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Ground State Properties of the Neutral Two-Dimensional Falicov-Kimball Model

by

Karl Paul Haller

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As members of the Final Examination Committee, we certify that we have read the dissertation prepared by Karl Paul HALLER

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and recommend that it be accepted as fulfilling the dissertation requirement for the Degree of Doctor of Philosophy

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	Date
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Final approval and acceptance of this dissertation is contingent upon the candidate's submission of the final copy of the dissertation to the Graduate College.

I hereby certify that I have read this dissertation prepared under my direction and recommend that it be accepted as fulfilling the dissertation requirement.

Dissertation Director Thomas G. Kennedy — July 9, 1998 Date

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SIGNED: Karl P. Hollis

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Dedication

This work is dedicated to my family. Their continuing support and encouragement have always been the main ingredients in the realization of my goals.

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Chapter 1
INTRODUCTION

1.1 The Falicov-Kimball Model

Experimentally it is found that matter orders itself at low temperature. This can be seen in the way matter forms a crystalline structure and in the long range order exhibited by magnetic systems. Many models have been used to study these phenomena, one of the simplest being the Ising model. This is a classical spin model whose Hamiltonian H is given by

$$H(S) = -\sum_{<x,y>} S_x S_y \tag{1.1}$$

where the sum is taken over all nearest neighbor pairs $< x, y >$ of lattice sites and $S_x = \pm 1$. The ground states are easily seen to be the configurations in which S_x is 1 for every x or S_x is -1 for every x. For dimensions ≥ 2 this long range order persists at low temperatures. However, the mechanism driving this is somewhat artificial in that the Ising Hamiltonian is designed to give preference, at least locally, to ordered states. To understand the physics of this ordering, the quantum mechanical properties of matter must be taken into account.

The Falicov-Kimball model is a quantum model involving two types of particles on a lattice. One type is allowed to hop between nearest neighbor sites, the other one does not and may be considered classical. At most one classical particle is allowed at each site and there is an on-site interaction between the hopping and classical particles. There are no terms explicitly favoring any kind of order incorporated into the Hamiltonian. The model is simple enough to obtain rigorous results, yet contains enough physics to produce long range order in the ground state configurations of the classical particles (and in the low temperature states as well [4, 5]). The order

comes about from the subtle interplay between the exclusion principle and the on-site interaction.

Since it was first proposed almost thirty years ago, the Falicov-Kimball model has been given many interpretations, and the motivations for studying it have become quite diverse. The original intent of Falicov and Kimball was to study metal-insulator transitions in transition-metal oxides [1]. In this case the hopping particles correspond to itinerant d-electrons while the classical particles represent localized f-electrons. The model may also serve as a simplified version of the Hubbard model [2]. In the Hubbard model both spin up and spin down electrons are allowed to hop, and the only interaction between the electrons is on-site. Thus the Falicov-Kimball model can be regarded as the Hubbard model in the special case where the spin up electrons are infinitely massive.

Another interpretation was introduced by Gruber and Macris [3]. They noted that the Falicov-Kimbal model may be viewed as one of a general class of models in which the electrons interact with a classical field. One obtains the Falicov-Kimbal model when this field takes on the values ± 1. In 1986 Kennedy and Lieb [4], and independently Brandt and Schmidt [5] proved that the model exhibited a phase transition at sufficiently low temperature. In [4] the classical particles are interpreted as ions and the hopping particles correspond to spinless electrons. With this interpretation, Falicov-Kimball can be viewed as a primitive model of matter, with which one can study the formation of atoms, molecules, and crystals. This is the point of view we take in this paper.

The Falicov-Kimball model is deceptively simple to write down. A variable v_x is assigned to each site x of a lattice Λ. It takes on the value 1 if x is occupied by an ion and 0 if x is unoccupied. The Hamiltonian for a single electron is the $|\Lambda| \times |\Lambda|$ matrix $T - 2UV$, where the 2 has been included for future convenience. The hopping term T is the lattice Laplacian with matrix elements T_{xy} where $T_{xy} = 1$ if $|x - y| = 1$, and $T_{xy} = 0$ otherwise. The matrix V is diagonal with entries v_x and U is a scalar

parameter. Since there is no interaction between the electrons, the Hamiltonian, H, is just the second quantized form of $T - 2UV$, given by

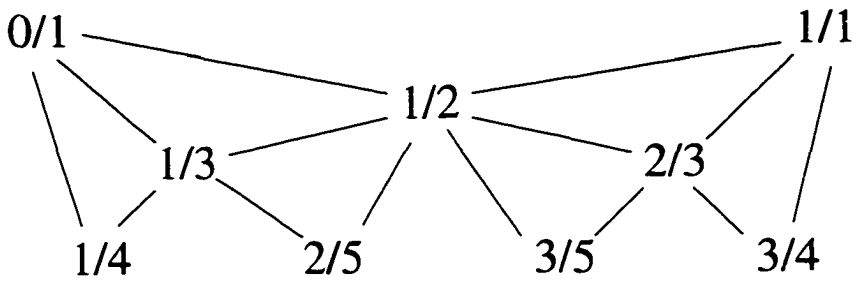
$$H = \sum_{<x,y>} c_x^\dagger c_y - 2U \sum_x c_x^\dagger c_x v_x \tag{1.2}$$

where $c_x^\dagger$ and c_y are the creation and annihilation operators of an electron at sites x and y, and $< x, y >$ represents a nearest neighbor pair of lattice sites. A "ground state" ion configuration is one that minimizes the lowest eigenvalue of H, or equivalently, the sum of the N_e lowest eigenvalues of $T - 2UV$ where N_e is the number of electrons. A particle-hole symmetry for each type of particle shows the equivalence of the ground states for models with parameters (U, N_i, N_e), $(-U, |\Lambda| - N_i, N_e)$, $(-U, N_i, |\Lambda| - N_e)$, and $(-U, |\Lambda| - N_i, |\Lambda| - N_e)$ where N_i is the number of ions. So in particular for the neutral case in which $N_i = N_e$, we may restrict ourselves to the case where $N_i \leq \Lambda/2$.

1.2 Previous Results

We denote the ion density by ρ_i and the electron density by ρ_e. The "neutral" case is defined by $\rho_i = \rho_e$, where the common density will be denoted simply by ρ. The ground states of the one dimensional neutral model for large U have been determined for all ρ by Lemberger [6]. Specifically he found that for all rational densities $\rho \in [0, 1]$ where $\rho = p/q$ with p and q relatively prime, there is a $U(q)$ such that if $U \geq U(q)$, the ground state is periodic with period q. These ground states are the "most homogeneous" in the sense that the ions are as spread out as possible over all length scales. The structure of these ground states follows the branching structure of the Farey tree [7], a portion of which is shown in figure 1.1. This tree is constructed using the rule that every pair of neighboring fractions p_1/q_1 and p_2/q_2, generates the fraction $(p_1 + p_2)/(q_1 + q_2)$. As the tree extends downward, every rational number between 0 and 1 is generated.

In an ion configuration, let us denote an unoccupied site by a "0" and an occupied



Farey Tree

FIGURE 1.1. The first few generations of the Farey tree. Each pair of neighboring fractions (those connected by a line segment) generates a new fraction.

site by a "1". Then the unit cell for the $\rho = 1/2$ ground state is given by (01). This cell is extended periodically on the lattice to give the ground state. From figure 1.1 we see that the cell (01) is simply the concatenation of the cells (0) and (1). These are the unit cells of the $\rho = 0$ and $\rho = 1$ ground states, where 0/1 and 1/1 are the "generators" of 1/2 in the Farey tree. Similarly we obtain the unit cell for the $\rho = 1/3$ ground state by concatenating the cells from the generators of 1/3, namely 0/1 and 1/2. The result is (001). The ground state for every density can be obtained in this manner.

It was conjectured that these ground states persist for all U. However in [8] Freericks, Gruber, and Macris proved that if $\rho_i < 1/4$ or $\rho_i > 3/4$ then for any value of ρ_e and for small enough $|U|$ the ground state is a mixture of the $\rho = 0$ (or $\rho = 1$) configuration with a configuration of period q, where q is such that $\rho_e = p/q$ with p and q relatively prime. Furthermore, it was shown that there exists a $\rho_c \approx 0.3710$ such that when $\rho_i = n/q \in [\rho_c, 1 - \rho_c]$, the ground state is the most homogeneous as described above. For all other ion densities in this interval the ground state is a mixture.

In [4] Kennedy and Lieb (see also [5]) showed that in the two-dimensional neutral

model with $\rho = 1/2$ and any $U \neq 0$. the ground state is the checkerboard configuration. They also showed that the model undergoes a phase transition and the long range order of the checkerboard configuration is preserved at low temperatures. In [9] Lebowitz and Macris extended this result to a region in the plane of the chemical potentials of the two types of particles.

By deriving a perturbation expansion in U^{-1} for the single electron Hamiltonian in the two-dimension neutral case, Gruber. Jedrzejewski, and Lemberger found the ground states for densities 1/3, 1/4 and 1/5 through fourth order [10]. In [11] Kennedy showed that these are indeed the ground states. These configurations are shown in figure 1.2.

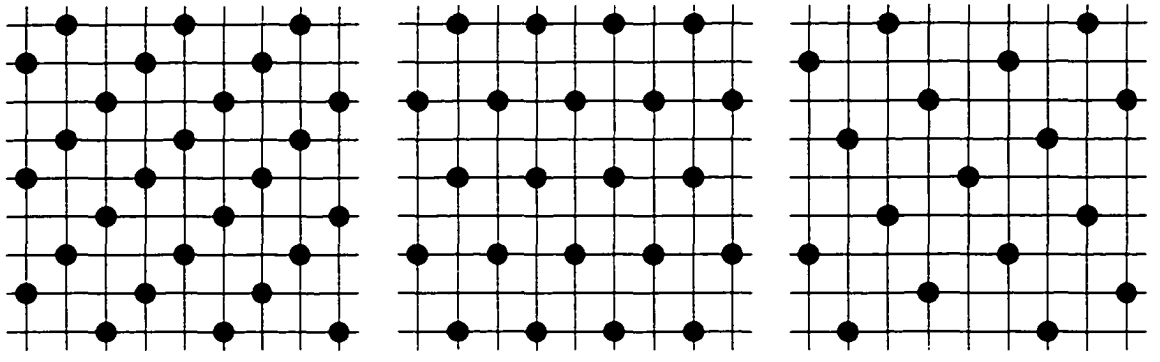


FIGURE 1.2. Ground states for densities 1/3, 1/4, and 1/5.

In [12] Kennedy showed that for rational densities in $(1/5, 2/9)$ and $(2/9, 1/4)$ there is phase separation in the neutral large U ground states. The 2/9 ground state was determined and shown to be periodic. In the interval $(1/5, 2/9)$ the phases consist of regions of either the 1/5 or 2/9 ground state. In $(2/9, 1/4)$ the result is similar with 1/5 replaced by 1/4. Unlike Lemberger's result for the neutral large U one-dimensional model, the phase separation has been shown to exist for all $U \geq U_0$ where U_0 is independent of the density. These results are very similar to our results in chapter 4, where the methods of both Kennedy [12] and Watson [13] have been

used extensively.

In [13] Watson studied a much simpler model which yielded remarkably similar results to the Falicov-Kimball model. The Hamiltonian he uses, which he calls the "greedy potential", is actually a rule for determining which of two given ion configurations costs less energy. The number of nearest neighbor pairs of ions is compared. The one with the fewest is declared to be less energetic. In the event of a tie, the number of pairs of ions separated by $\sqrt{2}$ is compared, and the one with the fewest is declared less energetic. If this results in a tie, we move on to ions separated by $\sqrt{5}$, then $\sqrt{8}$, and so on. Each tie moves the comparison to the next possible ℓ_2 distance. For the following densities it was found that the ground states of the greedy potential agreed with the known ground states of the large U neutral Falicov-Kimball model: 1/2, 1/3, 1/4, 1/5. Using our results this list may be extended to include all rational densities in $[1/3, 2/5]$ as well as 2/11. Furthermore, for "most" rational densities in $[1/5, 1/4]$ the greedy ground states are aperiodic. This is similar to Kennedy's result that the Falicov-Kimball ground states are aperiodic for all rational densities in $(1/5, 2/9)$ and $(2/9, 1/4)$ [12]. However, for rational densities in $(1/6, 2/11)$ the greedy ground states are periodic. We show that the corresponding Falicov-Kimball ground states phase-separate and are aperiodic.

So we see that for a range of densities, the greedy potential does a good job in capturing the effective ionic repulsion in the large U neutral Falicov-Kimball model. However, as is seen in the expansions in chapter 2, this effective repulsion depends heavily on the ℓ_1 metric rather than the ℓ_2 distances used by Watson.

In the non-neutral two-dimensional model Kennedy [11] showed that if U is large but fixed, then for $\rho \in \{1/2, 1/3, 1/4, 1/5\}$, there is an open region in the ρ_e, ρ_i plane, containing the point (ρ, ρ), such that the ground states for the densities in this region are "close" to the neutral ground state with density ρ. As U grows, we must shrink these regions to ensure closeness to the neutral ground state. In the one-dimensional model Lemberger [6] showed that for any fixed pair (ρ_e, ρ_i) with $\rho_e \neq \rho_i$ there exists

a $U_c(\rho_e/\rho_i)$ such that if $U \geq U_c(\rho_e/\rho_i)$ the ions in the ground state clump together forming a "segregated" configuration.

For analyses of the Falicov-Kimball model using the grand canonical formalism we refer the reader to [10, 14, 15, 16, 17, 18]. In [19], Datta, Messager, and Nachtergaele study the stability of interfaces in the three-dimensional model. We also mention a low temperature cluster expansion developed by Messager and Miracle-Sole [20] which they used to study the ground states and low temperature states in the plane of chemical potentials. An overview of the model and results may be found in [3].

1.3 Present Results

In this paper we focus on the two-dimensional Falicov-Kimball model in the neutral case with $U \gg 0$. We determine the ground state ion configurations for all rational densities in $[1/3, 2/5]$, as well as densities $1/6$ and $2/11$. We also determine the ground states for a sequence of densities starting at $1/5$ and converging to 0. On the interval $[1/3, 2/5]$ we show that the ground states are periodic, having the same structure as the one-dimensional ground states. For densities between $1/6$ and $2/11$ we show that the ground states exhibit a phase separation analogous to that found by Kennedy [12] for densities in $(1/5, 2/9)$ and $(2/9, 1/4)$.

In chapter 3 we show that for every even integer $N \geq 2$, the ground states for density $\rho = (\frac{N^2}{2} + N + 1)^{-1}$ are translations, reflections, and rotations of the configuration with ions at $m(\frac{N}{2}, \frac{N}{2} + 1) + n(\frac{N}{2} + 1, -\frac{N}{2})$ where m and n range over all integers. An example with $N = 4$ is shown in figure 1.3. The thicker lines show how the ions form the vertices of a tiling by squares. A similar tiling results from every ground state in our sequence, with the slopes of the sides of the squares converging to ± 1 as the density goes to 0. The dashed lines are inserted to show the similarity with the ℓ_1 sphere packing problem on a lattice. Each ground state in our sequence is distinguished by the fact that it is the unique (up to lattice symmetries) configuration

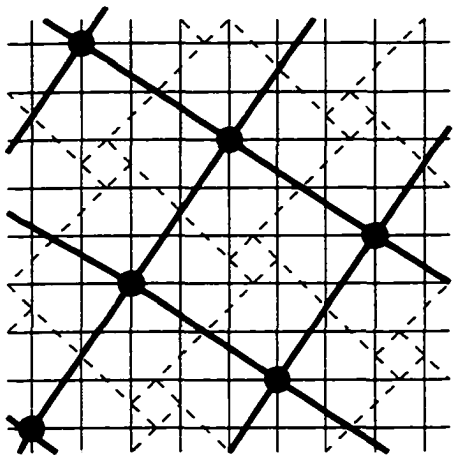


FIGURE 1.3. A portion of the ground state for density 1/13.

of density $(\frac{N^2}{2} + N + 1)^{-1}$ in which every pair of ions is separated by an ℓ_1 distance of at least $N + 1$.

In chapter 4 we prove that the ground states for densities 1/6 and 2/11 are those shown in figure 1.4. Following the method of Kennedy in [12], and based on the

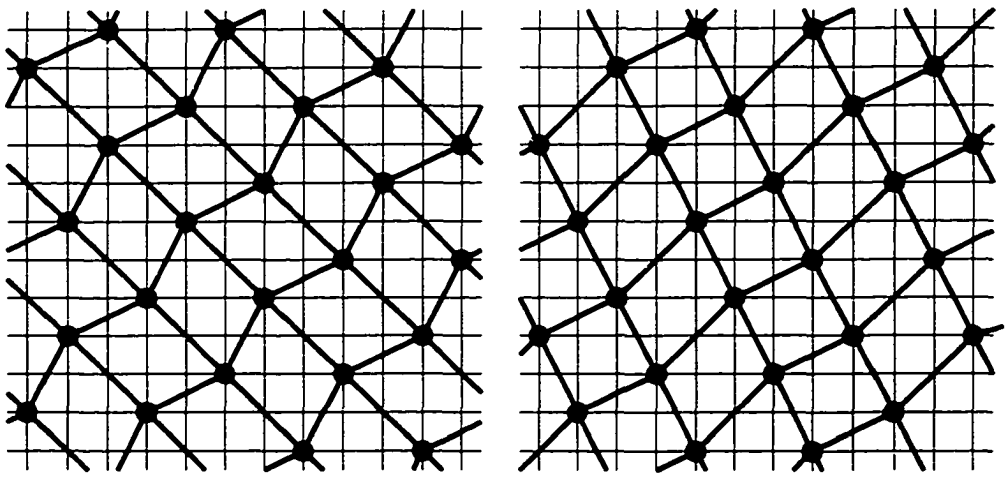


FIGURE 1.4. Left: ground state for density 1/6. Right: ground state for density 2/11. The thicker lines are a guide for the eye.

ideas of Watson in [13], we show that the ground states for densities between 1/6 and

2/11 are composed of large regions of the 1/6 ground state and large regions of the 2/11 ground state. However, the geometry of these two ground states prohibits them from mixing in a natural way, so the regions corresponding to the 1/6 ground state are separated from those corresponding to the 2/11 ground state by a relatively thin domain wall.

In chapter 5 we show that the ground states for all rational densities in $[1/3, 2/5]$ are periodic. In [11] Kennedy showed that if one only minimizes over periodic configurations, the ground states for densities in $[1/3, 1/2]$ must be constant on lines of slope ± 1 , i.e. site x is occupied by an ion $\Leftrightarrow$ site $x + (1, \eta 1)$ is occupied, where $\eta \in \{1, -1\}$ is constant throughout the configuration. We show that this "stripe" property persists when the minimization is over all configurations. For technical reasons we must restrict ourselves to densities in $[1/3, 2/5]$, however we feel it is safe to conjecture that the ground states for densities in $[2/5, 1/2]$ are periodic as well.

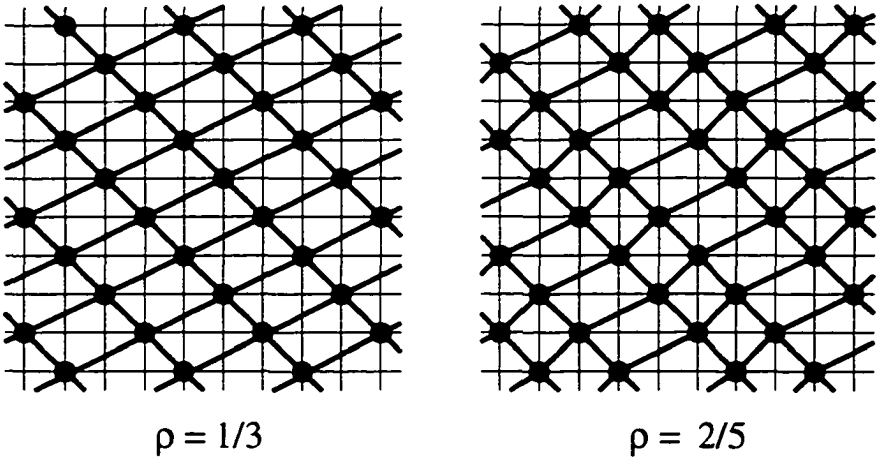


FIGURE 1.5. Left: ground state for density 1/3. Right: ground state for density 2/5. The thicker lines are a guide for the eye.

Given the stripe property, the problem becomes one-dimensional in the sense that all that remains is to determine the spacing between the stripes of occupied sites which minimizes the energy. Figure 1.5 shows the ground states for densities 1/3 and 2/5. We see that both are constant along lines of slope -1, but the spacing

between the occupied stripes is different. A modification of Lemberger's method for the one-dimensional case then shows that the stripe spacing in the two dimensional ground states is the same as the ion spacing in the one-dimensional ground states. The periodic structure of the ground states is then given by the Farey tree just as in one-dimension.

1.4 Future Work

There are many open problems involving the Falicov-Kimball model. We mention here a few possible extensions of our results. For densities in $[1/3, 2/5]$ as well as the sequence of densities we have determined the large U ground states. However, in all these cases the lower bound on U depends on the density. It is not known whether there exists a lower bound independent of the density over any interval. For some of the densities with periodic ground states it should be possible to to show the existence of multiple Gibbs states at low temperature using Pirigov-Sinai theory.

In nature, crystals are formed without the aid of a lattice. So crystallization should be studied using continuum models. One could modify the Falicov-Kimball model by changing the single particle Hamiltonian to something like

$$\Delta + U \sum_{i=1}^{N_i} W(x - x_i),$$

where W is, e.g., a square well potential whose support is centered about the origin, then minimize the sum of the N_e lowest eigenvalues of this operator over the locations x_i of the ions. Although the potential in this toy model is very artificial, it may be simple enough to yield rigorous results.

Chapter 2
EXPANSIONS

In this chapter we derive two expansions valid for the neutral case with large $U > 0$. To derive the expansions we change from the "occupation" variables, v_x, to the "spin" variables, s_x, defined by $v_x = \frac{1}{2}(s_x + 1)$. Then $s_x = 1$ when site x is occupied by an ion, and $s_x = -1$ when site x is unoccupied. We may then construct the $|\Lambda| \times |\Lambda|$ matrix $S = 2V - I$, so that

$$T - 2UV = T - US - UI . \tag{2.1}$$

Thus the use of the spin variables merely shifts the ground state energy by an amount UN_e.

If $U > 4$ the matrix $h = T - US$ has $|\Lambda|$ eigenvalues, $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{|\Lambda|}$, where $\lambda_i \in [-U-4, -U+4] \cup [U-4, U+4]$. We define

$$H(S) = \sum_{i=1}^{N_e} \lambda_i .$$

For $U > 4$ the number of negative eigenvalues of h is equal to the number of ions. So when the numbers of electrons and ions are equal, we have

$$H(S) = \sum_{\lambda_i < 0} \lambda_i . \tag{2.2}$$

2.1 Expansion 1

If C is a contour in the complex plane containing all the negative eigenvalues of h, then following Lemberger [6] we have

$$H(S) = \frac{1}{2\pi i} \oint_C Tr[z(z-h)^{-1}]\, dz . \tag{2.3}$$

By iterating the equation

$$(z-h)^{-1} = (z+US)^{-1} + (z+US)^{-1}T(z-h)^{-1}\,.$$

we may write equation 2.3 as

$$\begin{aligned} H(S) &= \sum_{k\geq 0} \frac{1}{2\pi i} \oint_C Tr([(z+US)^{-1}T]^k z(z+US)^{-1})\,dz \\ &= -UN_i + \sum_{k\geq 2} \frac{1}{2\pi i} \oint_C Tr([(z+US)^{-1}T]^k z(z+US)^{-1})\,dz. \end{aligned} \tag{2.4}$$

where N_i is the number of ions. The contour integral in equation 2.4 equals

$$\sum_{x_1,\ldots,x_k} T_{x_1x_2}\cdots T_{x_kx_1} \frac{1}{2\pi i} \oint_C \frac{z}{(z+US_{x_1x_1})^2} \prod_{j=2}^{k} \frac{1}{(z+US_{x_jx_j})}\,dz\,. \tag{2.5}$$

Denote the integrand in the above by $f(z)$, so

$$f(z) = \frac{z}{(z+U)^p(z-U)^r}\,.$$

where p is the number of times $+1$ appears in the sequence $(S_{x_1x_1},\ldots,S_{x_kx_k},S_{x_1x_1})$ and r is the number of times -1 appears in the same sequence. Note that if $p=0$ then f is analytic on the interior of C. Thus the integral is 0. Also, if $r=0$ the residue is 0. Thus for the integral in (2.5) to be non-zero, the above sequence must contain a 1 and a -1.

After evaluating this integral, (2.5) becomes

$$\frac{2U}{(-2U)^k} \sum_{x_1,\ldots,x_k}{}' T_{x_1x_2}\cdots T_{x_kx_1}(-1)^p \frac{(k-2)!}{(p-1)!(k-p)!} \frac{k-2p+1}{2}\,, \tag{2.6}$$

where $\sum'$ indicates that the sum is restricted to those sequences $(x_1,\ldots,x_k)$ in which the sequence $(S_{x_1x_1},\ldots,S_{x_kx_k})$ contains at least one 1 and one -1. Define m to be the number of times 1 appears in the sequence $(S_{x_1x_1},\ldots,S_{x_kx_k})$. Then $p = m + \frac{1+S_{x_1x_1}}{2}$. Let $\alpha_r = \frac{1+S_{x_rx_r}}{2}$. By summing over a particular $(x_1,x_2,\ldots,x_k)$

and all its cyclic permutations, we obtain

$$\frac{2U}{(-2U)^k}T_{x_1x_2}\cdots T_{x_kx_1}\sum_{\tau=1}^{k}(-1)^{m+\alpha_\tau}\frac{(k-2)!}{(m+\alpha_\tau-1)!(k-m-\alpha_\tau)!} \times\frac{k-2(m+\alpha_\tau)+1}{2}. \tag{2.7}$$

Note that α_τ will be 1 exactly m times, and 0 exactly $k-m$ times. Thus (2.7) becomes

$$\begin{aligned}\frac{2U(-1)^m}{(-2U)^k}T_{x_1x_2}\cdots T_{x_kx_1}\Big[&(k-m)\frac{(k-2)!}{(m-1)!(k-m)!}\frac{k-2m+1}{2}\\ &-m\frac{(k-2)!}{m!(k-m-1)!}\frac{k-2m-1}{2}\Big]\\ &=\frac{2U(-1)^m}{(-2U)^k}T_{x_1x_2}\cdots T_{x_kx_1}\frac{(k-2)!}{(m-1)!(k-m-1)!}.\end{aligned} \tag{2.8}$$

We may now write equation 2.3 as

$$H(S)=-UN_i+2U\sum_{k\geq 2}{\sum_{x_1,\ldots,x_k}}'\frac{(-1)^m}{k}(-2U)^{-k}T_{x_1x_2}\cdots T_{x_kx_1}\binom{k-2}{m-2}. \tag{2.9}$$

Since $T_{xy}=1$ if $|x-y|=1$ and 0 otherwise, the second sum on the right is over closed nearest neighbor walks, γ, on the lattice. These walks may be defined as functions $\gamma:\{0,1,2,\ldots\}\to\Lambda$ where $\gamma(n)$ and $\gamma(n+1)$ are nearest neighbor lattice sites. With $|\gamma|$ defined to be the number of steps taken by the walk, the fact that it is closed implies that $|\gamma|$ must be even and $\gamma(|\gamma|)=\gamma(0)$. We denote the set of lattice sites $\{\gamma(0),\gamma(1),\ldots,\gamma(|\gamma|-1)\}$ by $supp(\gamma)$. From the prime on the summation in equation 2.9 we see that each walk must visit both an occupied and an unoccupied site. We may now write

$$H(S)=-UN_i+\sum_{\gamma:|\gamma|\geq 2}\frac{(-1)^{m(S,\gamma)}}{|\gamma|}(2U)^{1-|\gamma|}\binom{|\gamma|-2}{m(S,\gamma)-1}, \tag{2.10}$$

where we have written "$m(S,\gamma)$" to stress the dependence of m on S and γ. An important feature of this expansion is that the $(-1)^{m(S,\gamma)}$ makes clear the sign of the contribution of a walk. One can see that a walk which makes an even number of visits to the occupied sites contributes a positive amount. Those which make an odd number of visits contribute a negative amount.

2.2 Expansion 2

In the neutral case, we may also express $H(S)$ as

$$H(S) = \frac{1}{2}\Big(Tr[h] - Tr\big[|h|\big]\Big). \tag{2.11}$$

where $|h| = \sqrt{h^2}$. Now

$$Tr[h] = U(|\Lambda| - 2N_i).$$

and

$$\begin{aligned} Tr\big[|h|\big] &= Tr\Big[\sqrt{(T - US)^2}\Big] \\ &= UTr\Big[\sqrt{I + ((U^{-1}T)^2 - (U^{-1}T)S - S(U^{-1}T))}\Big]. \end{aligned}$$

So we have

$$H(S) = U(\frac{\Lambda}{2} - N_i) - U\frac{1}{2}Tr\Big[\sqrt{I + ((U^{-1}T)^2 - (U^{-1}T)S - S(U^{-1}T))}\Big]. \tag{2.12}$$

For large enough U, following Gruber, Jedrzejewski, and Lemberger in [10], we may expand the square root in equation 2.12 to obtain

$$H(S) = -UN_i + \sum_{m \text{ even} \geq 2} U^{1-m} \sum_{X \subseteq \Lambda} h_{m,X} \prod_{x \in X} S_{xx}. \tag{2.13}$$

The coefficients $h_{m,X}$ are non-zero only when X is a subset of a closed nearest neighbor walk with m steps. Furthermore, there exists a positive constant c such that $|h_{m,X}| \leq c^m$.

It will be useful to express H in terms of the occupation variables V_{xx} where $S_{xx} = 2V_{xx} - 1$. Then

$$H(V) = -UN_i + \sum_{m \text{ even} \geq 2} U^{1-m} \sum_{\emptyset \neq X \subseteq \Lambda} c_{m,X} \prod_{x \in X} V_{xx} + E_\emptyset, \tag{2.14}$$

where

$$c_{m,X} = 2^{|X|} \sum_{B : X \subseteq B} (-1)^{|B \setminus X|} h_{m,B}, \tag{2.15}$$

and

$$E_\emptyset = \sum_{m \text{ even} \geq 2} U^{1-m} \sum_{B \subseteq \Lambda} (-1)^{|B|} h_{m,B} \tag{2.16}$$

is the ground state energy of the empty configuration. From equation 2.15 and the properties of the coefficients $h_{m,X}$, we see that the coefficients $c_{m,X}$ are non-zero only when X is a subset of a closed nearest neighbor walk with m steps, and there exists a constant c with $|c_{m,X}| \leq c^m$.

We now mention a technical note regarding constants and the mixing of expansion. In chapter 3 we use expansion 1 exclusively. In chapter 4 we only expansion 2 with the occupation variables (minus $E_\emptyset$). However, in chapter 5 we use expansion 2 (minus $E_\emptyset$) for orders 2 through 8, and expansion 1 for the higher orders. So to be completely accurate, the Hamiltonian in chapter 5 should be taken as itself plus the terms in $E_\emptyset$ at orders 2 through 8.

Chapter 3

SEQUENCE OF GROUND STATES

In this section we use the expansion derived in chapter 2 of the introduction to determine the ground states for a sequence of densities converging to 0. The key is that the function $m(S, \gamma)$ allows us to determine the sign of the contribution of a particular walk. If a walk makes only one visit to a single ion, $m(S, \gamma)$ will equal 1 and the walk will decrease the energy. Therefore, to minimize the second order term $H_2(S)$, we want S to have no nearest neighbor. Then every walk of length 2 hits an occupied and an unoccupied site which makes its contribution negative. Similarly, to minimize $H_2(S) + H_4(S)$, we would like each pair of ions to be separated by at least ℓ_1 distance 3. This assures us that any walk of length ≤ 4 visits only one ion, making its contribution negative.

Continuing this to higher orders, we see that we would like the ions to be as far apart from each other as possible. There is, however, a density constraint which at some point must stop the ions from getting too far apart. There are particular densities which allow us to proceed as above up to a certain order. For example, with $\rho = 1/5$, there is a configuration in which every pair of ions is separated by an ℓ_1 distance of at least 3. In fact, 1/5 is the largest density for which this can occur. This configuration is unique up to lattice symmetries, and has been shown to be the ground state for density 1/5. In this section we show how this is naturally extended to a sequence of densities starting from 1/5 and converging to 0. For each even n we demand that each pair of ions be separated by an ℓ_1 distance of at least $n + 1$. The lemma shows that there is a maximal density for which this can be achieved, and at that density such a configuration is unique up to lattice symmetries. The theorem proves that these are the ground states at this maximal density.

We should note that the proof of the theorem does not rely on the lemma. However, the lemma is stated and proved to give insight as to why this particular sequence of densities is a natural choice.

Lemma 3.1. *Let $N \geq 2$ be an even integer. Let the lattice Λ be $L \times L$ where L is a multiple of $\frac{N^2}{2} + N + 1$. Consider the set of configurations with the property that every two ions are separated by an ℓ_1 distance of at least $N + 1$. Then the density of any such configuration is at most $(\frac{N^2}{2} + N + 1)^{-1}$. Furthermore, there is a unique configuration (up to translations, rotations and reflections) in this set which attains this density.*

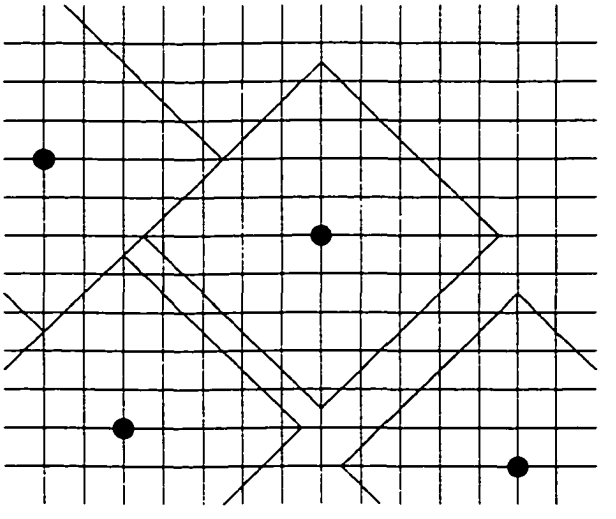


FIGURE 3.1. A portion of a configuration which satisfies the property in the lemma for $N = 8$.

Proof: Let S be a configuration satisfying the hypothesis of the lemma. If we center an ℓ_1 ball of radius $\frac{N+1}{2}$ about each ion, these balls will not overlap (see figure 3.1). The number of sites in each ball is $\frac{N^2}{2} + N + 1$, thus $\rho(S) \leq (\frac{N^2}{2} + N + 1)^{-1}$.

Let us now try to build a configuration which attains this density. Keeping in mind that the ℓ_1 balls described above must not overlap, we will try to pack them as close together as possible to obtain a disjoint covering of the lattice. By translation

invariance, we may start by placing an ion at the origin. In order to obtain our covering, we must place an ion at ℓ_1 distance $N+1$ from the origin, say (i,j), where $|i|+|j| = N+1$. There are many choices, but without loss of generality, we may assume our choice has $i \geq 0$ and $j \geq 0$. We now group these sites into three sets L, R and C. L contains the sites where $i \leq \frac{N}{2} - 1$, R has those with $i \geq \frac{N}{2} + 2$ and $C = \{(\frac{N}{2}, \frac{N}{2}+1), (\frac{N}{2}+1, \frac{N}{2})\}$ (see figure 3.2). Suppose we put an ion at a site (i,j)

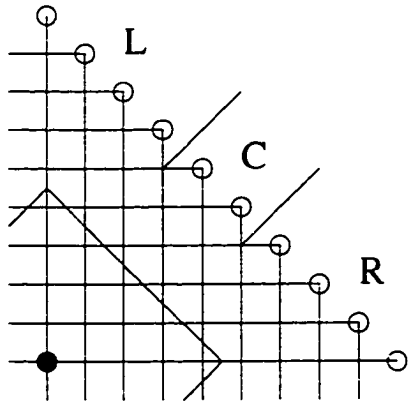


FIGURE 3.2. The sets L, R and C for the case $N = 8$. The solid dot is the ion at the origin.

in L and place one of our ℓ_1 balls of radius $\frac{N+1}{2}$ around it as well as the ion at the origin. We want to focus on the two sites $(i+1, j-\frac{N}{2})$ and $(i+1, j-\frac{N}{2}-1)$, which are as yet uncovered by a ball. These sites are circled in figure 3.3. In order to cover site $(i+1, j-\frac{N}{2})$ we must put an ion at $(i+\frac{N}{2}+1, j-\frac{N}{2})$. However, since we require a disjoint covering, this makes it impossible to cover $(i+1, j-\frac{N}{2}-1)$ (see figure 3.3). Similarly, covering $(i+1, j-\frac{N}{2}-1)$ leaves $(i+1, j-\frac{N}{2})$ uncovered. So we see that by placing an ion in L, we cannot avoid leaving sites uncovered and thus cannot hope to achieve our maximal density. A similar argument holds for sites in R. We are left with no where else to go but the set C.

Let us choose the site $(i,j) = (\frac{N}{2}, \frac{N}{2}+1)$ in C. Just as before, we want to make sure that $(i+1, j-\frac{N}{2})$ gets covered, so we place an ion at $(i+\frac{N}{2}+1, j-\frac{N}{2})$. We now have enough room to cover site $(i+1, j-\frac{N}{2}-1)$ by placing an ion at $(i+1, j-N-1)$.

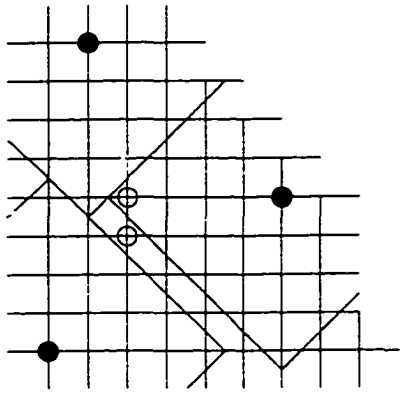


FIGURE 3.3. An ion has been placed in L. Attempting to cover the upper circled site leaves the lower circled site uncovered. Attempting to cover the lower circled site leaves the upper one uncovered.

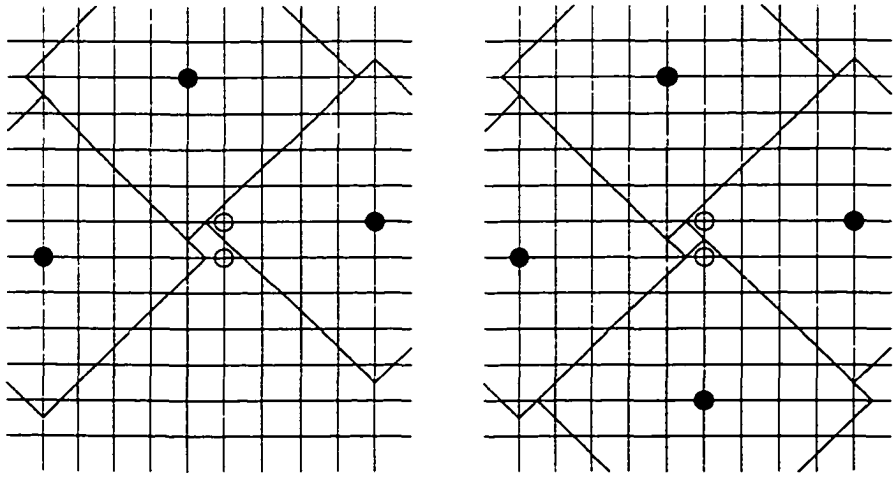


FIGURE 3.4. Left: the leftmost ion is the one at the origin, the uppermost is the one from C and the rightmost is necessary to cover the upper circled site. Right: completing the local arrangement in order to cover every site.

The result is shown in figure 3.4. Repeating this argument starting at each new ion we see that the pattern in figure 3.4 persists over the entire lattice. So we end up with a configuration with ions at $m(\frac{N}{2}, \frac{N}{2}+1) + n(\frac{N}{2}+1, -\frac{N}{2})$ where m and n range over all integers. Similarly, if at the beginning we started with the other site in C we would end up with ions at $m(\frac{N}{2}+1, \frac{N}{2}) + n(\frac{N}{2}, -\frac{N}{2}-1)$, a reflection of our original result. □

Theorem 3.1. *Let $N \geq 2$ be an even integer. Let the lattice Λ be $L \times L$ where L is a multiple of $\frac{N^2}{2}+N+1$ and the density $\rho = (\frac{N^2}{2}+N+1)^{-1}$. Then if we use periodic boundary conditions, the ground state configurations are translations, reflections, and rotations of the configuration with ions at $m(\frac{N}{2}, \frac{N}{2}+1) + n(\frac{N}{2}+1, -\frac{N}{2})$ where m and n range over all integers.*

When $N = 2$, $\rho = 1/5$. The ground state at this density is shown in figure 3.5. We note that this configuration corresponds to a tiling by squares. This is true for all the ground states covered by the theorem, where the slopes of the sides of the squares approach ± 1 as $N \to \infty$.

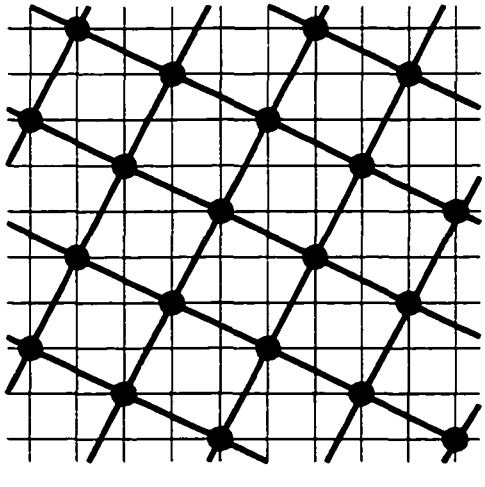


FIGURE 3.5. A portion of the ground state for density 1/5. The lines are a guide for the eye.

Proof of Theorem 3.1: Let S be a configuration with density $(\frac{N^2}{2}+N+1)^{-1}$. Let $I(S)$ be the set of sites with an ion. Let $x \in I$ and define

$$H_{n,x}(S) = (2U)^{1-n} \sum_{\substack{\gamma \\ |\gamma|=n \\ x \in supp(\gamma)}} \frac{1}{k(\gamma)} \frac{(-1)^{m(S,\gamma)}}{n} \binom{n-2}{m(S,\gamma)-1}.$$

where $k(\gamma)$ is the number of ions in $supp(\gamma)$. Then from equation 2.10 we have

$$H = \sum_{even\ n \geq 2} \sum_{x \in I} H_{n,x}.$$

Let $\tilde{S}$ be the configuration with density $(\frac{N^2}{2}+N+1)^{-1}$ and ions at $m(\frac{N}{2}, \frac{N}{2}+1) + n(\frac{N}{2}+1, -\frac{N}{2})$ where m and n range over all integers. The goal is to show that $H(S) - H(\tilde{S}) \geq 0$. We start by examining the lower order terms. We define

$$H_x^{\leq 2N} = \sum_{even\ n \geq 2}^{2N} H_{n,x}.$$

and

$$H^{\leq 2N} = \sum_{x \in I} H_x^{\leq 2N}.$$

Note that $0 \in I(\tilde{S})$. By the symmetry of $\tilde{S}$ and since H is invariant under rotations, reflections, and translations, we have

$$H_{n,x}(\tilde{S}) = H_{n,0}(\tilde{S})$$

for all n and $x \in I(\tilde{S})$. If S is any configuration with $|I(S)| = |I(\tilde{S})|$, this implies

$$H^{\leq 2N}(S) - H^{\leq 2N}(\tilde{S}) = \sum_{x \in I(S)} (H_x^{\leq 2N}(S) - H_0^{\leq 2N}(\tilde{S})). \tag{3.1}$$

Let $G_n(S) \subseteq I(S)$ be defined by $x \in G_n(S) \Leftrightarrow S$ restricted to $B_{\frac{n}{2}}(x)$ is the same as $\tilde{S}$ restricted to $B_{\frac{n}{2}}(0)$ up to a lattice symmetry. Then in particular, $x \in G_{2N}(S) \Leftrightarrow S$ has no other ions in $B_N(x)$. Suppose $x \in I(S) \setminus G_{2N}(S)$ and let d be the minimal ℓ_1

distance between x and any other occupied site. Then $d \leq N$ and $H_{n,x}(S) = H_{n,0}(\tilde{S})$ for $n \leq 2(d-1)$, which says that

$$H_x^{\leq 2N}(S) - H_0^{\leq 2N}(\tilde{S}) = O(U^{1-2d}).$$

Let us first assume $d \geq 2$, and consider $H_{2d,x}(S)$. Every term in this sum corresponds to a walk through x which hits ∂B_d at most once. There are three distinct possibilities for such a walk. (i) The walk does not hit ∂B_d. (ii) the walk hits ∂B_d at an unoccupied site, or (iii) the walk hits ∂B_d at an occupied site. Since S on $B_{d-1}(x)$ is the same as $\tilde{S}$ on $B_{d-1}(x)$, the contributions from the walks in case (i) cancel in $H_{2d,x}(S) - H_{2d,0}(\tilde{S})$. Similarly for case (ii), the contributions will cancel since there are no ions on ∂B_d in $\tilde{S}$. In case (iii), the walk in S visits exactly two ions giving a positive contribution to $H_{2d,x}(S)$, whereas in $\tilde{S}$, the walk visits one ion giving a negative contribution to $H_{2d,0}(\tilde{S})$, so $H_{2d,x}(S) - H_{2d,0}(\tilde{S})$ will be positive.

Now suppose $d = 1$ so that the ion at x has at least one nearest neighbor ion. Then either (i) all the sites neighboring x are occupied, or (ii) x has at least one unoccupied nearest neighbor. Recall that the walks which do not visit both an occupied and an unoccupied site do not contribute to H. So in case (i), $H_{2,x}(S) = 0$ while $H_{2,0}(\tilde{S})$ is negative making $H_{2,x}(S) - H_{2,0}(\tilde{S})$ positive. As for case (ii), the only walks that make a contribution to $H_{2,x}(S)$ are those which visit x and one of the neighboring unoccupied sites However, the contribution from each of these walks will cancel in $H_{2,x}(S) - H_{2,0}(\tilde{S})$ with the contribution from the corresponding walk in $\tilde{S}$. Since x has a neighboring ion there is at least one walk which does not contribute to $H_{2,x}(S)$, but makes a negative contribution to $H_{2,0}(\tilde{S})$. So in any case we have

$$H_x^{\leq 2N}(S) - H_0^{\leq 2N}(\tilde{S}) \geq CU^{1-2d} + O(U^{1-2(d+1)}), \tag{3.2}$$

where $C > 0$ is some constant depending on S only through d.

Looking at the right hand side of equation 3.1 we see that the only non-zero terms are those for which $x \in I(S) \setminus G_{2N}(S)$. By inequality 3.2 each of these terms may be

bounded below by CU^{1-2N} where $C > 0$ depends only on N. Thus

$$H^{\leq 2N}(S) - H^{\leq 2N}(\tilde{S}) \geq C|I(S) \setminus G_{2N}(S)|U^{-1-2N}. \tag{3.3}$$

From inequality 3.3 we may conclude that $\tilde{S}$ minimizes the Hamiltonian through order $2N$. We now show that the higher order terms do not mess this up.

We start with the definitions

$$H_x^{>2N} = \sum_{even \ \ n \geq 2(N+1)} H_{n,x}.$$

and

$$H^{>2N} = \sum_{x \in I} H_x^{>2N}.$$

Then we have the following two inequalities

$$\begin{aligned} \left| H^{>2N}(S) - \sum_{even \ \ n \geq 2(N+1)} \sum_{x \in G_n(S)} H_{n,x}(S) \right| &= \left| \sum_{even \ \ n \geq 2(N+1)} \sum_{x \in I(S) \setminus G_n(S)} H_{n,x}(S) \right| \\ &\leq \sum_{even \ \ n \geq 2(N+1)} c^n U^{-1-n} |I(S) \setminus G_n(S)|. \end{aligned}$$

and

$$\begin{aligned} \left| H^{>2N}(\tilde{S}) - \sum_{even \ \ n \geq 2(N+1)} \sum_{x \in G_n(S)} H_{n,x}(S) \right| &= \left| \sum_{even \ \ n \geq 2(N+1)} \sum_{x \in I \setminus G_n} H_{n,0}(\tilde{S}) \right| \\ &\leq \sum_{even \ \ n \geq 2(N+1)} c^n U^{-1-n} |I(S) \setminus G_n(S)|. \end{aligned}$$

Putting these together we have that

$$|H^{>2N}(\tilde{S}) - H^{>2N}(S)| \leq 2 \sum_{even \ \ n \geq 2(N+1)} c^n U^{-1-n} |I(S) \setminus G_n(S)|. \tag{3.4}$$

We must now obtain an upper bound on $|I(S) \setminus G_n(S)|$.

Let $F : I(\tilde{S}) \to I(S)$ be one to one and onto. Extend the domain of F to all of Λ by the following. For each $i \in \Lambda$ there is a unique $x \in I(\tilde{S})$ such that $\|x - i\|_1 \leq \frac{N}{2}$, i.e.

$i = x + (i_1, i_2)$ where $|i_1| + |i_2| \leq \frac{N}{2}$. Define $F(i) = F(x) + (i_1, i_2)$. Now suppose that $x \in I(S)$ with the property that every other $i \in B_{\frac{n}{2}}(x)$ has $|F^{-1}(i)| = 1$. Then clearly x is in G_n. So if x is not in G_n, there must be an $i_x \in B_{\frac{n}{2}}(x)$ with $|F^{-1}(i_x)| \neq 1$. Now, $i_x \in B_{\frac{n}{2}}(y)$ for at most $|B_{\frac{n}{2}}(0)|$ other sites y, so

$$|I(S) \setminus G_n(S)| \leq |B_{\frac{n}{2}}(0)||\{i : |F^{-1}(i)| \neq 1\}|.$$

Substituting this into 3.4 and using the fact that $|B_{\frac{n}{2}}(0)| \leq n^2$, we obtain

$$|H^{>2N}(\tilde{S}) - H^{>2N}(S)| \leq C'|\{i : |F^{-1}(i)| \neq 1\}|U^{1-2(N+1)}. \tag{3.5}$$

where $C' > 0$ depends only on N. We now return to the lower order terms and use inequality 3.3 to show that $H^{\leq 2N}(S) - H^{\leq 2N}(\tilde{S}) \geq C''|\{i : |F^{-1}(i)| \neq 1\}|U^{1-2N}$.

Suppose i is such that $|F^{-1}(i)| \geq 2$. Then there are occupied sites x and y with $\|x - i\|_1 \leq \frac{N}{2}$ and $\|y - i\|_1 \leq \frac{N}{2}$. Then $\|x - y\|_1 \leq N$, so $x \in I(S) \setminus G_{2N}(S)$. There can be at most $|B_{\frac{N}{2}}(0)|$ sites i with $\|x - i\|_1 \leq \frac{N}{2}$, so

$$|B_{\frac{N}{2}}(0)||I(S) \setminus G_{2N}(S)| \geq |\{i : |F^{-1}(i)| \geq 2\}|. \tag{3.6}$$

Now,

$$|\Lambda| = \sum_i |F^{-1}(i)| = |Range(F)| + \sum_{i:|F^{-1}(i)|\geq 2} (|F^{-1}(i)| - 1)$$

$$\Rightarrow \sum_{i:|F^{-1}(i)|\geq 2} (|F^{-1}(i)| - 1) = |\Lambda| - |Range(F)| = |\{i : |F^{-1}(i)| = 0\}|$$

$$\Rightarrow \sum_{i:|F^{-1}(i)|\geq 2} |F^{-1}(i)| = |\{i : |F^{-1}(i)| \neq 1\}|.$$

Since $|B_{\frac{N}{2}}(0)| \geq |F^{-1}(i)|$ we have

$$|B_{\frac{N}{2}}(0)||\{i : |F^{-1}(i)| \geq 2\}| \geq |\{i : |F^{-1}(i)| \neq 1\}|.$$

Combining this result with 3.6 we see that

$$|I(S) \setminus G_{2N}(S)| \geq \frac{1}{|B_{\frac{N}{2}}(0)|^2}|\{i : |F^{-1}(i)| \neq 1\}|.$$

Substituting this into 3.3 we see that

$$H^{\leq 2N}(S) - H^{\leq 2N}(\tilde{S}) \geq C''|\{i : |F^{-1}(i)| \neq 1\}|U^{1-2N}. \tag{3.7}$$

where $C'' > 0$ depends only on N.

Rewriting equations 3.7 and 3.5 we end up with

$$H^{\leq 2N}(S) \geq H^{\leq 2N}(\tilde{S}) + C''|\{i : |F^{-1}(i)| \neq 1\}|U^{1-2N}.$$

and

$$H^{>2N}(S) \geq H^{>2N}(\tilde{S}) - C'|\{i : |F^{-1}(i)| \neq 1\}|U^{1-2(N+1)}.$$

Adding these together we obtain

$$H(S) \geq H(\tilde{S}) + |\{i : |F^{-1}(i)| \neq 1\}|U^{1-2N}(C'' - C'U^{-2}).$$

which proves the theorem. □

Chapter 4

PHASE SEPARATION

For densities 1/6 and 2/11 we show that the ground states are configurations S^A and S^C respectively, as shown in figure 4.1. For densities between 1/6 and 2/11 we show that the ground states are made up of large regions which look like S^A and large regions which look like S^C, where these S^A and S^C regions are separated by a domain wall. This "phase separation" is similar to that found by Kennedy for densities in (1/5, 2/9) and (2/9, 1, 4). The precise statement of the theorem is as follows.

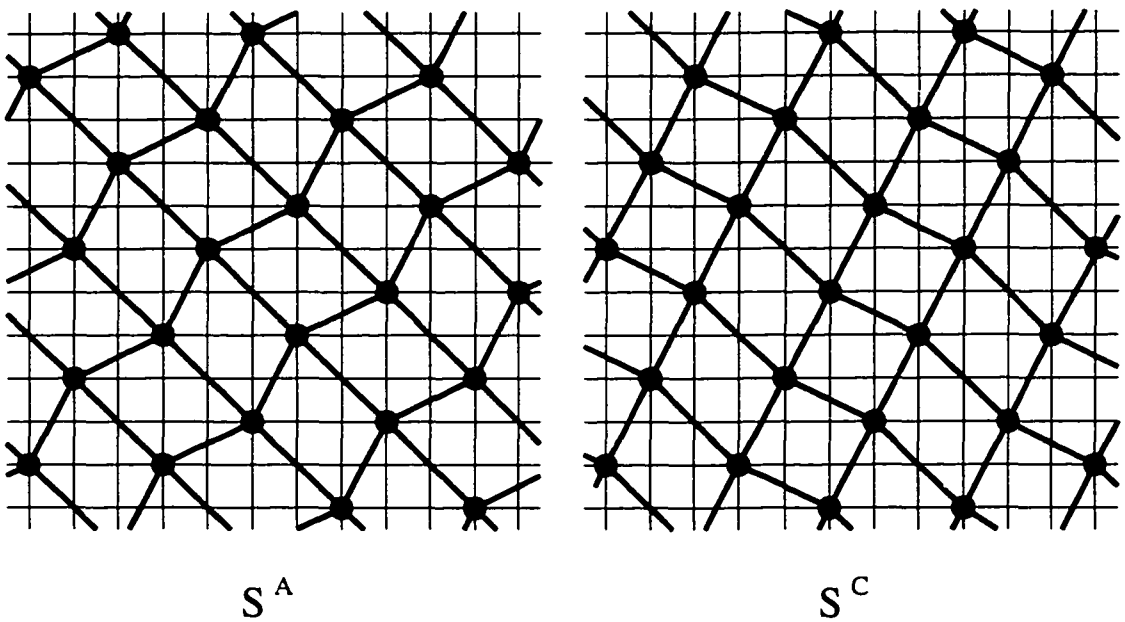


FIGURE 4.1. Left: the ground state for density 1/6. Right: the ground state for density 2/11.

Theorem 4.1. *We take the ion density, ρ, to be rational, and use periodic boundary conditions. Let the lattice Λ be $L \times L$ where L is a multiple of 66. Then there exists positive constants U_0 and c such that if $U \geq U_0$, (i) when $\rho = 1/6$, the ground*

state ion configurations are translations, rotations, and reflections of configuration S^A shown in figure 4.1, (ii) when $\rho = 2/11$, the ground state ion configurations are translations, rotations, and reflections of configuration S^C shown in figure 4.1, and (iii) when $1/6 < \rho < 2/11$, for every ground state ion configuration there is a set of sites Λ_0 with $|\Lambda_0| \leq cU^{10}L$, such that on every connected component of $\Lambda \setminus \Lambda_0$, the configuration is a rotation or reflection of either S^A or S^C from figure 4.1.

Although U is large, it remains fixed while L becomes arbitrarily large. The bound on the size of Λ_0 shows that $|\Lambda_0|$ is $O(L)$, while $|\Lambda| = L^2$. Thus for large L, Λ_0 is a tiny fraction of the lattice. So we see that in the ground states where ρ is between $1/6$ and $2/11$, the bulk of the lattice is occupied by "islands" on which the configuration agrees with either the $\rho = 1/6$ ground state or the $\rho = 2/11$ ground state.

We prove theorem 4.1 by determining the ground states through order 12, then showing that the higher orders "respect" these conclusions. To find the ground states through order 12, we minimize H order by order. Through sixth order, following the ideas of Watson, we find that the ground states correspond to tilings by squares, parallelograms, and kites, as shown in figure 4.3. We write the Hamiltonian as a function of the number of each type of tile. All tilings have the same energy through order 6. At eighth order we find that all square-parallelogram tilings have the same energy, but kites increase the energy. Thus through eighth order, the ground states correspond to square-parallelogram tilings.

At tenth order the tiles are too small to capture all the terms. However, the vertices in a square-parallelogram tiling can be one of only four types. These are shown in figure 4.5. At tenth order we may write H in terms of the number of each of these vertex types. At orders 10 and 12 we find that types A and C have the same energy, and types B and D have higher energy. Thus the ground state through order 12 must be a square-parallelogram tiling with only type A and C vertices. However, a type A vertex cannot be adjacent to a type C vertex. Thus we must separate the

A and C vertices to minimize the energy.

With $H = \sum_{even\ m \geq 2} U^{1-m} h_m$, we define $H_m = U^{1-m} h_m$, and

$$H^{\geq N} = \sum_{even\ m \geq N} H_m$$

for even N. The following theorem give us the inequalities necessary to prove theorem 4.1.

Theorem 4.2. *Let M be the number of 4×4 blocks in a configuration S which are not a reflection or rotation of one of those shown in figure 4.2. Let n_S, n_P, n_K be the number of squares, parallelograms and kites respectively (figure 4.3). Let n_A, n_B, n_C, n_D be the number of type A, B, C, and D ions respectively (figure 4.5). If the lattice has dimensions $L \times L$ and ρ is the ion density, then there are functions f_8, f_{12}, f_{14} of U and ρ, and constants a and b such that*

$$\frac{16}{3} U^{-5} M \leq H_2 + H_4 + H_6 + U^{-5}(a + b\rho) \leq 96 U^{-1} M . \tag{4.1}$$

$$H_8(S) - L^2 f_8 = 32 U^{-7} n_K + O(U^{-7}) M . \tag{4.2}$$

$$\begin{aligned} H_{10}(S) + H_{12}(S) - L^2 f_{12} = {} & 40 U^{-9} n_D + 5280 U^{-11} n_B + 20128 U^{-11} n_D \\ & + O(U^{-9}) M + O(U^{-9}) n_K , \end{aligned} \tag{4.3}$$

$$H^{\geq 14}(S) - L^2 f_{14} = O(U^{-13})(M + n_K + n_B + n_D) . \tag{4.4}$$

$O(U^{-k})$ denotes a quantity whose absolute value is bounded by a constant times U^{-k}.

Proof of (4.1) from Theorem 4.2: This is shown in appendix A.1. □

So we see that every 4×4 block which is not shown in figure 4.2 contributes at a positive amount of energy at order at most 6, and the configurations in which every 4×4 block is one of those in figure 4.2 have 0 energy through sixth order. Thus for

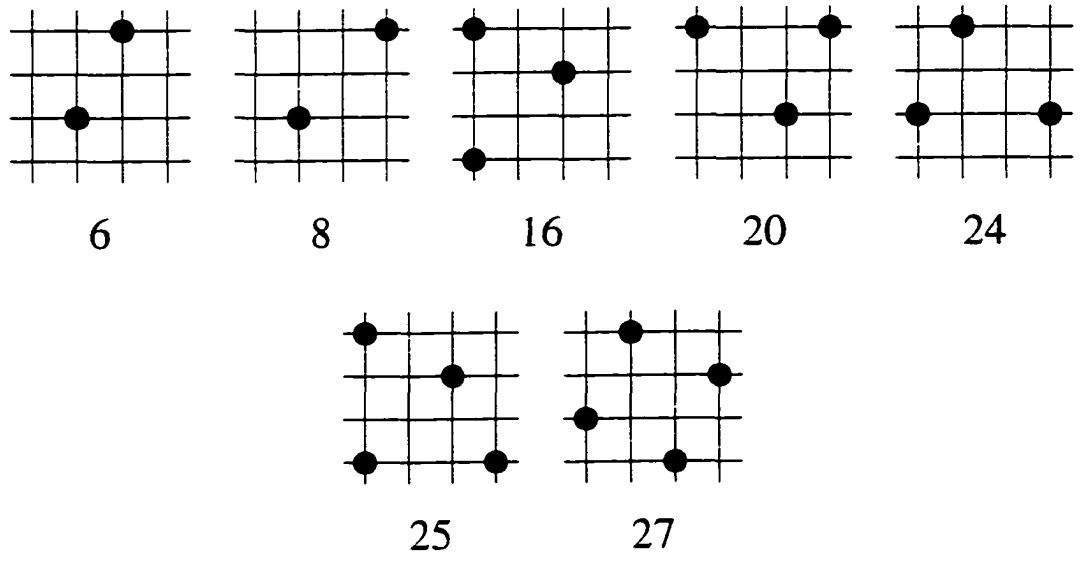


FIGURE 4.2. Configurations which minimize the energy locally.

a configuration to be a ground state through order 6, every 4×4 block must be a rotation or reflection of one of those from figure 4.2. The following lemma shows that these configurations form tilings by squares, parallelograms, and kites.

Lemma 4.1. *Let S be a configuration where every 4×4 block is one of those shown in figure 4.2. Then S corresponds to a tiling by squares, parallelograms, and kites as shown in figure 4.3.*

Proof: Let S be a configuration satisfying the hypothesis of the lemma. Consider any 2x2 square of unoccupied sites in S. The 4x4 block centered on this square must then be either type 24 or type 27. If it is type 27, then we see by connecting the dots that our 2x2 square is enclosed by a larger square of area 5. If it is type 24, then the 4x4 block directly below it must be another type 24 block, with two possible orientations. Connecting the dots in one orientation gives us a parallelogram of area 6, the other gives us a kite of area 6 (see figure 4.3).

The edges in these shapes are of length $\sqrt{5}$ or $\sqrt{8}$. We may fill in these edges in

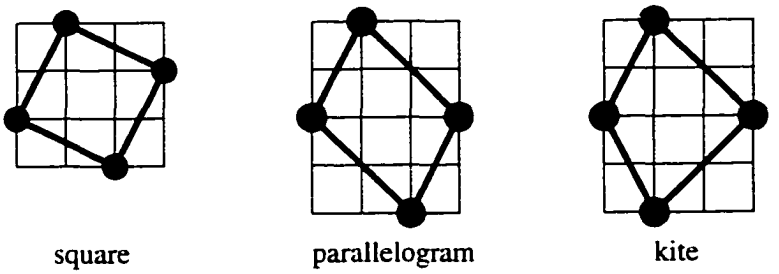


FIGURE 4.3. Shapes bounding an empty 2x2 block. Left: type 27 block. Middle and right: type 24 block above the two possible orientations of another type 24 block.

each of the seven possible 4x4 blocks. The result is shown in figure 4.4. From the posi-

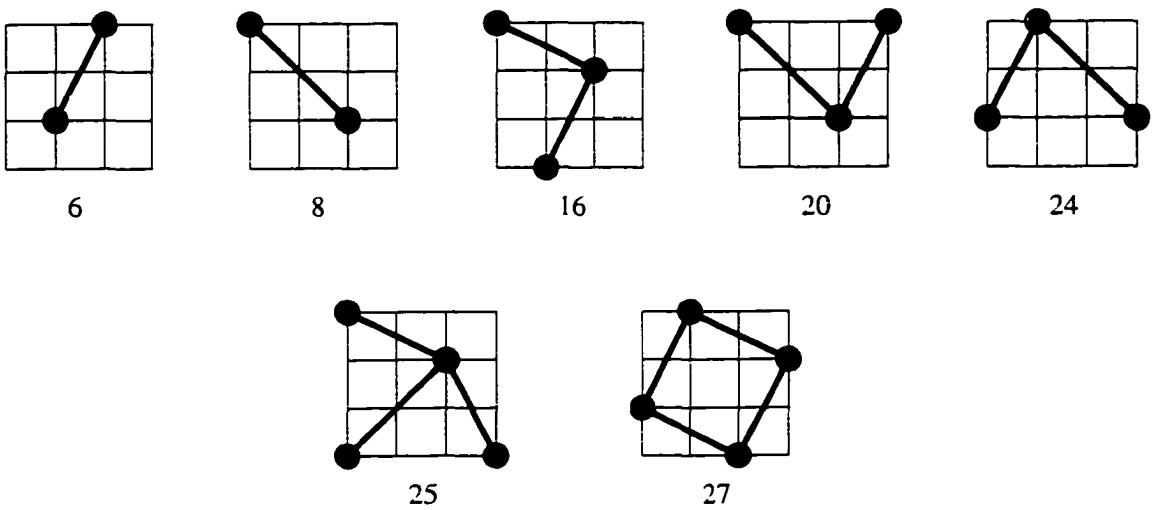


FIGURE 4.4. Possible 4x4 block configurations for the ground state of H_4 with $\frac{1}{5} > \rho > \frac{1}{6}$.

tions of the empty 2x2 squares in each of these seven blocks we see that each ion is the vertex of at least one of the three shapes and that each edge of length $\sqrt{8}$ is an edge of two shapes. Notice how the edge in a type 6 block connects the inner square of the 4x4 block with its perimeter without hitting one of the corners. One of the edges in a type 16 block also has this property. For any edge of length $\sqrt{5}$ there is a 4x4 block containing it with this property, so this block must be type 6 or 16. From the positions of the empty 2x2 in these two block types, we see that any edge of length $\sqrt{5}$ is an edge of two shapes. Since every edge borders two shapes and every ion is the vertex of

at least one shape. S must correspond to a tiling by the three shapes in figure 4.3. □

Proof of (4.2) from Theorem 4.2: If S is such a tiling, we would like to write $H_8(S)$ in terms of n_S, n_P and n_K, the number of squares, parallelograms and kites respectively. Suppose X is a subset of $I(S)$. Recall that if X is to give a non zero contribution to $H_8(S)$, X must be a set of ions which is contained in a closed nearest neighbor walk of eight steps. Referring to figure 4.3 we see that such a walk cannot possibly visit more than 2 ions, the tiles are just too big. Furthermore, if the walk does visit 2 ions, these ions must belong to the same tile. We are left with three possibilities for X: (a) X consists of a single ion, (b) X consists of 2 ions forming an edge of a tile (i.e. the ions are separated by $\sqrt{5}$ or $\sqrt{8}$) or (c) X consists of 2 ions on opposing vertices of a tile (i.e. the ions are separated by 3, $\sqrt{10}$, or 4). If X falls into case (a) define $\tilde{c}_{8,X} = \frac{1}{4}c_{8,X}$, for case (b) $\tilde{c}_{8,X} = \frac{1}{2}c_{8,X}$ and $\tilde{c}_{8,X} = c_{8,X}$ for case (c). For future reference, we note that all three cases may be written as $\tilde{c}_{8,X} = \frac{c_{8,X}}{\kappa(X)}$, where $\kappa(X)$ is the number of tiles containing X. κ is an over-counting factor which is required since, for example, one edge belongs to two tiles. Let us define

$$\epsilon_8^S = \sum_{X \subseteq square} \tilde{c}_{8,X} \,.$$

where "$X \subseteq square$" means that X is a subset of the ions in a particular square tile. This is the energy of a square at order 8. We define ϵ_8^P and ϵ_8^K similarly, being the energies of a parallelogram and kite respectively, at order 8. So we may write

$$H_8(S) = L^{-2}(n_S\epsilon_8^S + n_P\epsilon_8^P + n_K\epsilon_8^K)\,. \tag{4.5}$$

In such a tiling the quantity of each type of tile is not arbitrary. Since the area $= L^2$ we have

$$5n_S + 6n_P + 6n_K = L^2\,. \tag{4.6}$$

We are also keeping the number of ions to be fixed at ρL^2, so

$$n_S + n_P + n_K = \rho L^2\,. \tag{4.7}$$

The energies in equation 4.5 are

$$\epsilon_8^S = -400. \qquad \epsilon_8^P = 944. \qquad \epsilon_8^K = 976.$$

These are computed in appendix A.2. Using equations 4.6 and 4.7 to solve for n_S and n_P in terms of n_K, we have

$$H_8(S) - L^2 f_8(U, \rho) = 32U^{-7} n_K .$$

Recall that S was assumed to be a tiling. Of course in general, this will not be the case. So suppose S is not a tiling. Let M be the number of 4x4 blocks on which the configuration is not one of the 7 mentioned above. Then the number of sites in the region where S is not a tiling is at most $16M$. So the terms intersecting this region contribute at most $O(U^{-7})M$ to H_8. Equations 4.6 and 4.7 will no longer hold, but their error will be bounded by a constant times M. Thus for a general S, we may write

$$H_8(S) - L^2 f_8(U, \rho) = 32U^{-7} n_K + O(U^{-7})M . \quad \square$$

Proof of (4.3) from Theorem 4.2: We now want to obtain a similar expression for the energy at orders 10 and 12. At these orders, our original three tiles are too small to capture all the terms. We must define new variables, analogous to n_S, n_P, and n_K, to work with. To this end, we will classify ions according to the arrangement of tiles surrounding them. Type A, B, C, and D ions are defined in figure 4.5. Note that there are no kites in these ion types. This is because of the positive coefficient of n_K in equation 4.2. The kites increase the energy at order 8.

Let us restrict our attention, for the moment, on a configuration S which corresponds to a tiling by only squares and parallelograms. Then every ion in $I(S)$ is one of the types in figure 4.5. We define n_A, n_B, n_C, and n_D to be the number of type A,

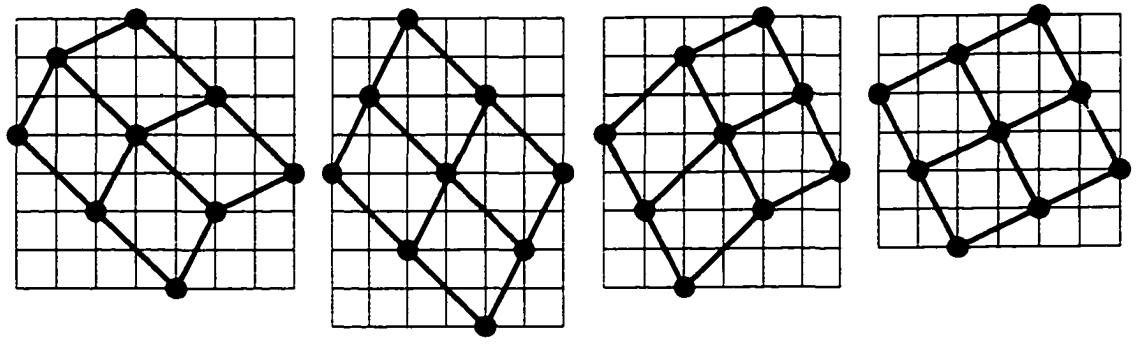


FIGURE 4.5. Local arrangements about the different ion types.

B, C, and D ions in $I(S)$. The energies at order m of these four ion types, e_m^A, e_m^C, e_m^C, and e_m^D, are defined in a manner similar to e_8^S, e_8^P, and e_8^K. They are calculated in appendix A.3 for $m = 10$ and 12. We then have that

$$H_{10}(S) + H_{12}(S) = U^{-9}(-36624n_A - 36624n_B - 63684n_C - 90704n_D) + U^{-11}(-158736n_A - 153456n_B + 355112n_C + 911088n_D).$$

As above, these four variables must satisfy

$$6n_A + 6n_B + \frac{11}{2}n_C + 5n_D = L^2. \tag{4.8}$$

and

$$n_A + n_B + n_C + n_D = \rho L^2. \tag{4.9}$$

Eliminating n_A and n_C we find that

$$H_{10}(S) + H_{12}(S) - L^2 f_{12}(U, \rho) = 40U^{-9}n_D + 5280U^{-11}n_B + 20128U^{-11}n_D.$$

This says that type B and D ions increase the energy at orders 10 and 12 Recall that our configuration S corresponds to a tiling by squares and parallelograms. Now consider a general configuration S. This configuration may contain kites as well as

regions which are not tilings. Using a similar argument as above, we may write

$$H_{10}(S) + H_{12}(S) - L^2 f_{12}(U,\rho) = 40U^{-9}n_D + 5280U^{-11}n_B + 20128U^{-11}n_D + O(U^{-9})M + O(U^{-9})n_K . \quad \square$$

Let us pause here to see what we can say about the ground states of the Hamiltonian truncated at order 12. In order to minimize $H_2 + H_4 + H_6$, we see from inequality 4.1 that M must be 0. M appears in equations 4.2 and 4.3 as a multiple of $O(U^{-7})$ and $O(U^{-9})$ terms, so for large enough U, to minimize the energy through order 12, we must have $M = 0$. The right hand side of 4.2 then becomes $32U^{-7}n_K$. In 4.3, n_K appears as a multiple of an $O(U^{-9})$ term. Thus we must have $n_K = 0$. From 4.3 we see that n_D and n_B make positive contributions at orders 10 and 12 respectively, so both of them must be 0. The only available ions we are left with are those of types A and C. We may conclude that if $\rho = 2/11$, in order to minimize the energy through order 12, every ion must be a type C. Similarly, for $\rho = 1/6$, every ion must be type A. Consider densities between 1/6 and 2/11. One can see from figure 4.5 that types A and C ions do not "fit" next to each other. That is, it is impossible to construct a configuration consisting only of these two ion types. This is the root of the phase separation. We now show that the higher order terms "respect" these conclusions.

Proof of (4.4) from Theorem 4.2: For any configuration S, we may write $H(S)$ as

$$H(S) = \sum_{\text{even } m \geq 2} U^{1-m} \sum_{x \in I(S)} \sum_{\substack{X \subseteq I(S): \\ x \in X}} \hat{c}_{m,X} ,$$

where $\hat{c}_{m,X} = \frac{c_{m,X}}{|X|}$. We can think of $U^{1-m} \sum_{\substack{X \subseteq I(S): \\ x \in X}} \hat{c}_{m,X}$ as the contribution to $H(S)$ from x at order m. Now let S^A be a configuration where every ion is type A. Because H is invariant under rotations and reflections, we see that $\sum_{\substack{X \subseteq I(S^A): \\ x \in X}} \hat{c}_{m,X}$ is the same for every $x \in I(S^A)$. The same may be said for S^C, a configuration in which every ion

is type C. Without loss of generality, we assume that 0 is in both $I(S^A)$ and $I(S^C)$. Let us then define

$$e_A = \sum_{\text{even } m \geq 14} U^{1-m} \sum_{\substack{X \subseteq I(S^A) \\ 0 \in X}} \hat{c}_{m,X} .$$

and

$$e_C = \sum_{\text{even } m \geq 14} U^{1-m} \sum_{\substack{X \subseteq I(S^C) \\ 0 \in X}} \hat{c}_{m,X} .$$

Let S be a configuration with $\frac{1}{6} \leq \rho \leq \frac{2}{11}$. For $x \in I(S)$ and m even, let $S_{x,m}$ denote the restriction of S to an ℓ^1 ball of radius $\frac{m}{2}$ centered at x. Let $A \subseteq I(S)$ denote the set of ions of type A, so $|A| = n_A$. For even m ≥ 14, define $A_m \subseteq A$ by $x \in A_m \Leftrightarrow S_{x,m}$ is a rotation or reflection of $S^A_{0,m}$. Clearly then $A \supseteq A_{14} \supseteq A_{16} \supseteq A_{18} \ldots$. The sets C and C_m are defined similarly for type C ions, with $|C| = n_C$.

Let $H^{\geq 14} = H - \sum_{\text{even } m \geq 14} H_m$. Then

$$\begin{aligned} &\left| H^{\geq 14}(S) - \sum_{\text{even } m \geq 14} U^{1-m} \sum_{x \in A_m \cup C_m} \sum_{\substack{X \subseteq I(S) \\ x \in X}} \hat{c}_{m,X} \right| \\ &= \left| \sum_{\text{even } m \geq 14} U^{1-m} \sum_{x \in I(S) \setminus (A_m \cup C_m)} \sum_{\substack{X \subseteq I(S) \\ x \in X}} \hat{c}_{m,X} \right| \\ &\leq \sum_{\text{even } m \geq 14} U^{1-m} |I(S) \setminus (A_m \cup C_m)| c^m . \end{aligned} \tag{4.10}$$

Similarly,

$$\left| n_A e_A - \sum_{\text{even } m \geq 14} U^{1-m} \sum_{x \in A_m} \sum_{\substack{X \subseteq I(S) \\ x \in X}} \hat{c}_{m,X} \right| \leq \sum_{\text{even } m \geq 14} U^{1-m} |A \setminus A_m| c^m , \tag{4.11}$$

and

$$\left| n_C e_C - \sum_{\text{even } m \geq 14} U^{1-m} \sum_{x \in C_m} \sum_{\substack{X \subseteq I(S) \\ x \in X}} \hat{c}_{m,X} \right| \leq \sum_{\text{even } m \geq 14} U^{1-m} |C \setminus C_m| c^m . \tag{4.12}$$

Note that both $A \setminus A_m$ and $C \setminus C_m$ are contained in $I(S) \setminus (A_m \cup C_m)$, so both $|A \setminus A_m|$ and $|C \setminus C_m|$ are $\leq |I(S) \setminus (A_m \cup C_m)|$. Since A_m and C_m are disjoint, we may add 4.11 and 4.12 to obtain

$$\left| n_A e_A + n_C e_C - \sum_{even\ m \geq 14} U^{-1-m} \sum_{x \in A_m \cup C_m} \sum_{\substack{X \subseteq I(S) \\ x \in X}} \hat{c}_{m,X} \right|$$

$$\leq 2 \sum_{even\ m \geq 14} U^{-1-m} |I(S) \setminus (A_m \cup C_m)| c^m . \tag{4.13}$$

We must now estimate the size of $|I(S) \setminus (A_m \cup C_m)|$. Let $x \in |I(S) \setminus (A_m \cup C_m)|$. Then either (i) $S_{x,m}$ is not contained in a part of S which is a square-parallelogram-kite tiling, or $S_{x,m}$ intersects a kite in S; or (ii) $S_{x,m}$ is contained in a part of S which is a square-parallelogram tiling, and $S_{x,m}$ contains a type B or D ion; or (iii) $S_{x,m}$ is contained in a part of S which is a square-parallelogram tiling, and $S_{x,m}$ contains both a type A and C ion. In case (i), $S_{x,m}$ must intersect a 4×4 block which is not shown in figure 4.2, or intersect a kite. Note that if a square-parallelogram tiling contains a type A ion, then all the tiles must be parallelograms. Thus case (iii) is impossible. So we may associate each $x \in |I(S) \setminus (A_m \cup C_m)|$ with a "bad" 4×4 square, a kite, a type B ion, or a type D ion. The number of sites associated with any one of these objects is bounded by dm^2 for some constant d. So we see that

$$|I(S) \setminus (A_m \cup C_m)| \leq dm^2 (M + n_K + n_B + n_D) . \tag{4.14}$$

Thus (4.10) and (4.13) are

$$\leq 2 \sum_{even\ m \geq 14} U^{1-m} c^m dm^2 (M + n_K + n_B + n_D) = O(U^{-13})(M + n_K + n_B + n_D) , \tag{4.15}$$

which means that

$$|H^{\geq 14}(S) - n_A e_A - n_C e_C| = O(U^{-13})(M + n_K + n_B + n_D) . \tag{4.16}$$

Combining equations 4.8 and 4.9 with equation 4.16, we have that

$$H^{\geq 14}(S) - L^2 f_{14}(U, \rho) = O(U^{-13})(M + n_K + n_B + n_D) . \quad \square \tag{4.17}$$

We now use the inequalities in theorem 4.2 to prove theorem 4.1.

Proof of Theorem 4.1: Let us first consider part (i) of theorem 4.1 where $\rho = 1/6$. In configuration S^A, $M = n_K = n_B = n_C = 0$. The equations in theorem 4.2 then imply that S^A is a ground state. Any other ground state must also have $M = n_K = n_B = n_C = 0$, and therefore correspond to a square-parallelogram tiling with no type B or C ions. The only such tiling with $\rho = 1/6$ is configuration S^A. Thus the ground states for $\rho = 1/6$ are the translations, reflections, and rotations of configuration S^A. A similar argument shows that S^C is the unique ground state, up to a lattice symmetry, for $\rho = 2/11$.

Now consider part (iii) of theorem 4.1 where $1/6 < \rho < 2/11$. We construct a trial configuration as follows. Divide the $L \times L$ square into two rectangles and put S^A on one side and S^C on the other. The areas of these rectangles may then be chosen to give the configuration any rational density between 1/6 and 2/11. In this trial configuration, we see that $(M + n_K + n_B + n_D)$ is bounded by a constant times L. Theorem 4.2 then tells us that $H + U^{-5}(a + b\rho) - L^2(f_8 + f_{12} + f_{14}) \leq O(U^{-1})L$. In a ground state the same inequality must hold. More explicitly, in a ground state we must have that

$$\frac{16}{3}U^{-5}M + 32U^{-7}n_K + 40U^{-9}n_D + 5280U^{-11}n_B + 20128U^{-11}n_D$$
$$+ O(U^{-7})M + O(U^{-9})n_K + O(U^{-13})(M + n_K + n_B + n_D) \leq O(U^{-1})L\,,$$

which we may rewrite as

$$M\left[\frac{16}{3}U^{-5} + O(U^{-7}) + O(U^{-13})\right] + n_K\left[32U^{-7} + O(U^{-9}) + O(U^{-13})\right]$$
$$+ n_B\left[5280U^{-11} + O(U^{-13})\right] + n_D\left[40U^{-9} + 20128U^{-11} + O(U^{-13})\right] \leq O(U^{-1})L.$$

If U is large enough, we can obtain a crude bound on $M + n_K + n_B + n_D$ by multiplying both sides of this inequality by U^{11}. We then see that any ground state must satisfy

$$M + n_K + n_B + n_D \leq cU^{10}L\,,$$

where c is a positive constant. Define Λ_0 to be the union of all the 4×4 blocks which are not one of those in figure 4.2, together with any site within ℓ^1 distance 6 of a type B or D ion, and any site contained in a kite. Then in $\Lambda \setminus \Lambda_0$, the configuration must correspond to a square-parallelogram tiling with no type B or D ions. However, in any square-parallelogram tiling it is not possible to have a type A ion adjacent to a type C ion, that is, separated by $\sqrt{5}$ or $\sqrt{8}$. Within $\Lambda \setminus \Lambda_0$, it is still possible to have a large region of type A ions connected to a large region of type C ions by a single line of sites. To insure that each connected component of $\Lambda \setminus \Lambda_0$ does not contain both type A and type C ions, we simply enlarge Λ_0 by an ℓ_1 distance of d. If d is large enough we can then be sure that each connected component of $\Lambda \setminus \Lambda_0$ contains only type A or type C ions. $\square$

Chapter 5
PERIODIC GROUND STATES

In this section we determine the large U ground states for densities between 1/3 and 2/5. These ground states are periodic with structure very similar to the one dimensional ground states. In fact, at any particular density in this region, the restriction of the ground state to any horizontal or vertical line is the one dimensional ground state at that density.

Theorem 5.1. *Suppose $\rho = p/q \in [1/3, 2/5]$ where p and q are relatively prime. We assume the lattice Λ is $L \times L$ where L is a multiple of $4q$. Then there exists $U(q) > 0$ such that for all $U \geq U(q)$, the ground states are translations, reflections, and rotations of the configuration S defined by the following properties: S is constant along lines of slope $+1$, and S restricted to any vertical or horizontal line is the same as the one dimensional large U ground state with density ρ.*

The remainder of the section is dedicated to the proof of this theorem.

First we give an overview of the proof. We start by considering 3×3 blocks of sites. Through fourth order, Kennedy has shown that each block which looks like one of those shown in figure 5.2 contributes the same amount of energy, while any other block contributes a higher amount of energy. So if a configuration exists in which every 3×3 block looks like one of those from figure 5.2, it must minimize H through fourth order. It turns out that such configurations do exist. In fact, Watson [13] has shown that they correspond to tilings by squares and parallelograms as shown in figure 5.3. In such a tiling the configuration must be constant on lines of slope ± 1, where the sign for the entire configuration is determined by the slope of the short sides of one of the parallelograms.

Up to rotations and reflections, the vertices of such a tiling must be one of the three types shown in figure 5.3. We may write the energy through order eight in terms of the number of each vertex type. Through sixth order we find that every tiling has the same energy. At eighth order, tilings with only type B and C vertices have the same energy, but type A vertices increase the energy. So if there exists configurations that correspond to square-parallelogram tilings with no type A vertices, they minimize H through order eight. It turns out that such configurations do exist for densities in $[1/3, 2/5]$.

When we include the higher order terms, the most we can say at this point is that the ground state consists primarily of large regions corresponding to a square-parallelogram tiling with no type A vertices. Because of the lack of type A vertices, these regions must contain parallelograms. Furthermore, the slopes of the short sides of these parallelograms must be the same throughout each individual region. This means that within each region, the configuration must be constant on lines of slope $+1$ or -1, but not both, as it would in a region consisting entirely of type A vertices.

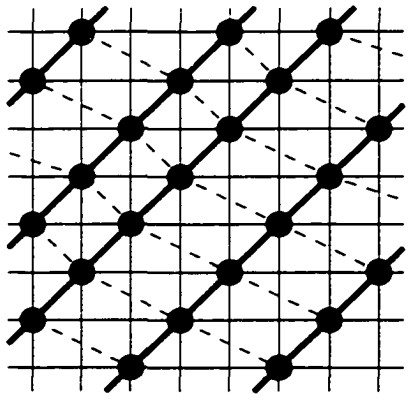


FIGURE 5.1. A typical example of a piece of one of the "+" regions. The thicker lines are the "stripes" of occupied sites. The dotted lines are inserted to show the squares and parallelograms.

One will note that on each of these "+" and "−" regions, the problem essentially

becomes one-dimensional, since we are now only concerned with the spacing between these "stripes" of occupied sites (see figure 5.1). It is tempting to try to apply a procedure to each region, similar to that of Lemberger for the one-dimensional case, in order to determine the cheapest stripe arrangement. However, there are two difficulties that arise. First there is the problem of the shape of these regions. Their boundaries may be very irregular whereas an extension of Lemberger's method would require applying periodic boundary conditions to a fairly regular shape such as a square or rectangle. Second there is a density constraint. Even if we could say something about the configuration in each + and − region, this would not take into account the ions lying outside these regions, so we effectively lose track of the original ion density. We must therefore find more regular regions to work with that allow us to keep track of the original density.

The first step in overcoming these difficulties is to partition the lattice into diamonds containing 8 sites, as shown in figure 5.4. If one of these diamonds intersects a 3×3 block not shown in 5.2, or it contains a type A ion, it may be associated with an increase in energy through order eight. We call such diamonds "bad." Each of the remaining "good" diamonds is contained in one of the + or − regions mentioned above. In a + region (− region), we group the diamonds into $-45°$ strips ($+45°$ strips) in such a way that the strips are bounded on each of the short sides by a bad diamond. This is shown in figure 5.7.

If we were to apply periodic boundary conditions to a particular strip and compare the resulting energy with that of the contribution of the strip to $H(S)$, it would seem that this difference would be proportional to the size of the boundary of the strip. However, consider one of the $45°$ strips of − diamonds. Inside the strip, the configuration is constant on lines of slope -1. These stripes persist through the long sides of the strip, and continue in S until they encounter a bad diamond. By definition, the short sides of the strip are also sides of bad diamonds. This allows us to show that the difference between the contribution of the strip to $H(S)$ and the

energy of the strip with periodic boundary conditions is $O(\Gamma)$, where Γ is the number of bad diamonds.

We then glue all the strips of good diamonds together with the bad diamonds, end to end, to form one long thin strip. We apply periodic boundary conditions to the configuration on this strip, call it S_1. Starting from S_1, we construct a sequence of configurations by rearranging the ions in S_1, in order to obtain a configuration S_K, having no bad 3×3 blocks and no type A ions. All of this is done in such a way as to give $|H(S_1) - H(S_K)| \leq c\Gamma U^{-9}$. We may then conclude that $H(S) \geq c\Gamma U^{-7} + H(S_K)$. Now starting with S_K, we use Lemberger's method [6] to construct another finite sequence of configurations with $H(S_i) \geq H(S_{i+1})$. Then with S^* being the last member of this sequence, we have $H(S) \geq c\Gamma U^{-7} + H(S^*)$. We will see that S^* does not depend on S. If we restrict S^* to any horizontal or vertical line we retrieve the one-dimensional ground state with density that of S^*. If we construct a configuration on our original lattice with this property, call it S^*_Λ, we find that $\Gamma = 0$ and $H(S^*_\Lambda) = H(S^*)$, showing that S^*_Λ is a ground state.

Proof of Theorem 5.1: With $H = \sum_{even\ m \geq 2} U^{1-m} h_m$, we define $H_m = U^{1-m} h_m$. Let M be the number of 3×3 blocks in a configuration S which are not a reflection or rotation of one of those shown in figure 5.2. In appendix B.1 we show that

$$\alpha M U^{-3} \leq H_2(S) + H_4(S) + U^{-3} L^2 (a + b\rho) \leq \beta M U^{-1}, \tag{5.1}$$

where $\alpha > 0$, $\beta > 0$, a, and b are constants. So we see that every 3×3 block which is not shown in figure 5.2 contributes a positive amount of energy at order at most 4, and the configurations in which every 3×3 block is one of those in figure 5.2 have zero energy through fourth order. The following lemma gives us a geometric interpretation of a configuration in which every 3×3 block is one of those shown in figure 5.2.

Lemma 5.1. (Watson) *Let S be a configuration where every 3×3 block is one of those shown in figure 5.2. Then there exists a tiling by squares and parallelograms as*

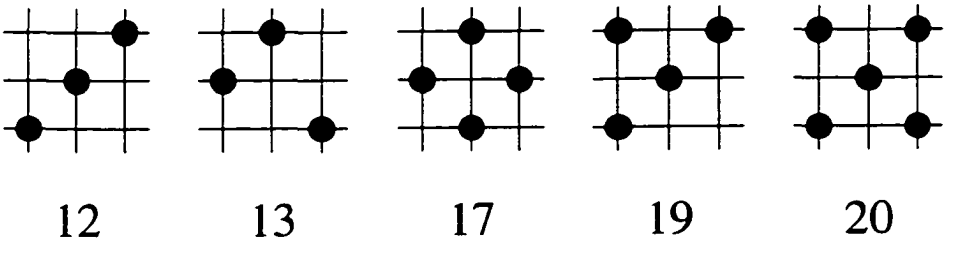


FIGURE 5.2. Configurations which minimize the energy locally.

shown in figure 5.3, in which every vertex corresponds to an ion in S.

Proof: Let S be a configuration satisfying the hypothesis of the lemma. Consider any occupied site. It is the center of a type 12, 19, or 20 block. By inspection, one may now work outwards and determine the allowable local ion arrangements. These turn out to be rotations and reflections of the three arrangements in figure 5.3. □

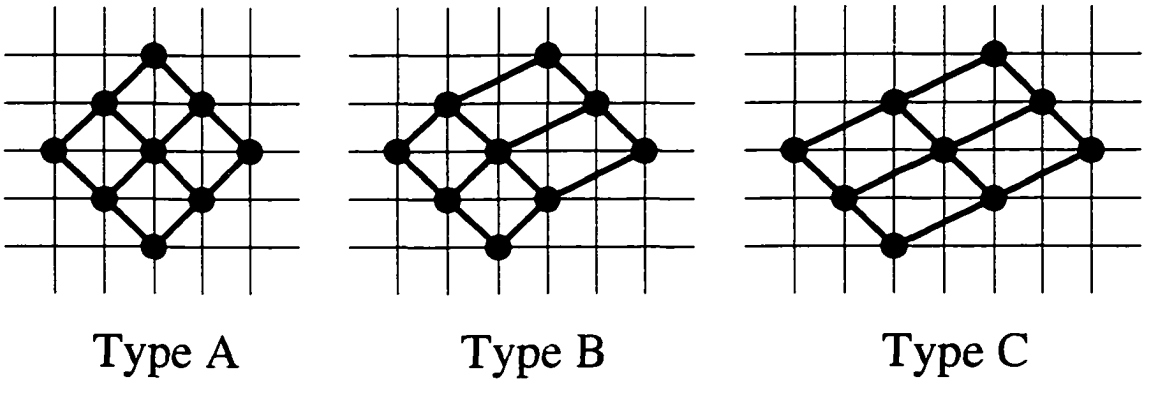


FIGURE 5.3. Possible local ion arrangements for a configuration in which every 3×3 block is one of those in figure 5.2.

From the lemma and equation 5.1, we see that the configurations which minimize the energy through fourth order correspond to tilings by squares and parallelograms. However, the densities one can obtain from such tilings is restricted. A configuration in which every ion is type C has density 1/3. One in which every ion is type A has density 1/2. We may construct a configuration having any rational density between 1/3 and 1/2 by placing an interface of slope ± 1 between a region of type A ions and a region of type C ions, the size of each region being chosen to give the desired

density. The ions on the interface will then be type B. So we see that from these square-parallelogram tilings, one may obtain any rational density in $[1/3, 1/2]$.

If S is such a tiling, we would like to write $H_6(S) + H_8(S)$ in terms of n_A, n_B, and n_C, the number of type A, B, and C ions respectively. Suppose X is a subset of $I(S)$. Recall that if X is to give a non zero contribution to $H_6(S) + H_8(S)$, it must be a set of ions contained in a closed nearest neighbor walk of eight steps. So there must be at least one ion $x \in I(S)$ with the property that for every $y \in X$, x and y are vertices of the same tile. In other words, X is a subset of the "local arrangement" about x. There may be more than one such x. For example, if X consists of a single ion, X will be contained in 9 local arrangements. To compensate for this over counting, we define $\tilde{c}_{m,X} = \frac{c_{m,X}}{\kappa(X)}$ where $\kappa(X)$ is the number of ions whose local arrangement contains X. We may now define, for even $m \leq 8$,

$$e_m^A = \sum_{X \subseteq type\ A} \tilde{c}_{m,X} .$$

where "$X \subseteq$ *type A*" means that X is a subset of the local arrangement about a type A ion. e_m^A is then the energy of a type A ion at order m. e_m^B and e_m^C are defined similarly. So if $H_m(S)$ is the energy of S at order m, we may write for even $m \leq 8$,

$$H_m(S) = L^{1-m}(n_A e_m^A + n_B e_m^B + n_C e_m^C) . \tag{5.2}$$

In such a tiling, the numbers n_A, n_B, and n_C are not independent. Since the area $= L^2$, we have

$$2n_A + \frac{5}{2}n_B + 3n_C = L^2 . \tag{5.3}$$

We are also keeping the number of ions fixed at ρL^2, so

$$n_A + n_B + n_C = \rho L^2 . \tag{5.4}$$

The energies in 5.2 for orders 6 and 8 are

$$e_6^A = -3200, \qquad e_8^A = 98000, \qquad e_6^B = -1520, \qquad e_8^B = 33600,$$
$$e_6^C = 160, \qquad e_8^C = -15120.$$

These numbers are calculated in appendix B.2. Using 5.3 and 5.4 to solve for n_B and n_C in terms of n_A, we have

$$H_6(S) + H_8(S) - L^2 f(U, \rho) = 15680U^{-7} n_A .$$

Recall that S was assumed to be a tiling. In general, this will not be the case. Suppose S is not a tiling and M is the number of 3×3 blocks which are not rotations or reflections of those in figure 5.2. Then the number of sites in the region where S is not a tiling is at most $9M$. So the terms intersecting this region contribute at most $O(U^{-5})M$ to $H_6 + H_8$. Equations 5.3 and 5.4 will no longer hold, but the difference between the right and left hand sides will be bounded by a constant times M. Thus for a general S, we may write

$$H_6(S) + H_8(S) - L^2 f(U, \rho) = 15680U^{-7} n_A + O(U^{-5})M . \tag{5.5}$$

We may now determine the ground states through order 8. From inequality 5.1 we see that any configuration with $M = 0$ will minimize the energy through fourth order. In equation 5.5 M appears at order 6. So for large enough U we want $M = 0$. Since the coefficient of n_A is positive in equation 5.5, we also want $n_A = 0$. So the configurations which minimize the energy through order 8 are those where every ion is type B or C. These configurations correspond to square-parallelogram tilings with no adjacent $\pm 45°$ strips of squares. They have zero energy through order 8. Any other configuration will have "bad" 3×3 blocks or type A ions which increase the energy. The point is that there exists a positive constant c so that this energy increase may be bounded from below by cU^{-7} times the number of these "local defects" in the configuration. We now move on to the higher order terms.

Recall that $\rho = p/q \in [1/3, 2/5]$ where p and q are relatively prime, and the lattice Λ is $L \times L$ where L is a multiple of $4q$. We partition Λ into diamonds containing 8 sites. This is shown in figure 5.4.

We define a diamond b to be *bad* if it contains a type A ion or intersects a bad 3×3 block. Otherwise, b is *good*. We let Γ denote the number of bad diamonds. The

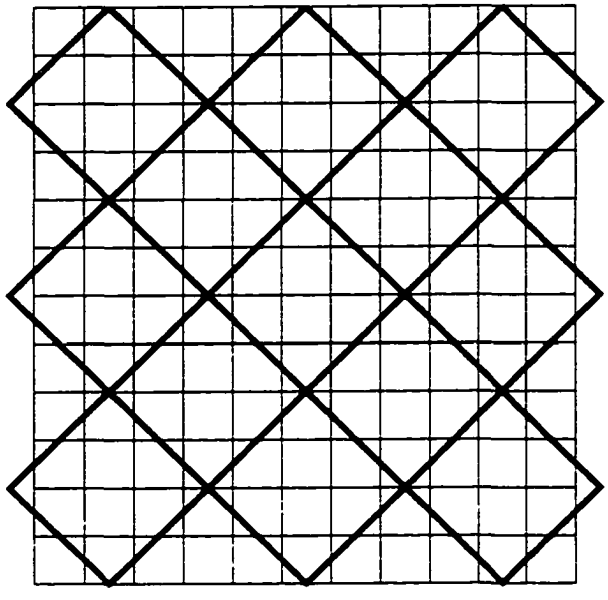


FIGURE 5.4. Partitioning of the lattice into diamonds containing 8 sites.

idea is this. A *good* diamond is one which is contained in a region of the configuration corresponding to a square-parallelogram tiling with no type A ions. We know from the above that the energy through order 8 is bounded below by a term proportional to the number of bad 3×3 blocks plus the number of type A ions, which is proportional to Γ. So through order 8, inequality 5.1 and equation 5.5 tell us that

$$\sum_{\text{even } n=2}^{8} H_n + U^{-3}L^2(a+b\rho) - L^2 f(U,\rho) \geq c\Gamma U^{-7}, \tag{5.6}$$

where $c > 0$ is a constant. For future convenience, we define $\tilde{H} = H + U^{-3}L^2(a + b\rho) - L^2 f(U,\rho)$.

Let S be a configuration with density $\rho(S) \in [\frac{1}{3}, \frac{2}{5}]$. We label a parallelogram in S with a $+$ if its short ends have slope $+1$, and a $-$ if its short ends have slope -1. Now, every good diamond must contain a type B or C ion, both of which are the vertex of a parallelogram. Any other parallelogram intersecting this diamond must have the same sign. We may thus carry our labelling over to the good diamonds themselves.

Consider a 45° strip of good diamonds. Suppose one diamond in this strip is $+$.

Then, as shown in figure 5.5, the + parallelogram in this diamond must propagate throughout the strip, causing all the diamonds to be +. This shows that the diamonds in a 45° strip may not change sign without containing a bad diamond. The same is true for a −45° strip.

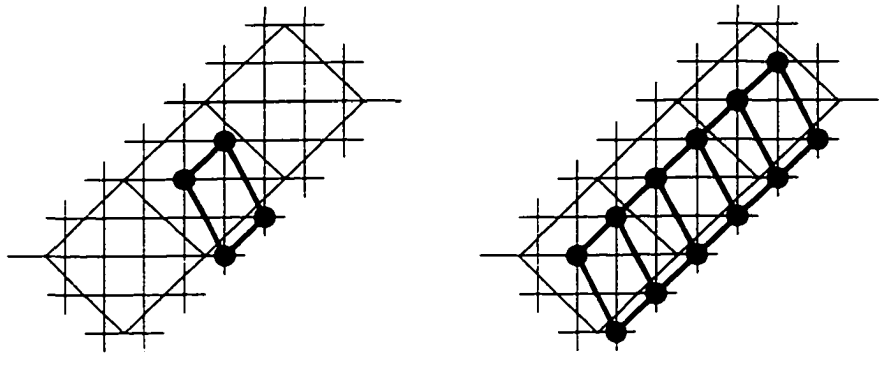


FIGURE 5.5. Left: a strip of slope +1 nearest neighbor diamonds, the middle one being +. Right: If all the diamonds in the strip are good, they must all be +.

One may think of S as being divided into regions where the diamonds are +, regions where the diamonds are −, and regions of bad diamonds. From the above, we see that a + region and a − region must be separated by a region of bad diamonds. In each good region, S is constant along lines of slope ± 1. We call this the *stripe* property. Indeed, inside every + (−) region, S is constant on lines of slope +1 (−1). More, however, may be said about the arrangement of the occupied stripes inside each good region. Since every ion must be type B or C, each pair of occupied stripes must be separated by one or two unoccupied stripes. Also, since there are no type A ions, we may not have consecutive stripes corresponding to the following occupation sequence: occupied, unoccupied, occupied, unoccupied, occupied. This rules out the checkerboard configuration, the sign of which is ambiguous. When a region has the stripe property with no type A ions, we say that the stripes are *correctly spaced*.

We now divide up the − regions into 45° strips as follows. Choose any good diamond whose sign is −. As shown in figure 5.6, we extend this set in the directions $\pm(1,1)$ until we hit a bad diamond. Every diamond in this 45° strip is good, and,

since one of them is $-$, they must all be $-$. We may then carry our labelling one step further and label this strip with a $-$. After doing this for every good $-$ diamond, we see that every $-$ diamond is contained in exactly one such $-$ strip. By changing all

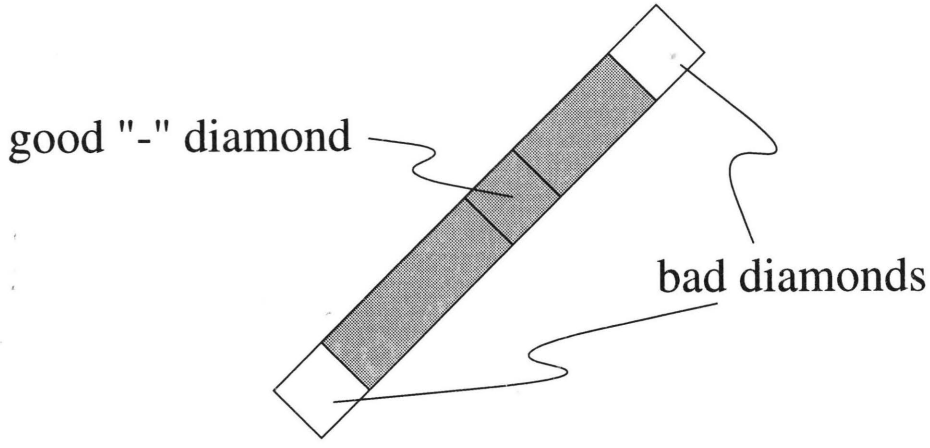


FIGURE 5.6. A good "$-$" diamond is chosen. The sites in the shaded region are contained in good "$-$" diamonds.

the signs in this construction, we end up with $-45°$ strips of good $+$ diamonds. We label these strips with a $+$. See figure 5.7

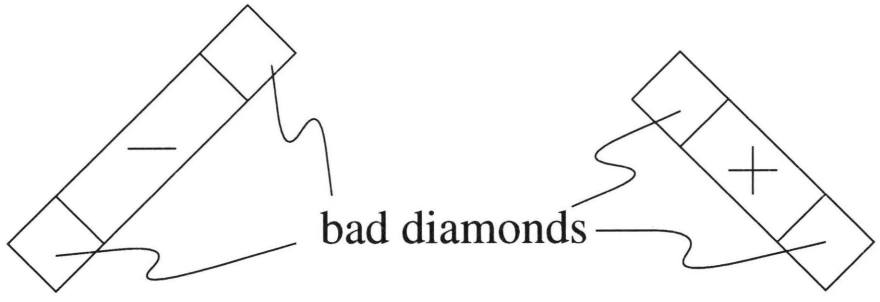


FIGURE 5.7. Left: a $-$ strip. Right: a $+$ strip. The configuration inside the $-$ strip ($+$ strip) is constant along lines of slope -1 ($+1$).

Let us now take these strips and glue them together, end to end, to form one long thin strip. Of course the orientation of the $+$ and $-$ strips is different in S, but we can simply rotate say the $-$ strips to line up with the $+$ strips. Now glue the bad diamonds onto one end to form an even longer strip. This is shown in figure 5.8. In

the region of this strip which contains the bad diamond, the configuration may not satisfy the stripe property. However, in the statement of the theorem L was assumed to be a multiple of $4q$. Thus the total number of ions is a multiple of $4p$. There are an even number of ions in each $+$ and $-$ strip, so there must be an even number of ions in the bad region of our thin strip. Therefore we may rearrange the configuration in this portion of the strip so that it satisfies the stripe property. We now glue the short ends together and the long ends together to form a torus, call it T. Let S_1 denote the resulting configuration on T. We want to bound $|\tilde{H}(S) - \tilde{H}(S_1)|$. As we shall see, we will only need to estimate this difference at orders ≥ 10.

FIGURE 5.8. The thin strip obtained by gluing together the $+$ and $-$ strips as well as the bad diamonds.

We define the contribution of a walk to H by

$$w(\gamma) = \frac{(-1)^{m(S,\gamma)}}{|\gamma|}(2U)^{1-|\gamma|}\binom{|\gamma|-2}{m(S,\gamma)-1}.$$

It then follows from equation 2.10 that

$$H = \sum_{\gamma} w(\gamma).$$

Consider a closed nearest neighbor walk γ_1 in S_1 with N steps. Suppose $\gamma_1(0)$ is a site in the "good" region of S_1 and it does not cross one of the cuts where the $+$ and $-$ strips were glued together. Then we may associate γ_1 in a natural way with a walk γ in S. This correspondence is shown in figure 5.9. Recall that the stripes in the good strips in S will persist until a bad diamond is encountered. So $w(\gamma_1) = w(\gamma)$ unless there is a bad diamond in S which is relatively close to γ. In appendix B.3 we show that if $w(\gamma_1) \neq w(\gamma)$ then there must be a bad diamond within ℓ_1 distance $|\gamma| = N$ of some site in $supp(\gamma)$.

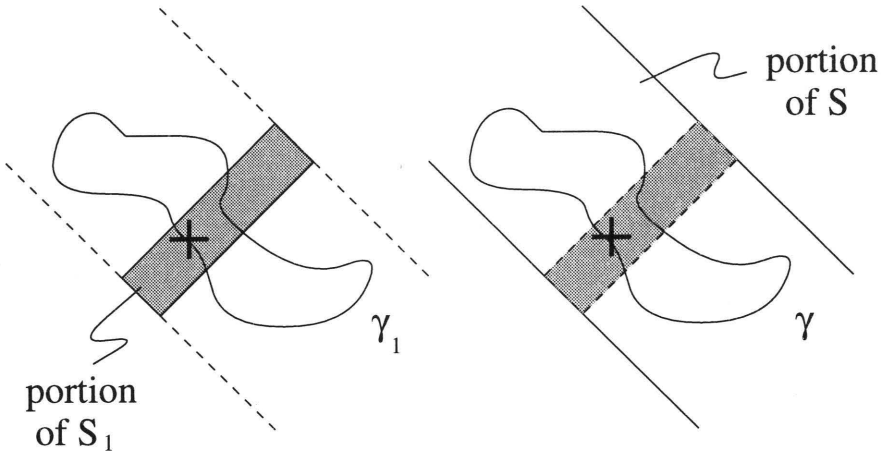


FIGURE 5.9. The shaded regions correspond to the original strip of good diamonds. Left: the portion of S_1 has been "unraveled" for clarity. Right: the corresponding portion of S. The "+" marks the origin of the walk.

In the remainder of this chapter, "c" will denote a constant independent of U and L. Let C_N denote the set of all closed nearest neighbor walks in S_1 with N steps such that $\gamma_1 \in C_N \Leftrightarrow \gamma_1(0)$ is a site in the "good" region of S_1 and it does not cross one of the cuts where the + and − strips were glued together. Since $|w(\gamma)| \leq U^{1-|\gamma|}2^{|\gamma|}$ the above implies that

$$\sum_{\gamma_1 \in C_N} |w(\gamma_1) - w(\gamma)| \leq U^{1-N} c^N N^2 \Gamma\,, \tag{5.7}$$

where γ is the walk in S corresponding to γ_1 as shown in figure 5.9. If a walk of length N in S_1 is not a member of C_N, it must cross one of the cuts where the strips were glued together, or enter a bad diamond. Now, if it crosses a cut, it must hit one of the four sites adjacent to the cut. Each cut may be associated with a bad diamond. There are at most 12Γ sites in S_1 which are adjacent to a cut or contained in a bad diamond. Thus the walks of length N in S_1 which are not in C_N contribute at most $U^{1-N}c^N\Gamma$ to $|\tilde{H}(S) - \tilde{H}(S_1)|$. Combining this result with inequality 5.7 we see that at order N,

$$\left|\tilde{H}_N(S) - \tilde{H}_N(S_1)\right| \leq U^{1-N} c^N N^2 \Gamma\,. \tag{5.8}$$

Note that although S_1 satisfies the stripe property, its stripes may not be correctly spaced. The idea now is to form a finite sequence of configurations, $\{S_i\}_{i=1}^{K}$, with

$$\left|\tilde{H}_N(S_{i+1}) - \tilde{H}_N(S_i)\right| \leq U^{1-N}c^N ,$$

$K = O(\Gamma)$, and the stripes in S_K being correctly spaced. The strategy is this. The reason why the stripes in S_1 may not be correctly spaced is because of the introduction of the bad diamonds, as well as the cuts. There are $O(\Gamma)$ stripes in the bad region of S_1 and $O(\Gamma)$ cuts, so we may hope to make $O(\Gamma)$ modifications, each modification costing at most $U^{1-N}c^N$ at order N.

The key then lies in how we make these modifications. We must be sure that each one fixes an "fault" in S_i without creating a similar fault. All the modifications follow the same basic procedure. We illustrate this by considering a pair of adjacent occupied stripes in S_1. Since the density of S_1 is $\leq 2/5$, if there is a pair of adjacent occupied stripes, there must be a pair of adjacent unoccupied stripes. This is shown in figure 5.10 where W is the portion of the strip between the markers. With the

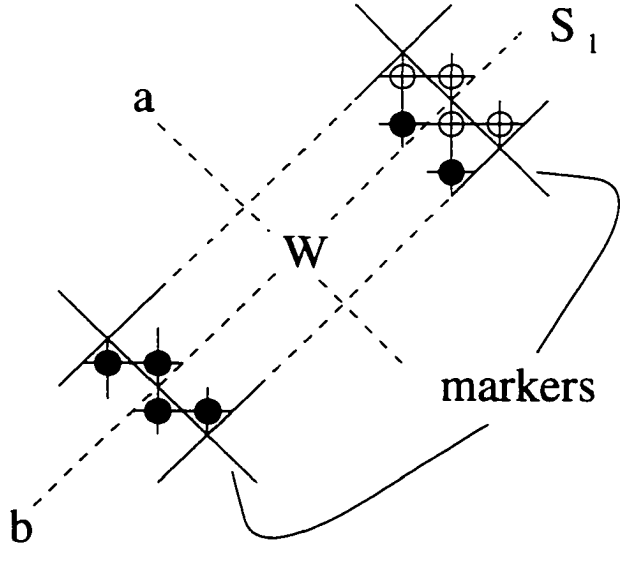


FIGURE 5.10. W is rotated about axis a and, if necessary, axis b.

two axis of rotation a and b as shown in figure 5.10, we form W^{-1} by rotating W

about the axis a. We then replace W by W^{-1} and, if necessary, rotate W^{-1} about the axis b so it fits into place. This is shown in figure 5.11. S_2 is then the modified configuration. Any walk which gives a non zero contribution to $\tilde{H}_N(S_2) - \tilde{H}_N(S_1)$ must cross one of the markers, and so must visit one of the 8 sites adjacent to the markers. So we have that $\left|\tilde{H}_N(S_2) - \tilde{H}_N(S_1)\right| \leq U^{1-N}c^N$.

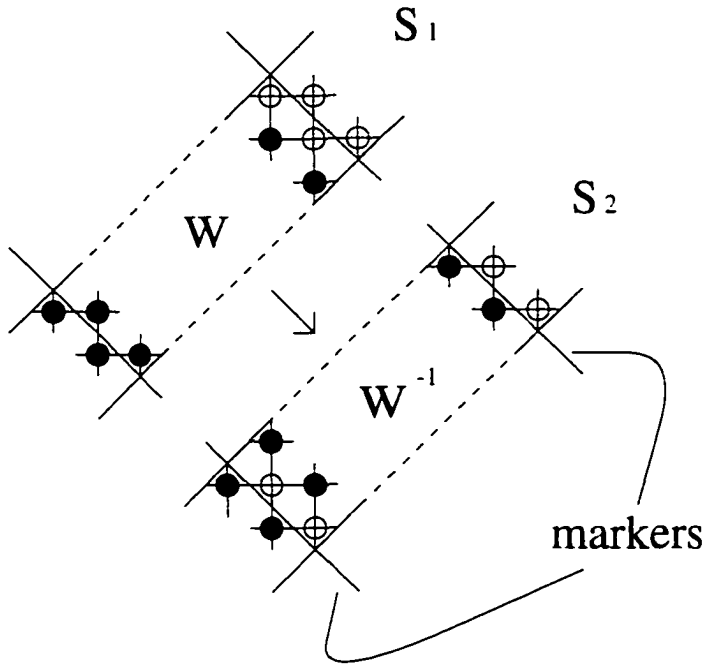


FIGURE 5.11. Separating a pair of neighboring occupied stripes.

Our modification has allowed us to separate a neighboring pair of occupied stripes without creating a new pair, all at an affordable cost. So we see that we can get rid of all such pairs with $O(\Gamma)$ modifications.

The next problem we focus on is the possibility of more than two consecutive unoccupied stripes. If this occurs, since the density is $\geq 1/3$ there must be at least one pair of occupied stripes separated by a single unoccupied stripe. Figure 5.12 shows how, in a similar manner as above, we may reduce the number of adjacent unoccupied stripes by one.

Since we could have at most $O(\Gamma)$ of these problems to start with, we can get rid of

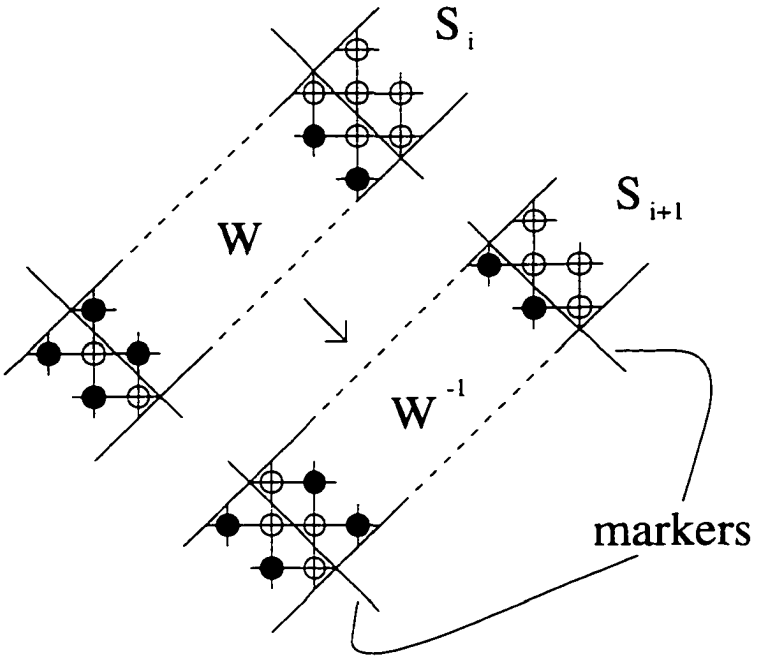


FIGURE 5.12. Reducing the number of consecutive unoccupied stripes.

all of them with $O(\Gamma)$ modifications. So after $O(\Gamma)$ modifications, we are to the point where every pair of occupied stripes is separated by one or two unoccupied stripes. We now face the possibility of our configuration containing type A ions. These ions could have come from S_1 or they could have been formed by the modifications above. But we only made $O(\Gamma)$ modifications, and S_1 contained at most $O(\Gamma)$ type A ions. So our configuration can contain at most $O(\Gamma)$ type A ions. We let a "1" denote an occupied stripe and a "0" denote an unoccupied stripe. The stripe sequence signifying a type A ion is then: 1, 0, 1, 0, 1. If this occurs, since the density is $\leq 2/5$ there must exist the following stripe sequence: 1, 0, 0, 1, 0, 0, 1. In figure 5.13 we see how the same procedure used above can get rid of these type A ions.

At first glance, it may seem that this last modification, although removing a type A ion at the left of W in S_1, may have created a type A ion at the right end of W^{-1} in S_{i+1}. However, if we do get a type A ion in S_{i+1} after the inversion of W, it must have been there before the inversion, in S_i. Thus the number of type A ions really is

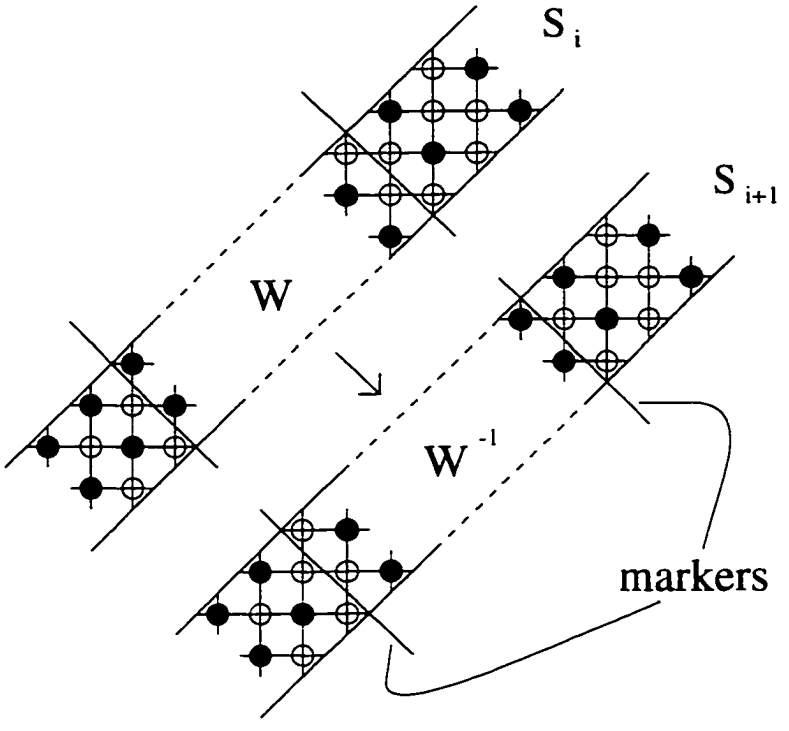


FIGURE 5.13. Removing the type A ions.

reduced.

We end up with the configuration S_K whose stripes are correctly spaced. Furthermore, $K = O(\Gamma)$ and $\left|\tilde{H}_N(S_{i+1}) - \tilde{H}_N(S_i)\right| \leq U^{1-N}c^N$ for each consecutive pair in our sequence. This gives us the following telescoping sum

$$\tilde{H}(S) - \tilde{H}(S_K) = \left[\tilde{H}(S) - \tilde{H}(S_1)\right] + \sum_{i=1}^{K-1}\left[\tilde{H}(S_i) - \tilde{H}(S_{i+1})\right]. \tag{5.9}$$

By the way our sequence of configurations was constructed above, and recalling inequality 5.8, we see that for $N \geq 10$

$$\sum_{n \text{ even} \geq 10} \left|\tilde{H}_n(S) - \tilde{H}_n(S_K)\right| \leq \Gamma \sum_{n \text{ even} \geq 10} U^{1-n}c^n n^2 \leq c\Gamma U^{-9}. \tag{5.10}$$

Since S_K satisfies the stripe property and its stripes are correctly spaced, we know that $\sum_{\text{even}}^{8} \tilde{H}_n(S_K) = 0$. So recalling inequality 5.6 and using inequality 5.10 for the

higher order terms, from inequality 5.9 we have

$$\tilde{H}(S) \geq \tilde{H}(S_K) + \alpha\Gamma U^{-7} - c\Gamma U^{-9}. \tag{5.11}$$

Consider the torus, T, on which S_K lives. We claim that among all configurations on this torus having density $\rho(S)$ and satisfying the stripe property, there is, up to lattice symmetries, a unique such configuration with minimal energy for large enough U. To show this, we use a method due to Lemberger, which he used to find the one-dimensional large U ground states.

Let us briefly summarize Lemberger's method for determining these ground states. These configurations turn out to be the "most homogeneous" in the sense that the ions are spaced as far apart as possible on all length scales. We then show how his ideas easily adapt to 2-d configurations having the stripe property. We will use σ to represent a 1-d configuration.

Let x and y be two sites on the 1-d lattice. The shortest closed nearest neighbor walks which visit both of these sites visit x and y exactly once, and hit every site between x and y exactly twice. So any ion between x and y increases $m(\sigma, \gamma)$ by 2. Thus $m(\sigma, \gamma)$ is even when x and y are both occupied or unoccupied, and it is odd when exactly one of x or y is occupied. Since $m(\sigma, \gamma)$ determines the sign of $w(\gamma)$ in $H(\sigma)$, it plays a key role in the following discussion.

With this in mind, consider a 1-d configuration, σ_1. For the sake of clarity, let us assume that the density of σ_1 is 2/5. As before, this guarantees us that if σ_1 contains a nearest neighbor pair of occupied sites, it must also contain a nearest neighbor pair of unoccupied sites. This situation is shown in figure 5.14 where W is the part of σ_1 between the markers. W^{-1} is defined as before. If a walk is to make a non-zero contribution to the difference $H(\sigma_2) - H(\sigma_1)$, it must cross a marker. The shortest such walks are those with two steps, going back and forth between the sites adjacent to the markers. In σ_1, the sites these walks hit are both occupied or both unoccupied, so their contribution to $H(\sigma_1)$ is 0. In σ_2, these walks go back and forth between an

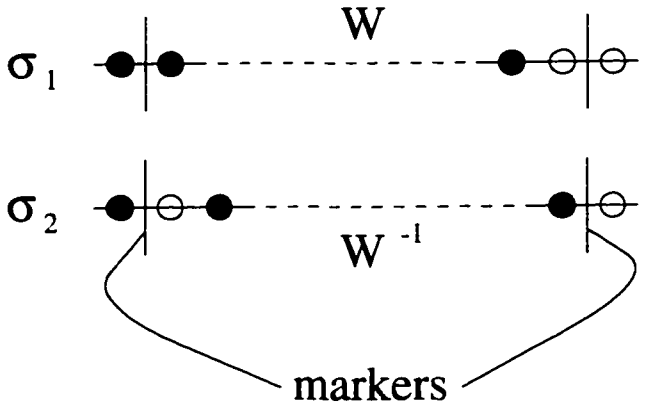


FIGURE 5.14. Separating nearest neighbor ions.

occupied and unoccupied site. So $m(\sigma_2, \gamma)$ is odd for both these walks, making their contribution to $H(\sigma_2)$ negative. Thus at leading order, $H(\sigma_2) - H(\sigma_1)$ is negative, so for large U this modification has decreased the energy.

We see that we can get rid of all the nearest neighbor pairs of ions, while reducing the energy at each step. Next we consider the situation where σ_i contains more than two consecutive unoccupied sites. Since the density is 2/5, there must be an unoccupied site with occupied nearest neighbors. The method here is a generalization of that above. σ_i is shown in figure 5.15, where we see that another pair of markers has been introduced. W is that part of σ_i between the longer markers. The set of sites between the shorter markers is denoted by J. In this case, the contribution of a walk will cancel if its support lies entirely in either the complement of J, or the set of sites in W. In other words, a walk can give a non-zero contribution to $H(\sigma_{i+1}) - H(\sigma_i)$ only if it crosses a short marker and a long marker. The shortest such walks are easily seen to be those with four steps, whose center site is between a short and long marker. In σ_i, the end sites of these walks are either both occupied or both unoccupied, so their contribution to $H(\sigma_i)$ is non-negative. In σ_{i+1}, exactly one end site is occupied, so these walks make a negative contribution to $H(\sigma_{i+1})$. Thus at leading order, $H(\sigma_{i+1}) - H(\sigma_i)$ is negative.

In general, the number of sites between a short and long marker will vary. In figure

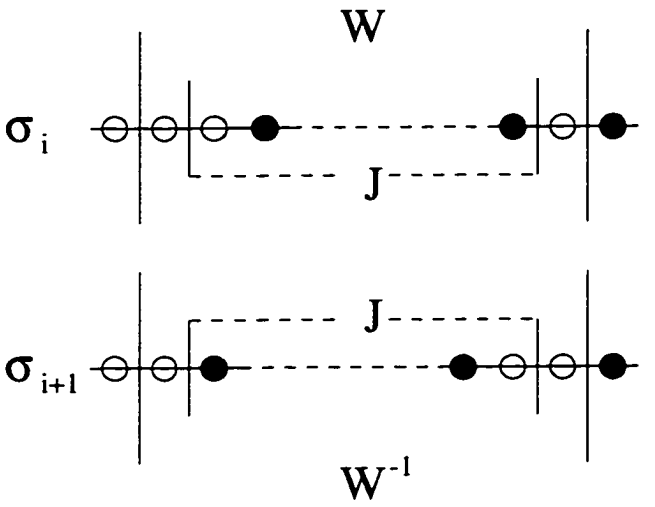


FIGURE 5.15. Reducing the number of consecutive unoccupied sites.

5.14, there are no such sites, while in figure 5.15 there is 1. The process, however, remains the same. In σ_i, both sites on either side of the region between a short and long marker will either be occupied or unoccupied, while in σ_{i+1}, exactly one will be occupied. This is the key to the energy decrease.

To summarize, we started with σ_1, an arbitrary configuration of density 2/5. We end up with a configuration σ_K of lower energy and equal density, where the gaps between consecutive ions consist of one or two unoccupied sites. For any fixed lattice size and density, it is easily demonstrated that if a configuration only has gaps of lengths d and $d+1$, the number of gaps of length d is unique, as well as those of length $d+1$. Furthermore, requiring that these numbers be ≥ 0 is enough to uniquely determine d. Lemberger calls such configurations *homogeneous*.

We must now concern ourselves with the ordering of these gaps. Lemberger handles this by associating each homogeneous configuration, σ, with a "rescaled" configuration, $F(\sigma)$. This new configuration is defined on a new lattice where the number of sites is equal to the number of ions in σ. Each ion in $F(\sigma)$ corresponds to a gap of one unoccupied site in σ, and each unoccupied site in $F(\sigma)$ corresponds to a gap of two unoccupied sites in σ. This is shown in figure 5.16. The above procedure may

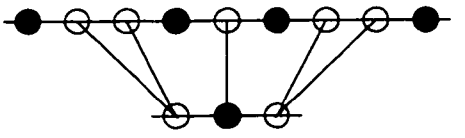


FIGURE 5.16. Top: a portion of a homogeneous configuration, σ. Bottom: corresponding portion of $F(\sigma)$.

now be performed starting from this new configuration, $\sigma'_1 \equiv F(\sigma_K)$. Of course the density may now be different, but we still end up with a homogeneous configuration in which every pair of consecutive ions is separated by a gap of d or $d+1$ unoccupied sites. We then re-scale as before, and begin the procedure again. After the n^{th} rescaling, we may use F^{-n} to map $\sigma_i^{(n)}$ back to a configuration of density $2/5$ on the original lattice. Lemberger showed by induction that $H(F^{-n}(\sigma_{i+1}^{(n)})) - H(F^{-n}(\sigma_i^{(n)}))$ is negative, demonstrating that the energy still decreases when the process is carried out over larger length scales. The induction hypothesis basically states that if we start with σ_i and σ_{i+1} as shown in figure 5.15, in the sense that the sites adjacent to the markers have the correct occupations to give us the energy decrease, then applying F^{-1} preserves this property. So after applying F^{-n} and ending up back on the original lattice, we may be certain that our "shortest walk" argument will hold.

As the process is continued, we eventually arrive at a configuration, σ^*, with the property that $F^n(\sigma^*)$ is homogeneous for all n. This configuration is called the *most homogeneous*, and is clearly the ground state. In our case where the density is $2/5$, σ^* corresponds to the configuration where the size of the gaps alternates between one and two. This is shown in figure 5.17. We note that the unit cell for the $\rho = 2/5$

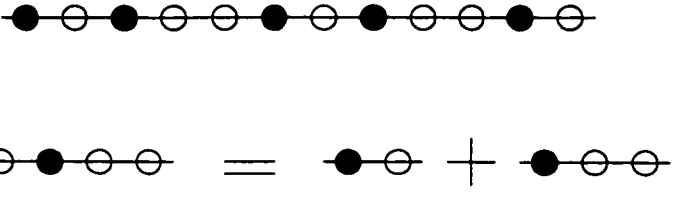


FIGURE 5.17. Top: a portion of σ^* for $\rho = 2/5$. Bottom: the unit cell for the $2/5$ ground state is the concatenation of the $1/2$ and $1/3$ unit cells.

ground state is simply just the concatenation of the unit cell for the $\rho = 1/2$ ground state with the unit cell for the $\rho = 1/3$ ground state.

Before returning to two dimensions, it should be noted that in each step of the above process, the number of sites between a short and a long marker never need exceed q, where the density is p/q with p and q relatively prime. Thus there is a constant c such that each step in the process reduces the energy as long as $U \geq c^q$. So in this proof, the necessary "largeness" of U depends on the density.

We now return to the 2-D case. Configurations which have the stripe property, such as S_K, naturally project onto a one-dimensional configuration, as shown in figure 5.18. Suppose γ is a closed nearest neighbor walk in the 2-D region shown in figure

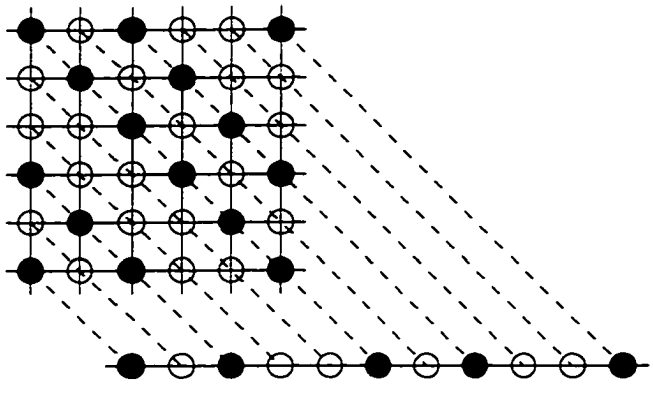


FIGURE 5.18. Projecting a two-dimensional "striped" region onto a one dimensional configuration.

5.18. We can identify $\gamma(i)$ with a site on the 1-d strip by simply following the dotted line. In this way we obtain a nearest neighbor walk, $\tilde{\gamma}$, on the 1-d configuration with the very nice property that $\gamma(i)$ is occupied if and only if $\tilde{\gamma}(i)$ is occupied. So if S is a 2-D configuration with the stripe property and σ its 1-d projection, for any γ in S we have that $m(S, \gamma) = m(\sigma, \tilde{\gamma})$. This equality is the main ingredient in adapting Lemberger's method for 1-d to the 2-D situation.

Figure 5.19 shows the 2-D analogue of the situation in figure 5.15. In S_i we wish to get rid of that portion of the strip with three consecutive unoccupied stripes. In

σ_i, the 1-d projection of S_i, this corresponds to getting rid of the three consecutive unoccupied sites. We proceed exactly as in the 1-d situation. We must check that

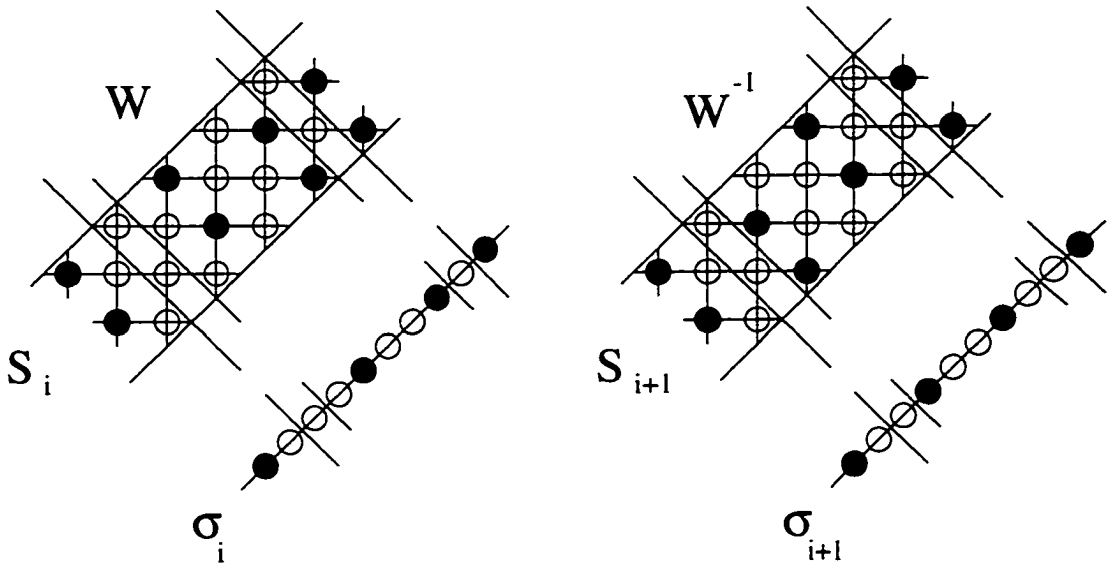


FIGURE 5.19. Lowering the energy by reducing the number of consecutive unoccupied stripes.

the "shortest walk" argument will give us $H(S_{i+1}) - H(S_i) \leq 0$. If a 2-D walk γ is to make a non-zero contribution to this difference, it must cross a short and a long marker, and so must its projected 1-d walk, $\tilde{\gamma}$. The shortest such 2-D walks project down to the shortest such 1-d walks, which we know will give the right values of m. But $m(S, \gamma) = m(\sigma, \tilde{\gamma})$, so for large enough U, $H(S_{i+1}) - H(S_i) \leq 0$.

So we may apply the Lemberger procedure to our strips starting from S_K. We will end up an energy minimizing configuration, S^*, having the same density as S_K, namely p/q. So from inequality 5.11, we may write

$$H(S) \geq H(S^*) + \alpha\Gamma U^{-7} - c\Gamma U^{-9}. \tag{5.12}$$

This equation will hold for any S with density ρ.

The stripe arrangement in S^* follows the Farey tree, just as the ion arrangement in the 1-d case. So S^* consists of a unit cell of length q, which is periodically extended to

cover the torus. Our original square lattice Λ has sides whose lengths are multiples of $4q$. So we may build the configuration S^*_Λ on Λ which has the same stripe arrangement as S^*, which will satisfy $H(S^*_\Lambda) = H(S^*)$. We may then rewrite inequality 5.12 as

$$H(S) \geq H(S^*_\Lambda) + \alpha\Gamma U^{-7} - c\Gamma U^{-9}. \tag{5.13}$$

If S does not satisfy the stripe property with the stripes correctly spaced, $\Gamma > 0$ so $H(S) > H(S^*_\Lambda)$. If S is such that $\Gamma = 0$, then we know from the Lemberger argument that $H(S) \geq H(S^*_\Lambda)$, with equality holding only when $S = S^*_\Lambda$. Thus for large enough U, S^*_Λ is the ground state. $\square$

Appendix A
PHASE SEPARATION

A.1 M-Potential

In the occupation variables, $H_2 + H_4 + H_6$ may be written as

$$H_2 + H_4 + H_6 = U^{-1}\Big[8 \sum_{<xy>:|x-y|=1} V_x V_y - 16 \sum_x V_x\Big]$$
$$+ U^{-3}\Big[64 \sum_{<xy>:|x-y|=\sqrt{2}} V_x V_y + 16 \sum_{<xy>:|x-y|=2} V_x V_y - 16 \sum_x V_x + \sum_{X \in E_4} c_{4,X} V_x\Big]$$
$$+ U^{-5}\Big[64 \sum_x V_x + 216 \sum_{<xy>:|x-y|=\sqrt{5}} V_x V_y + 24 \sum_{<xy>:|x-y|=3} V_x V_y + \sum_{X \in E_6} c_{6,X} V_x\Big],$$

where E_4 is the collection of sets X appearing at fourth order which contain a pair of sites x and y with $|x - y| = 1$, and E_6 is the collection of sets X appearing at sixth oder which contain a pair of sites x and y with $|x - y| \in \{1, \sqrt{2}, 2\}$. Note that the three terms involving $\sum_x$ contribute an amount which is proportional to the ion density. Since we are considering this density to be fixed, these terms may be dropped.

Let B be a 4×4 block of 16 sites. Define

$$H_B = U^{-1}\frac{2}{3} \sum_{\substack{<xy>\subset B: \\ |x-y|=1}} V_x V_y$$
$$+ U^{-3}\Big[\frac{64}{9} \sum_{\substack{<xy>\subset B: \\ |x-y|=\sqrt{2}}} V_x V_y + 2 \sum_{\substack{<xy>\subset B: \\ |x-y|=2}} V_x V_y + \sum_{\substack{X \subset B: \\ X \in E_4}} \frac{c_{4,X}}{\tau_X} V_X\Big]$$
$$+ U^{-5}\Big[36 \sum_{\substack{<xy>\subset B: \\ |x-y|=\sqrt{5}}} V_x V_y + 6 \sum_{\substack{<xy>\subset B: \\ |x-y|=3}} V_x V_y + \sum_{\substack{X \subset B: \\ X \in E_6}} \frac{c_{6,X}}{\tau_X} V_X\Big],$$

where τ_X is the number of translates of X which are contained in B. Note that if $X \in E_4$ with $V_X \neq 0$, then there is a pair of sites x, y in X with $|x - y| = 1$ and

$V_x V_y = 1$. This gives a contribution of $\frac{2}{3}U^{-1}$ to H_B which is much larger than the order U^{-3} contribution from $\frac{c_{4,X}}{\tau_X}$. If $X \in E_6$ with $V_X \neq 0$, then there is a pair of sites x, y in X with $|x-y| \in \{1, \sqrt{2}, 2\}$ and $V_x V_y = 1$. This gives a positive contribution at order 2 or 4 which is much larger than the order U^{-5} contribution from $\frac{c_{6,X}}{\tau_X}$. Figure A.1 shows, up to rotations and reflections, all possible ion arrangements in a 4×4 block with no two ions separated by 1, $\sqrt{2}$, or 2.

Now, H_B was defined so that

$$\sum_B H_B = H_2 + H_4 + H_6 . \tag{A.1}$$

The idea is to find a function, K_B, defined on a 4×4 block so that $\sum_B K_B$ is proportional to the density, and $H_B + U^{-5} K_B$ is minimized by configurations 6, 8, 16, 20, 25, and 27 in figure A.1. The difference between $\sum_B (H_B + U^{-5} K_B)$ and $H_2 + H_4 + H_6$ will then be proportional to the density. Furthermore, if a configuration exists with the property that every 4×4 block is one of 6, 8, 16, 20, 25, or 27 from figure A.1, then it minimizes $H_2 + H_4 + H_6$.

Let S_B be configuration on a 4×4 block B. Consider the set of configurations obtained by rotating and reflecting configuration 1 in figure A.2. There are four elements in this set, say S_1^1, S_2^1, S_3^1 and S_4^1. Define

$$k_B^1(S_B) = \sum_j 1(I(S_j^1) \subseteq I(S_B)) .$$

where $1(I(S_j^1) \subseteq I(S_B))$ is the indicator function. In general, if $\{S_j^i\}$ is the set of configurations obtained by rotating and reflecting configuration i in figure A.2, we define

$$k_B^i(S_B) = \sum_j 1(I(S_j^i) \subseteq I(S_B)) .$$

Now let

$$K_B = 192 - 174k_B^1 - 78k_B^2 - 18k_B^3 - 24(k_B^4 - k_B^5) - 24(k_B^6 - k_B^7) - 18(k_B^8 - k_B^9) .$$

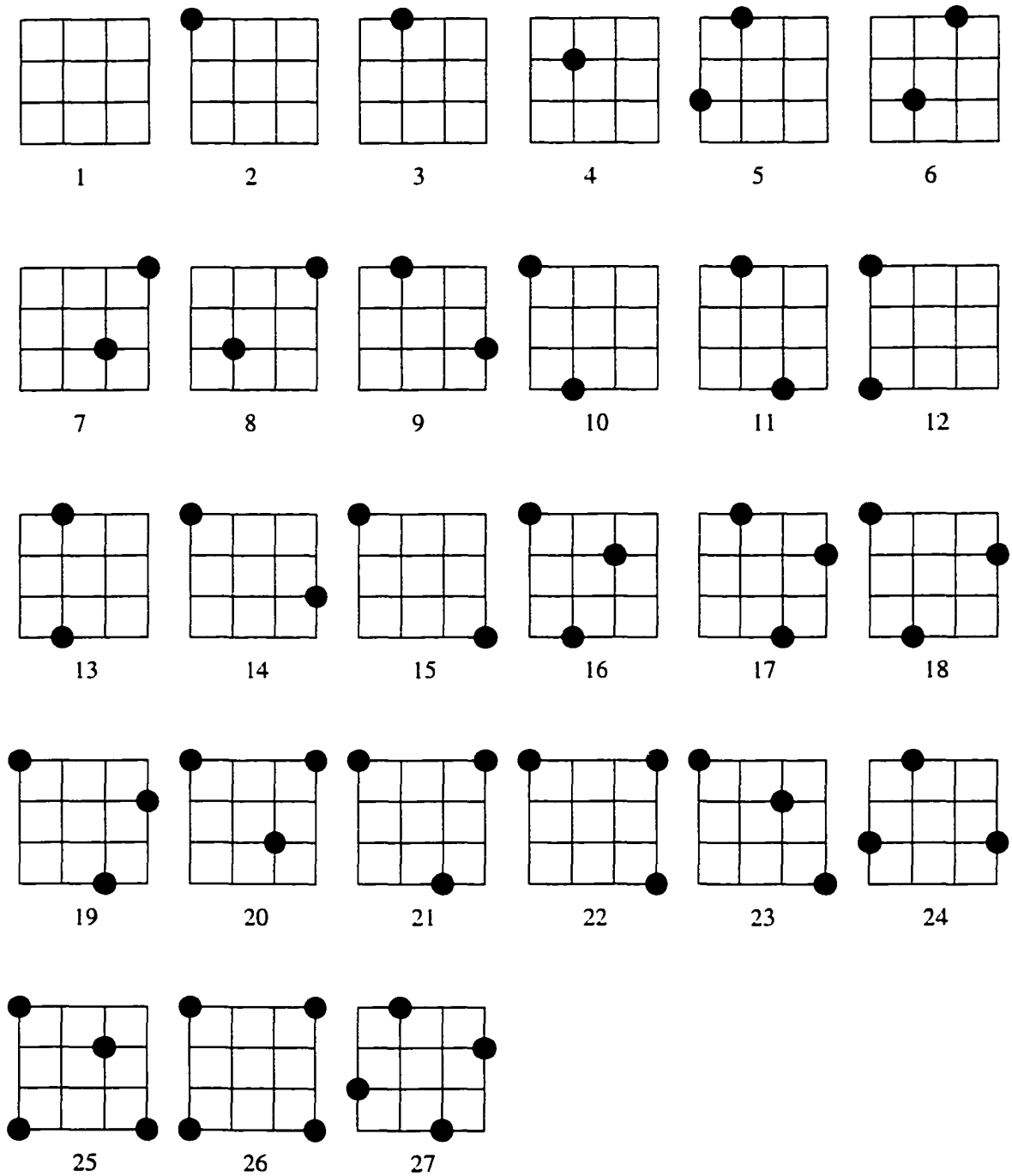


FIGURE A.1. All possible ion arrangements (up to lattice symmetries) in a 4×4 block of a configuration that minimizes $H_2 + H_4$.

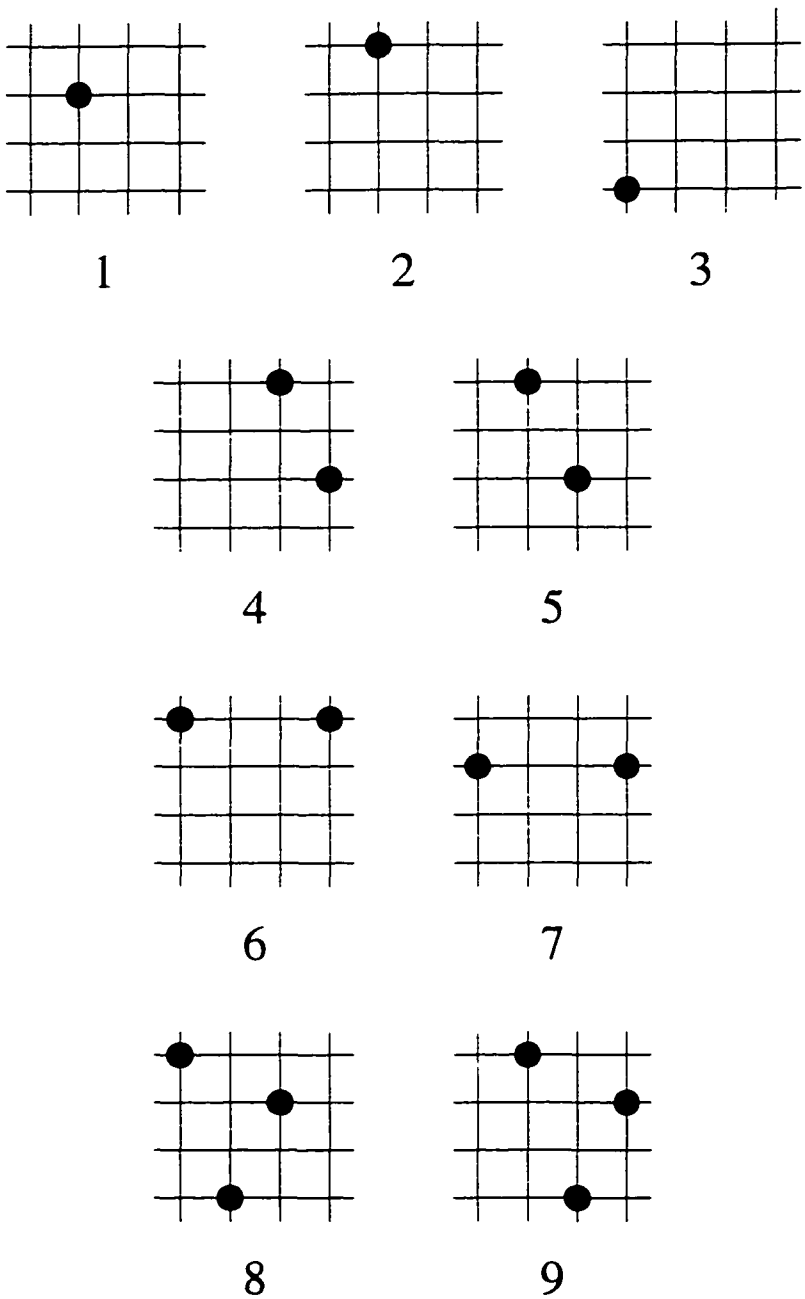


FIGURE A.2. Configurations in a 4×4 block used to define the m-potential.

Then $\sum_B K_B$ is a multiple of the density.

The function $H_B + U^{-5}K_B$ applied to blocks 6, 8, 16, 17, 20, 24, 25, and 27 in figure A.1 gives 0. The value on all the other blocks is $\geq 18U^{-5}$. Notice how block 17 contains a 3×3 sub-block having only one ion in a corner. This type of 3×3 sub-block does not appear in blocks 6, 8, 16, 20, 24, 25, or 27. The 4×4 block directly below block 17 cannot be another type 17 block, and because of this "bad" 3×3 sub-block, it cannot be a type 6, 8, 16, 20, 24, 25, or 27 block. So each type 17 block actually increases K_B.

Any block containing a pair of ions x, y with $|x - y| \in \{1, \sqrt{2}, 2\}$ makes a positive contribution at order 2 or 4. From above, we see that any other block which is not one of 6, 8, 16, 20, 24, 25, or 27 from figure A.1, contributes 0 at orders 2 and 4, but makes a positive contribution at order 6. This proves inequality 4.1.

A.2 Energies For Order 8

In a tiling of squares, parallelograms, and kites, there are only a few subsets $X \subset I(S)$ which contribute at order 8. They are shown, up to rotations and reflections, in figure A.3.

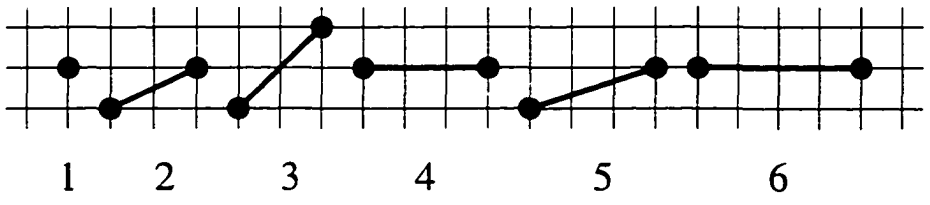


FIGURE A.3. All possible subsets of $I(S)$ (up to lattice symmetries) which contribute to the energy at eighth order when S corresponds to a square-parallelogram-kite tiling. The lines serve to distinguish the subsets.

In chapter 4 we defined

$$e_8^S = \sum_{X \subseteq square} \tilde{c}_{8,X} ,$$

which we may rewrite as

$$\epsilon_8^S = \sum_{\substack{X \in figure\ A.3: \\ X \subseteq square}} \tau_{S,X} \tilde{c}_{8,X} .$$

where "$X \in$ *figure* A.3" means that X is a rotation or reflection of one of the arrangements from figure A.3, and $\tau_{S,X}$ is the number of translates of X appearing in a square. ϵ_8^P and ϵ_8^K may be written in a similar manner.

Recall that $\kappa(X) = \frac{c_{8,X}}{\tilde{c}_{8,X}}$. The last three columns of table A.1 give the numbers $\frac{\tau_{S,X}}{\kappa(X)}$, $\frac{\tau_{P,X}}{\kappa(X)}$, and $\frac{\tau_{K,X}}{\kappa(X)}$ respectively, for each X in figure A.3. So we see, for example,

X	$c_{8,X}$	square	para.	kite
1	112	1	1	1
2	-768	2	1	1
3	1152	0	1	1
4	448	0	1	1
5	512	2	0	0
6	32	0	0	1

TABLE A.1. Values of $c_{m,X}$ used to calculate the eighth order energy contributions from a square, kite, and parallelogram.

that $\epsilon_8^S = 112 \times 1 - 768 \times 2 + 512 \times 2 = -400$.

A.3 Energies For Orders 10 and 12

Let S correspond to a tiling by squares and parallelograms. The subsets $X \subset I(S)$ which contribute at orders 10 and 12 are shown, up to rotations and reflections, in figure A.4. Recall that the local arrangement about an ion in $I(S)$ must look like one of the four shown in figure 4.5. We define $\tilde{c}_{m,X} = \kappa^{-1}(X) c_{m,X}$, where $\kappa(X)$ is the number of ions whose local arrangement contains X. We then have that

$$\epsilon_m^A = \sum_{X \subseteq type\ A} \tilde{c}_{m,X} .$$

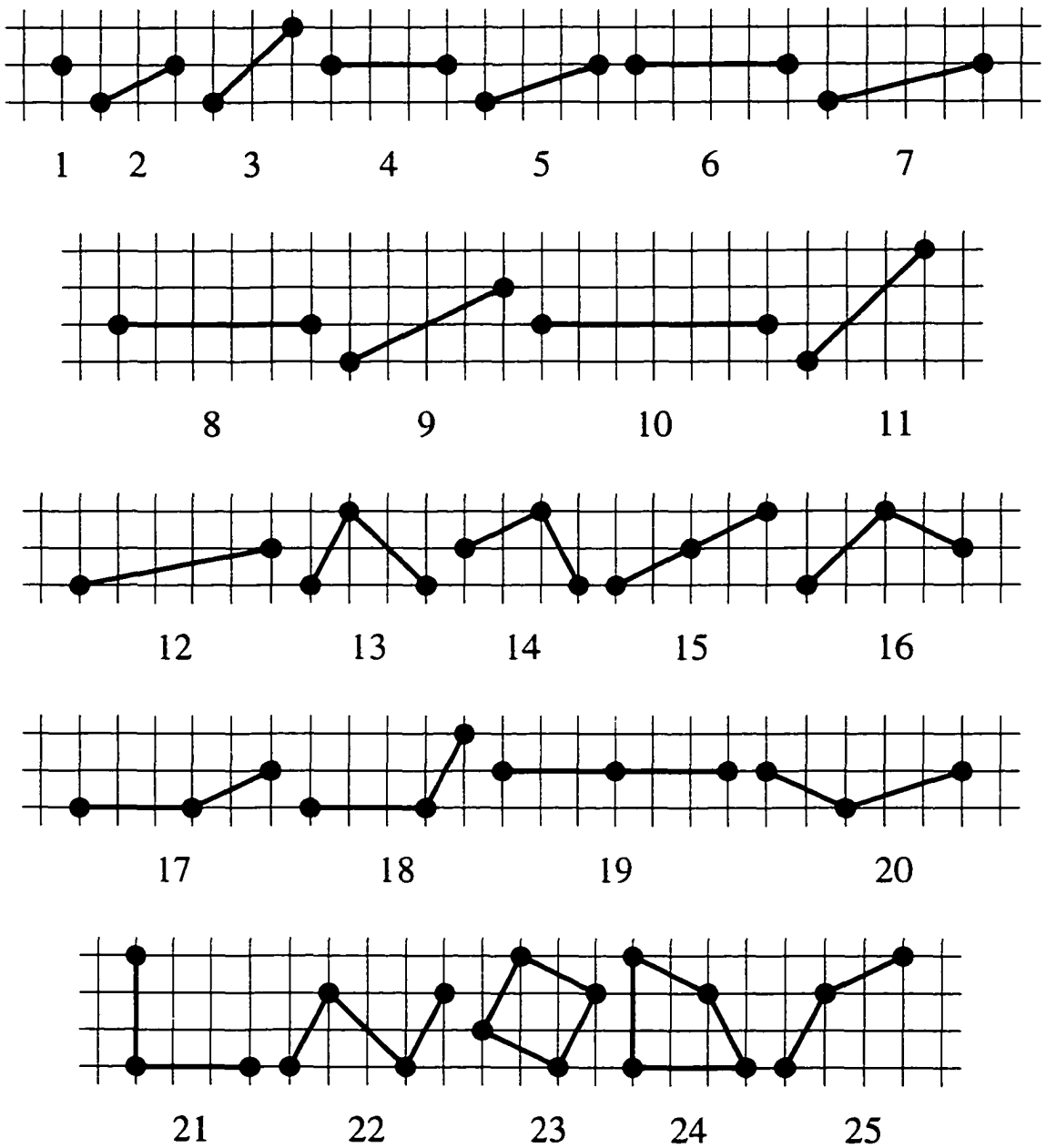


FIGURE A.4. All possible subsets of $I(S)$ (up to lattice symmetries) which contribute to the energy at orders 10 and 12 when S corresponds to a square-parallelogram tiling. The lines serve to distinguish the subsets.

where "$X \subseteq$ *type* A" means that X is contained in the local configuration about a type A ion. This may be written as

$$e_m^A = \sum_{\substack{X \in figure\ A.4. \\ X \subseteq type\ A}} \tau_{A,X} \tilde{c}_{m,X} .$$

where "$X \in$ *figure* A.4" means that X is a rotation or reflection of one of the arrangements from figure A.4, and $\tau_{A,X}$ is the number of translates of X appearing in the local configuration about a type A ion. The energies e_m^B, e_m^C, and e_m^D may be written in a similar manner.

Recall that $\kappa(X) = \frac{c_{m,X}}{\tilde{c}_{m,X}}$. The last four columns of table A.2 give the numbers $\frac{\tau_{A,X}}{\kappa(X)}$, $\frac{\tau_{B,X}}{\kappa(X)}$, $\frac{\tau_{C,X}}{\kappa(X)}$, and $\frac{\tau_{D,X}}{\kappa(X)}$ respectively, for each X in figure A.4. So we see, for example, that $e_{10}^D = -704 \times 1 - 14000 \times 2 + 640 \times 2 + 40 \times 2 - 15840 \times 4 = -90704$.

X	$c_{10,X}$	$c_{12,X}$	A	B	C	D
1	-704	-1344	1	1	1	1
2	-14000	110616	1	1	3/2	2
3	-5760	-66816	1	1	1/2	0
4	-1320	-43144	1	1	1/2	0
5	640	-47424	0	0	1	2
6	1120	5184	0	0	0	0
7	1000	8160	1	1	1/2	0
8	40	2208	0	0	1/2	2
9		10800	0	2	1	2
10		48	0	2	1/2	0
11		19200	1	0	0	0
12		1728	2	0	1	0
13	-7920	-50544	2	2	1	0
14	-15840	121680	0	0	2	4
15		33696	0	1	1	2
16		-56160	2	2	1	0
17		1872	2	0	1	0
18		-14976	0	2	1	0
19		832	0	1	0	0
20		-7488	0	0	0	4
21		-11024	1	0	0	0
22		26208	0	1	1/2	0
23		235872	0	0	1/2	1
24		26208	1	0	0	0
25		5616	1	0	0	0

TABLE A.2. Values of $c_{m,X}$ used to calculate the energy of types A, B, C, and D ions at orders 10 and 12.

Appendix B
PERIODIC GROUND STATES

B.1 M-Potential

In the occupation variables, $H_2 + H_4$ may be written as

$$H_2 + H_4 = U^{-1}\Big[8 \sum_{<xy>:|x-y|=1} V_x V_y - 16 \sum_x V_x\Big]$$
$$+ U^{-3}\Big[64 \sum_{<xy>:|x-y|=\sqrt{2}} V_x V_y + 16 \sum_{<xy>:|x-y|=2} V_x V_y - 16 \sum_x V_x + \sum_{X \in E_4} c_{4,X} V_X\Big] .$$

where E_4 is the collection of sets X appearing at fourth oder which contain a pair of sites x and y with $|x-y| = 1$. Note that the two terms involving $\sum_x$ contribute an amount which is proportional to the ion density. Since we are considering this density to be fixed, these terms may be dropped.

Let B be a 3×3 block of 9 sites, with z being its center site. Define

$$H_B = U^{-1}\frac{4}{3} \sum_{\substack{<xy> \subset B \\ |x-y|=1}} V_x V_y$$
$$+ U^{-3}\Big[16 \sum_{\substack{<xy> \subset B \\ |x-y|=\sqrt{2}}} V_x V_y + \frac{16}{3} \sum_{\substack{<xy> \subset B \\ |x-y|=2}} V_x V_y + \sum_{\substack{X \subset B \\ X \in E_4}} \frac{c_{4,X}}{\tau_X} V_X\Big] ,$$

where τ_X is the number of translates of X which are contained in B. Note that if $X \in E_4$ with $V_X \neq 0$, then there is a nearest neighbor pair x, y in X with $V_x V_y = 1$. This gives a contribution of $\frac{4}{3}U^{-1}$ to H_B which is much larger than the order U^{-3} contribution from $\frac{c_{4,X}}{\tau_X}$. Figure B.1 shows, up to rotations and reflections, all possible ion arrangements in a 3×3 block with no nearest neighbor ions.

Now, H_B was defined so that

$$\sum_B H_B = H_2 + H_4 . \qquad \text{(B.1)}$$

The idea is to find a function, K_B, defined on a 3×3 block so that $\sum_B K_B$ is proportional to the density, and $H_B + U^{-3} K_B$ is minimized by configurations 12, 13, 17, 19, and 20 in figure B.1. The difference between $\sum_B (H_B + U^{-3} K_B)$ and $H_2 + H_4$ will then be proportional to the density. Furthermore, if a configuration exists with the

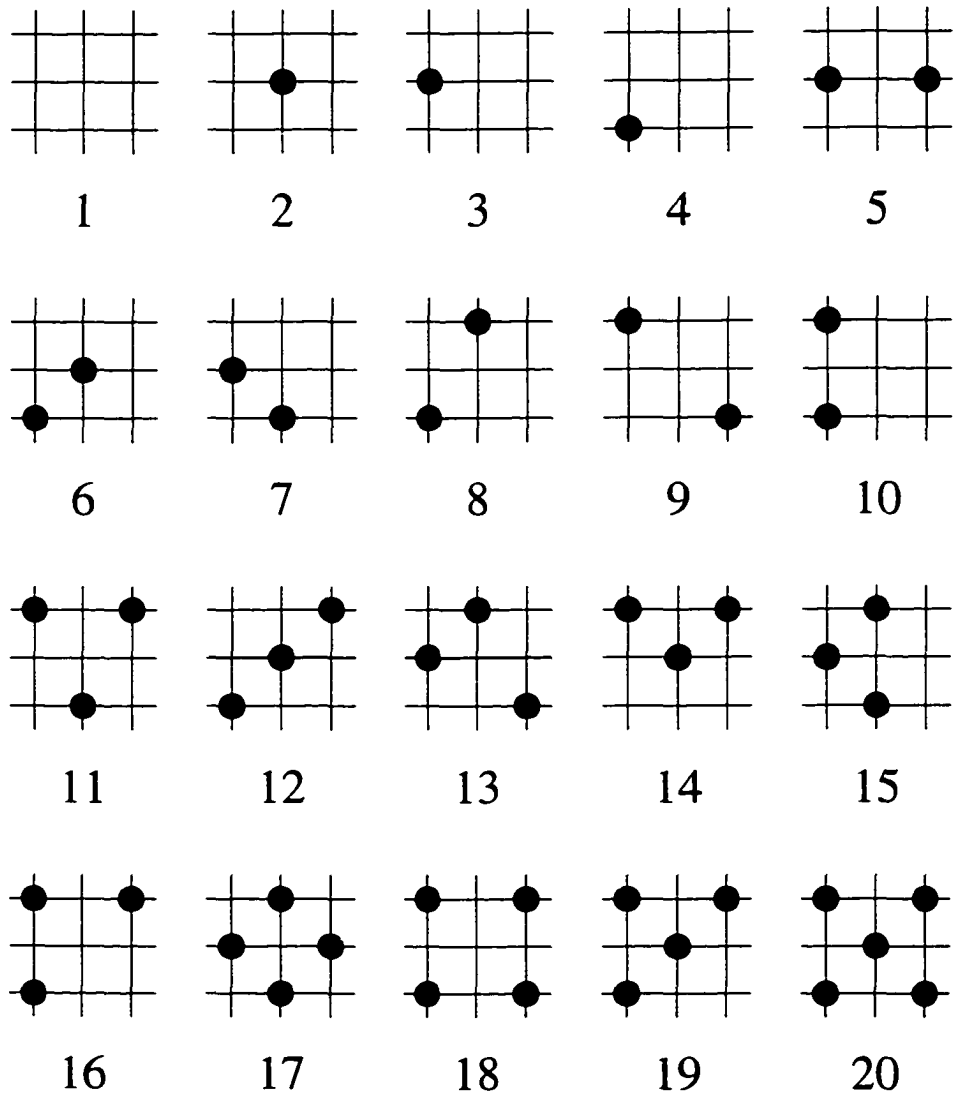


FIGURE B.1. All possible ion arrangements (up to lattice symmetries) in a 3×3 block of a configuration that minimizes H_2.

property that every 3×3 block is one of 12, 13, 17, 19, or 20 from figure B.1, then it minimizes $H_2 + H_4$.

Define

$$K_B = 96 - \frac{128}{3} \sum_{x \in B : |x-z|=1} V_x - \frac{80}{3} \sum_{x \in B : |x-z|=\sqrt{2}} V_x - \frac{224}{3} V_z .$$

Then clearly $\sum_B K_B$ is proportional to the ion density. A few simple calculations show that $H_B + U^{-3} K_B$ applied to the configurations in blocks 12, 13, 17, 19, and 20 of figure B.1 gives 0. The results of this calculation on the remaining blocks are given in table B.1, where $E_B = 3U^{-3}(H_B + U^{-3} K_B)$.

block	1	2	3	4	5	6	7	8	9	10	11	14	15	16	18
E_B	288	64	160	208	32	32	80	80	128	144	16	16	16	80	32

TABLE B.1. Energies through fourth order of the different block types after including the m-potential.

Any block containing a nearest neighbor pair of ions makes a positive contribution at order 2. From the results in table B.1, we see that any other block which is not one of 12, 13, 17, 19, or 20 from figure B.1, contributes 0 at order 2 but makes a positive contribution at order 4. This proves inequality 5.1.

B.2 Energies For Orders 6 and 8

Let S correspond to a tiling by squares and parallelograms. The subsets $X \subset I(S)$ which contribute at orders 6 and 8 are shown, up to rotations and reflections, in figure B.2. Recall that the local arrangement about an ion in $I(S)$ must look like one of the three shown in figure 5.3. We define $\tilde{c}_{m,X} = \kappa^{-1}(X) c_{m,X}$, where $\kappa(X)$ is the number of ions whose local arrangement contains X. We then have that

$$e_m^A = \sum_{X \subseteq type\ A} \tilde{c}_{m,X} ,$$

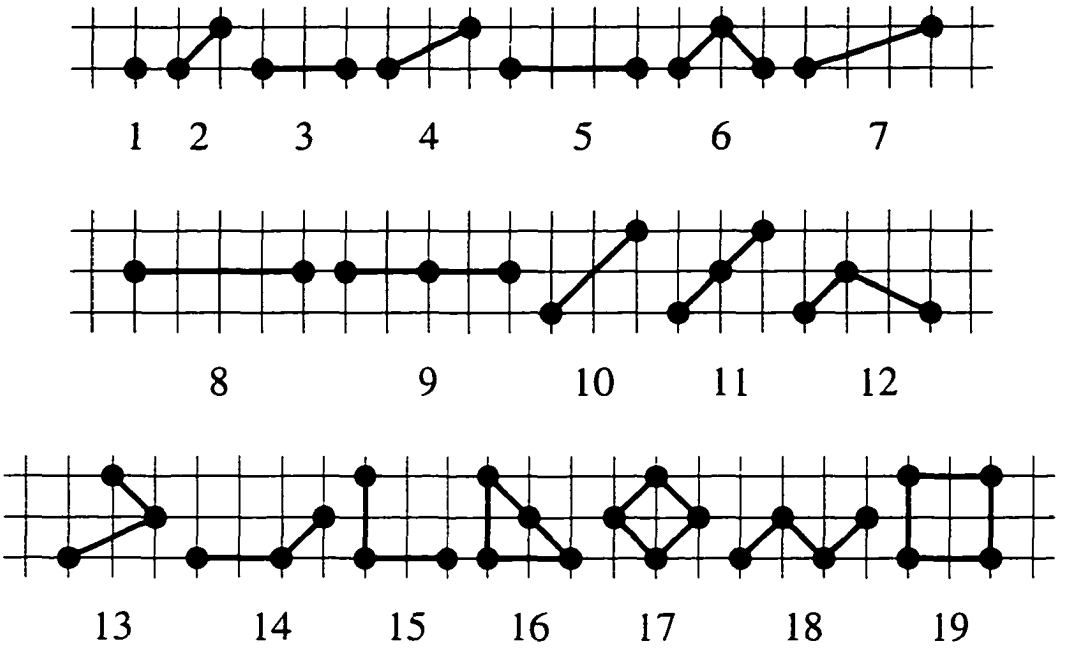


FIGURE B.2. All possible subsets of $I(S)$ (up to lattice symmetries) which contribute to the energy at orders 6 and 8 when S corresponds to a square-parallelogram tiling. The lines serve to distinguish the subsets..

where "$X \subseteq$ *type* A" means that X is contained in the local configuration about a type A ion. This may be written as

$$\epsilon_m^A = \sum_{\substack{X \in figure\ B.2. \\ X \subseteq type\ A}} \tau_{A,X} \tilde{c}_{m,X} \,.$$

where "$X \in$ *figure* $B.2$" means that X is a rotation or reflection of one of the arrangements from figure B.2, and $\tau_{A,X}$ is the number of translates of X appearing in the local configuration about a type A ion. The energies e_m^B and e_m^C may be written in a similar manner.

The last three columns of table B.2 give the numbers $\frac{\tau_{A,X}}{\kappa(X)}$, $\frac{\tau_{B,X}}{\kappa(X)}$, and $\frac{\tau_{C,X}}{\kappa(X)}$, respectively, for each X in figure B.2.

So we see, for example, that $e_6^A = 64 \times 1 - 384 \times 2 + 96 \times 2 - 674 \times 4 = -3200$.

X	$c_{6,X}$	$c_{8,X}$	A	B	C
1	64	112	1	1	1
2	-384	768	2	3/2	1
3	96	-1360	2	1	0
4	216	-768	0	1	2
5	24	448	0	1	2
6	-672	11520	4	2	0
7		512	4	1	0
8		32	2	0	0
9		192	2	0	0
10		1152	2	1	1
11		768	2	1	1
12		-1728	0	2	4
13		-5184	0	1	2
14		-384	8	2	0
15		-1248	4	1	0
16		3840	4	1	0
17		23040	1	1/2	0
18		3840	4	1	0
19		960	1	0	0

TABLE B.2. Values of $c_{m,X}$ used to calculate the energy of types A, B, and C ions at orders 6 and 8.

B.3 Bound

Lemma B.1. *Let γ_1 be a closed nearest neighbor walk of length N in C_N. Let γ be its corresponding walk in S. Suppose there are no bad diamonds within ℓ_1 distance N of γ. Then $w(\gamma_1) = w(\gamma)$.*

Proof: We know that $\gamma(0)$ is contained in some strip of good diamonds, say R. Without loss of generality, assume R is a $-$ strip. Define $\bar{R}$ to be the set of sites of the form $x + n(-1, 1)$ where x is a site in R and n is any integer. Let $\hat{b}$ be a diamond which intersects γ. Then by hypothesis, $\hat{b}$ is a good diamond. Consider the strip of diamonds between $\hat{b}$ and T in the "direction" of γ, as shown in figure B.3. Each one

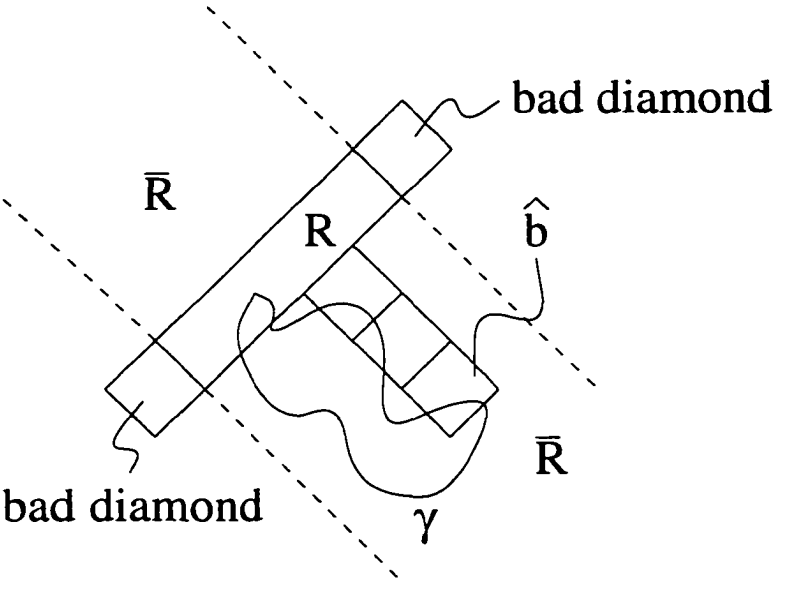


FIGURE B.3. The strip of diamonds referred to in the proof are those between $\hat{b}$ and R.

of these diamonds must be within N of γ, so by hypothesis all these b's must be good. Thus the stripe arrangement in R persists through these good diamonds and so $\hat{b}$ has the same stripe arrangement as R. Since this holds for all $\hat{b}$ intersecting γ we see that $w(\gamma_1) = w(\gamma)$.

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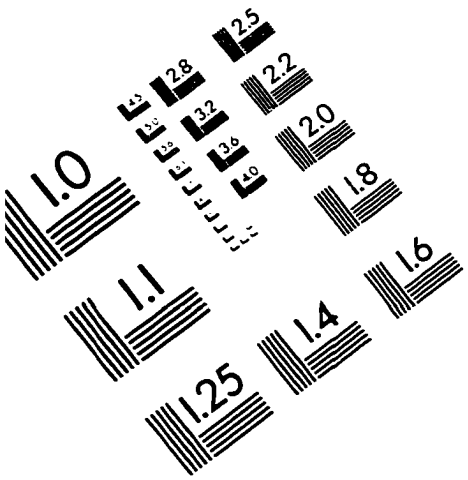
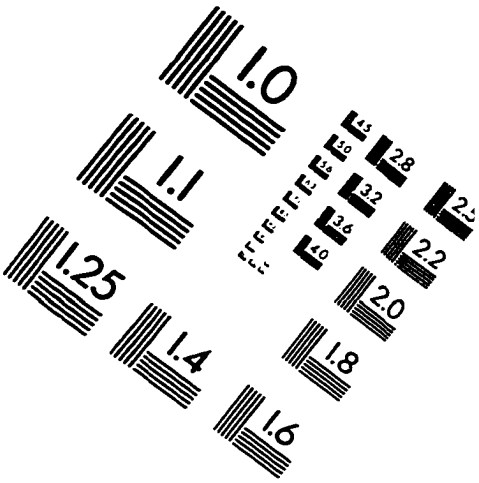
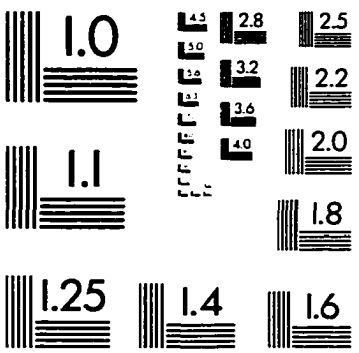
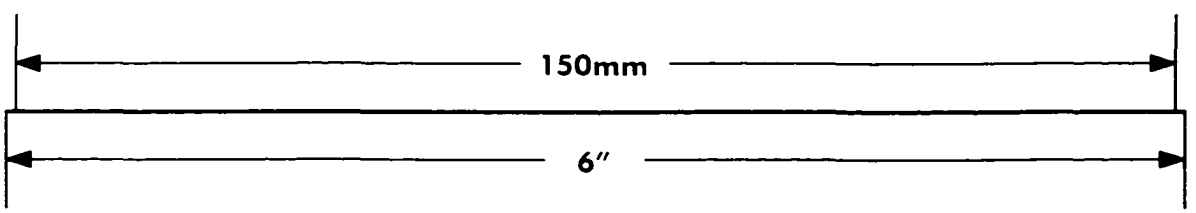
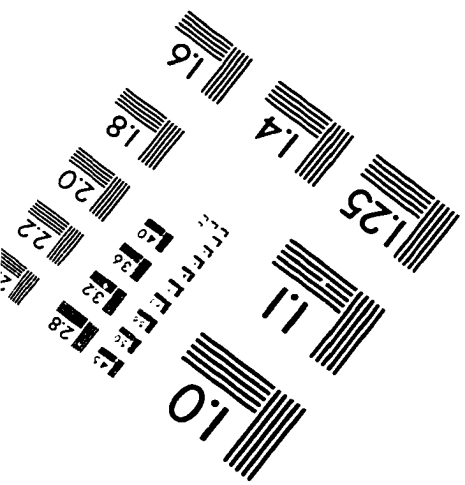
IMAGE EVALUATION TEST TARGET (QA-3)

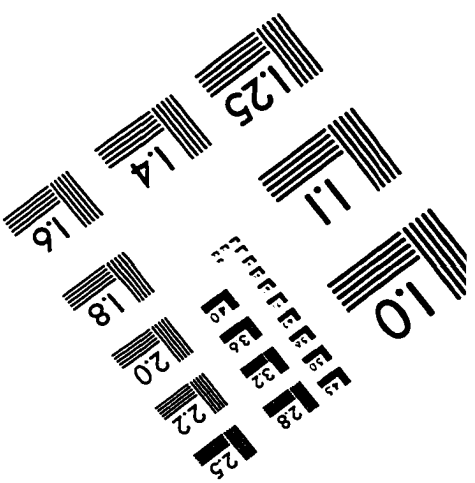












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