nuclei are separated by one or two empty sites and one extends using period $(1, 1)$. ∎

Proof of lemma 2.5:

Recall that in figure 2 we only show one configuration from each symmetry class. In figure 4 we show all the configurations on a three by three block that are equivalent to configurations 2,5,6,11,12, or 13 in figure 2. So the hypothesis of lemma 2.5 is that only the configurations in figure 4 can occur.

We begin by defining 8 statements that could hold for the configuration. The labelling of these statements is for later convenience. We will abbreviate statements like “the three by three block centered at x is H” to simply “H at x”.

1a: H at x_0, M at $x_0 + (0, 1)$

2a: H at x_0, L at $x_0 + (0, -1)$

1b: J at x_0, O at $x_0 + (0, -1)$
2b: J at x_0, N at $x_0 + (0, 1)$
3a: I at x_0, N at $x_0 + (1, 0)$
4a: I at x_0, M at $x_0 + (-1, 0)$
4b: K at x_0, O at $x_0 + (1, 0)$
3b: K at x_0, L at $x_0 + (-1, 0)$
Then the following implications hold.
1a $\Rightarrow$ H at $x_0 + (-2n, n)$, M at $x_0 + (-2n, n+1)$, G at $x_0 + (-2n-1, n+1)$ $\forall$ integers n.
2a $\Rightarrow$ H at $x_0 + (-2n, -n)$, L at $x_0 + (-2n, -n-1)$, D at $x_0 + (-2n-1, -n-1)$ $\forall$ integers n.
1b $\Rightarrow$ J at $x_0 + (2n, -n)$, O at $x_0 + (2n, -n-1)$, E at $x_0 + (2n+1, -n-1)$ $\forall$ integers n.
2b $\Rightarrow$ J at $x_0 + (2n, n)$, N at $x_0 + (2n, n+1)$, F at $x_0 + (2n+1, n+1)$ $\forall$ integers n.
3a $\Rightarrow$ I at $x_0 + (n, 2n)$, N at $x_0 + (n+1, 2n)$, D at $x_0 + (n+1, 2n+1)$ $\forall$ integers n.
4a $\Rightarrow$ I at $x_0 + (-n, 2n)$, M at $x_0 + (-n-1, 2n)$, E at $x_0 + (-n-1, 2n+1)$ $\forall$ integers n.
4b $\Rightarrow$ K at $x_0 + (n, -2n)$, O at $x_0 + (n+1, -2n)$, G at $x_0 + (n+1, -2n-1)$ $\forall$ integers n.
3b $\Rightarrow$ K at $x_0 + (-n, -2n)$, L at $x_0 + (-n-1, -2n)$, F at $x_0 + (-n-1, -2n-1)$ $\forall$ integers n.

The proofs of all eight cases are similar, so we only consider 1a. The given blocks yield the following sequence of implications.

$$\begin{pmatrix} & & \\ & & M \\ & & H \end{pmatrix} \Rightarrow \begin{pmatrix} & & \\ & & M \\ & P & H \end{pmatrix} \Rightarrow \begin{pmatrix} & & \\ & G & M \\ J & P & H \end{pmatrix} \Rightarrow \begin{pmatrix} & O & \\ H & G & M \\ J & P & H \end{pmatrix} \Rightarrow \begin{pmatrix} M & O & \\ H & G & M \\ J & P & H \end{pmatrix}$$

The blocks involved in the above may overlap. For example, the first "matrix" says that there is H at x_0 and M at $x_0 + (0, 1)$. This is just the statement 1a. The first implication comes about as follows. Given that there is an H at x_0, when we look at the configurations in figure 4we see that the only possibility for $x_0 + (-1, 0)$ is P. The subsequent implications are proved in the same fashion.

The above sequence of implications shows that H at x_0 implies H at $x_0 + (-2, 1)$, M at $x_0 + (-2, 2)$, and G at $x_0 + (-1, 1)$ Keeping in mind the periodicity of the pattern, the desired implication now follows by induction.

We will use 1 as shorthand for the statement "1a or 1b holds for some site x_0"; 2,3,4 are defined similarly. In both 1a and 1b the pattern propagates along a line in the (-2,1) direction. In 2,3,4 it propagates along lines in the (2,1),(1,2),(1,-2) directions respectively. If two of 1,2,3,4 happen, then the resulting patterns must intersect and one can show that is a site where the block must be two different patterns. This contradiction shows at most one of 1,2,3,4 occur.

Since at most one of 1,2,3,4 can occur, we have four cases. We consider the case where none of 1,2,3 occur. The other cases are similar. Note that none of 1,2,3 occurring means that for every site x_0 none of 1a,1b,2a,2b,3a,3b occur.

If the block at x is H, then the block at $x + (0, 1)$ must be either J or M and the block at $x + (0, -1)$ must be either J or L. Since neither of 1a or 2a occur, whenever there is an H at x then there must be J's at $x + (0, 1)$ and $x + (0, -1)$. Similarly, since neither 1b nor 2b occur, whenever there is a J at x then there are H's at $x + (0, 1)$ and $x + (0, -1)$.

Thus if the configuration contains at least one J or one H then it contains a vertical line which alternates between J and H. One can then show that this vertical line determines the entire configuration. It is

$$\begin{pmatrix} J & P & H & A \\ H & A & J & P \\ J & P & H & A \\ H & A & J & P \end{pmatrix}$$

repeated periodically. This pattern satisfies the conclusions of the lemma. The remaining possibility is that neither of J nor H appear in the configuration.

If neither of J nor H appear, then P cannot appear since P at x always implies H at $x + (1, 0)$. Suppose D appears somewhere in the configuration. Then keeping in mind that J,H and P are forbidden, we have

$$\begin{pmatrix} & \\ D & \end{pmatrix} \Rightarrow \begin{pmatrix} I & \\ D & L \end{pmatrix} \Rightarrow \begin{pmatrix} I & N \\ D & L \end{pmatrix}$$

But this means that 3a occurs, but that is not allowed. Thus there are no D's in the configuration.

Now suppose B appears at x. Remembering that D is forbidden, we have

$$\begin{pmatrix} & \\ & B \end{pmatrix} \Rightarrow \begin{pmatrix} & L \\ N & B \end{pmatrix} \Rightarrow \begin{pmatrix} B & L \\ N & B \end{pmatrix}$$

By induction and the periodicty of the configuration, there is a B at $x + (-n, n)$, an L at $x + (-n, n + 1)$ and an N at $x + (-n - 1, n)$ for all integers n. It is easy to show that this determines the entire configuration. It is

$$\begin{pmatrix} B & L & N \\ N & B & L \\ L & N & B \end{pmatrix}$$

This configuration satisfies the conclusions of the lemma.

The remaining possibility is that B never appears. Recall that D and J are already forbidden. Suppose there is a nuclei at x. Consider the 3 by 3 block with x in the lower right corner. Since B,D and J are excluded, the only possibilities for this block are K and M. They both have a nuclei at $x + (-1, 2)$. Thus if there is a nuclei at x then there is a nuclei at $x + (-1, 2)$. The configuration is periodic, so this proves that it has period $(-1, 2)$. ∎

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Tables

	k_B^1	k_B^2	k_B^3	k_B^4	k_B^5	k_B^6	k_B^7
K_B^1	0	0	0	-45	-50	0	160
K_B^2	0	0	0	51	-120	0	-450
K_B^3	0	0	0	75	-130	0	-640
K_B^4	0	0	0	135	-150	0	-960
K_B^5	0	0	90	315	-210	0	-1920
K_B^6	0	720	120	0	0	240	-2700
K_B^7	-420	0	-90	450	0	0	-3360

Table 1: The functions K_B^i used in the proof of lemma 2.3. Each K_B^i is a linear combination of the k_B^j. For example, $K_B^1 = -45k_B^4 - 50k_B^5 + 160k_B^7$.

Figure Captions

Figure 1. The ground state configuration for the neutral model for densities (a) 1/3, (b) 1/4, and (c) 1/5. These ground states were derived nonrigorously in [8].

Figure 2. All possible configurations for the nuclei in a three by three block are shown (up to rotations and reflections of the block). Lemma 2.3 says which configurations can appear in the ground state for various ranges of densities.

Figure 3. The configurations used in the proof of lemma 2.4.

Figure 4. The configurations used in the proof of lemma 2.5.