Low-Temperature Phase Diagrams of Quantum Lattice Systems. III. Examples.

By Jürg Fröhlich[1] and Luc Rey-Bellet[2]

Institut für Theoretische Physik, ETH-Hönggerberg
8093 Zürich, Switzerland

Abstract. We use the low-temperature expansion and the extension of Pirogov-Sinai theory developed in [1], and the perturbation theory of [2] to describe the phase diagrams of two families of fermionic lattice systems at low-temperature: the balanced model and a variant of the $t-J$ model.

1 Introduction

In this paper, we illustrate the methods developed in two previous papers [1, 2] to analyze the low-temperature phase diagrams of quantum lattice systems in terms of two classes of models, the balanced model and the $t-J$ models (of interest in connection with high-temperature superconductivity). In this paper, we describe our main results and discuss the key ideas of the proofs, but we do not present all the details of our calculations. Furthermore, we permit ourselves to describe various conjectures. Methods similar to those in [1] have been developed by Borgs, Kotecky and Ueltschi, [3], for quantum spin systems.

[1]e-mail: juerg@itp.phys.ethz.ch

[2]Present adress: Section de mathématiques, Université de Genève,
case postale 240, 1211 Genève 24, Switzerland. e-mail: rey@divsun.unige.ch

1.1 The models

We consider two spin-1/2 models on a two-dimensional lattice, (but our methods can be used in any dimension $d \geq 2$).

(i) *The balanced model.*
The Hamiltonian of the model, for a finite subset Λ of $\mathbb{Z}^2$, is given by

$$\begin{aligned} H_{bal}(t) &= \sum_{\substack{\|x-y\|=1 \\ \langle xy\rangle\subset\Lambda}} \left(J\sigma_x^{(3)}\sigma_y^{(3)}\right) n_x n_y + \sum_{\substack{\|x-y\|=\sqrt{2} \\ \langle xy\rangle\subset\Lambda}} \left(J'\sigma_x^{(3)}\sigma_y^{(3)}\right) n_x n_y \\ &\quad + \sum_{x\in\Lambda} U n_{x\uparrow} n_{x\downarrow} - \sum_{\substack{\|x-y\|=1 \\ \langle xy\rangle\subset\Lambda}} \sum_{\sigma\in\{\uparrow,\downarrow\}} t\left(c_{x\sigma}^{\dagger} c_{y\sigma} + h.c.\right), \end{aligned} \tag{1}$$

where $\sigma_x^{(i)}$, $i = 1, 2, 3$, are the Pauli matrices acting on the spin space at site $x \in \Lambda$, $c_{x\sigma}^{\dagger}$ and $c_{x\sigma}$ are the creation and annihilation operators for a particle with spin σ at site x, $n_{x\sigma}$ is the number operator for a particle with spin σ at site x, and $n_x = n_{x\uparrow} + n_{x\downarrow}$ is the total particle number operator at site x. The Hilbert space at each lattice site $x \in \Lambda$ is isomorphic to $\mathbb{C}^4$. As a basis for $\mathbb{C}^4$, we choose $\{|\uparrow\downarrow\rangle, |\uparrow\rangle, |\downarrow\rangle, |0\rangle\}$.

We shall consider the antiferromagnetic case, i.e., $J > 0$ and $J' > 0$, and a large on-site repulsive interaction, $U \gg J$, $U \gg J'$. The word "balanced" refers to the condition $J' = J/2$. At half-filling, $H_{bal}(0)$ has an infinite number of groundstates and does not satisfy the Peierls condition. The hopping term, $H_{bal}(t) - H_{bal}(0)$, is treated as a perturbation. By using a variant of perturbation theory developed in [2], we shall show that the hopping term lifts the infinite degeneracy of the groundstate energy of $H_{bal}(0)$ in order t^2. Two Néel states will turn out to be the groundstates of $H_{bal}(t)$, and long-range order survives at finite temperature.

(ii) *A variant of the $t - J$ model*
The Hamiltonian of this model is given by

$$\begin{aligned} H_{t-J}(\lambda, t) &= \sum_{\substack{\|x-y\|=1 \\ \langle xy\rangle\subset\Lambda}} \left[\frac{1}{2}\left(J\sigma_x^{(3)}\sigma_y^{(3)} + v\right) + \lambda\left(\sigma_x^{(1)}\sigma_y^{(1)} + \sigma_x^{(2)}\sigma_y^{(2)}\right)\right] n_x n_y \\ &\quad - \sum_{\substack{\|x-y\|=1 \\ \langle xy\rangle\subset\Lambda}} \sum_{\sigma\in\{\uparrow,\downarrow\}} t\left(c_{x\sigma}^{\dagger} c_{y\sigma} + h.c.\right) + \sum_{\substack{\|x-y\|=\sqrt{2} \\ \langle xy\rangle\subset\Lambda}} v' n_x n_y - \sum_{x\in\Lambda} \mu n_x. \end{aligned} \tag{2}$$

We require an infinitely strong on-site repulsive interaction, i.e, we forbid double occupancy. The Hilbert space each lattice site $x \in \Lambda$ is isomorphic to $\mathbb{C}^3$. A convenient basis for $\mathbb{C}^3$ is $\{|\uparrow\rangle, |\downarrow\rangle, |0\rangle\}$.

We study the antiferromagnetic case, i.e, $J > 0$. Since the unitary transformation $\prod_{x\in\Lambda_e} \sigma_x^{(3)}$, where Λ_e is the even sublattice of Λ, changes the sign of λ, we may assume, without loss of generality, that $\lambda > 0$. We do not impose any restriction on the values of v and v'. We study this model with the help of perturbative methods (see [2]) which are applicable only in the regime where λ/J and a suitable dimensionless version of t is small.

This model describes the motion of holes in an antiferromagnetic background. It is a variant of the $t - J$ model which may describe some features of high-T_c superconductors. The plain $t - J$ model corresponds to the parameters values $v = -J, v' = 0$ and can be derived from the Hubbard model in the strong coupling limit. Although the physically relevant parameter ranges are $\lambda \approx J/2$ and $t \approx J$, it appears to be of interest to study the model in the limit of strong anisotropy and weak hopping where rigorous results can be obtained, with the hope that such results can be extrapolated

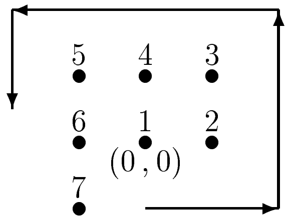

Figure 1: Spiral order in $\mathbb{Z}^2$

to the physical domain. For example these results indicate in which domain of parameter space Fermi liquids or a superconducting phase might appear.

1.2 The methods

For the convenience of the reader we briefly recall the results obtained in [1, 2]. The perturbation theory of [2] will serve to cast the Hamiltonians defined in (1) and (2) in a form that enables us to apply the low-temperature expansion (Pirogov-Sinai) theory of [1] to our models.

Standard references for the general formalism of quantum lattice systems are [4, 5, 6]. In this paper, we consider lattice gases of fermions and we require a slight modification of the usual formalism. Indeed fermionic creation and annihilation operators at different lattice sites do not commute but anticommute. But we have in the sequel commutativity (or locality) conditions.

A quantum lattice system is defined by the following data:

(i) To each $x \in \mathbb{Z}^d$ is associated an Hilbert space $\mathcal{H}_x$ which is isomorphic, for all x, to a fixed, finite-dimensional Hilbert space $\mathcal{H}$. We choose an ordering on $\mathbb{Z}^d$, for example the spiral ordering depicted in Figure 1 for $d = 2$ (and an analogous ordering for $d \geq 3$). This ordering is chosen to have the property that, for any finite set X, the set $\overline{X} := \{z \in \mathbb{Z}^\nu, z \preceq X\}$ of lattice sites which are smaller than X, or belong to X, is finite. The Hilbert space associated to a finite subset $X = \{x_1 \prec \cdots \prec x_{|X|}\} \subset \mathbb{Z}^d$ is the ordered tensor product

$$\mathcal{H}_X = \mathcal{H}_{x_1} \otimes \cdots \otimes \mathcal{H}_{x_{|X|}}\,.$$

and we denote $\mathcal{L}(\mathcal{H}_X)$ the algebra of all bounded operators on $\mathcal{H}_X$.

(ii) For any finite subset $X \subset \mathbb{Z}^d$ two operators algebras acting on $\mathcal{H}_X$ are given

- The (local) *field algebra* $\mathcal{F}_X \subset \mathcal{L}(\mathcal{H}_{\overline{X}})$,
- The (local) *observable algebra* $\mathcal{A}_X \subseteq \mathcal{F}_X$,

which satisfy the following properties.

(a) If $X \subset Y$ and $x \prec y$, for all $x \in X$ and all $y \in Y \setminus X$, then there is a natural embedding of $\mathcal{F}_X$ into $\mathcal{F}_Y$ and, in the following, we write B for both $B \in \mathcal{F}_X$ and $B \otimes \mathbf{1}_{\mathcal{H}_{Y\setminus X}}$ in $\mathcal{F}_Y$.

(b) For the infinite system, the (quasilocal) field and operator algebras are the C^*-algebras given by

$$\mathcal{A} = \overline{\bigcup_{X \nearrow \mathbb{Z}^\nu} \mathcal{A}_X}^{\text{norm}}\,, \quad \mathcal{F} = \overline{\bigcup_{X \nearrow \mathbb{Z}^\nu} \mathcal{F}_X}^{\text{norm}}\,,$$

(the limit taken through a sequence of increasing subsets of $\mathbb{Z}^d$, where increasing refers to the spiral ordering defined above).

(c) The elements of the field and observable algebras satisfy the commutativity condition: If $X \cap Y = \emptyset$, then for any $A \in \mathcal{F}_X$, $B \in \mathcal{A}_Y$

$$[A, B] = 0 . \tag{3}$$

For fermions, as in our examples, the field algebra, $\mathcal{F}_X$, is the algebra generated by creation and annihlation operators at lattice sites $x \in X$ and the observable algebra, $\mathcal{A}_X$, may be taken to the subalgebra of $\mathcal{F}_X$ consisting of gauge-invariant operators. For example, for spin 1/2 fermions, we take $\mathcal{H}_x \simeq \mathbb{C}^2 \otimes \mathbb{C}^2$, for all $x \in \mathbb{Z}^d$, with the basis

$$\begin{aligned} |0\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \quad |\uparrow\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ |\downarrow\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \quad |\uparrow\downarrow\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} . \end{aligned} \tag{4}$$

Creation and annihilation operators are given in terms of a Klein-Jordan-Wigner transformation

$$\begin{aligned} c^*_{x\uparrow} &= \otimes_{y \prec x} \left(\sigma^3_{y1} \otimes \sigma^3_{y2} \right) \otimes \sigma^+_{x1} & \qquad c_{x\uparrow} &= \left(c^*_{x\uparrow} \right)^* \\ c^*_{x\downarrow} &= \otimes_{y \prec x} \left(\sigma^3_{y1} \otimes \sigma^3_{y2} \right) \otimes \sigma^3_{x1} \otimes \sigma^+_{x2} & \qquad c_{x\downarrow} &= \left(c^*_{x\downarrow} \right)^* , \end{aligned}$$

where $\sigma^+_{xi}, \sigma^-_{xi}, \sigma^3_{xi}$, $x \in \mathbb{Z}^d$, $i = 1, 2$ are the Pauli matrices acting at lattice site x on the first or second factor of $\mathbb{C}^2 \otimes \mathbb{C}^2$. This representation makes explicit the non-local character of creation and annihilation operators: $c^*_{x\sigma}$, $c_{x\sigma}$, $\sigma \in \{\uparrow, \downarrow\}$ belong to $\mathcal{L}(\mathcal{H}_{\overline{x}})$. With this representation it is straightforward to check the commutativity condition (3).

The methods of [1] can applied to Hamiltonians of the form

$$H = H_0(\underline{\mu}) + V,$$

defined on the Hilbert space $\mathcal{H}_{\overline{\Lambda}}$, where Λ is a finite (arbitrarily large) subset of the lattice $\mathbb{Z}^\nu$. We assume that both operators, $H_0(\underline{\mu})$ and V, can be written as sums of local operators which belong to the *observable algebras*:

$$\begin{aligned} H_0(\underline{\mu}) &= \sum_{X \subset \Lambda} \phi^0_X(\underline{\mu}) , & \qquad \phi^0_X(\underline{\mu}) &\in \mathcal{A}_X \\ V &= \sum_{X \subset \Lambda} V_X , & \qquad V_X &\in \mathcal{A}_X . \end{aligned}$$

We consider translation-invariant lattice systems, i.e. systems satisfying

$$\phi^0_X(\underline{\mu}) = \phi^0_{X+a}(\underline{\mu}), \;\; V_X = V_{X+a} ,$$

for all $X \subset \mathbb{Z}^d$, $a \in \mathbb{Z}^d$.

Furthermore, $\underline{\mu} \in \mathbb{R}^{P-1}$ parametrizes "external fields" (chemical potentials, magnetic field, ...). Our assumptions on $H_0(\underline{\mu})$ are the following: there is a domain $\mathcal{O} \subset \mathbb{R}^{P-1}$ such that the conditions **H1-H4** below are satisfied.

- **H1.** $H_0(\underline{\mu})$ **is a finite-range classical Hamiltonian**.
  (a) The operators $\{\phi^0_X(\underline{\mu})\}$ have finite range r, i.e.,

$$r := \max_{\substack{X : \Phi^0_X(\underline{\mu}) \neq 0 \\ x, y \in M, \, 1 \leq i \leq \nu}} |x_i - y_i|, \tag{5}$$

is finite.

(b) There exists a basis $\{e^x_{j_x}\}_{j_x\in I}$, where $I=\{1,\ldots,N\}$, $N=\dim\mathcal{H}_x$, is a finite set independent of x, such that, for all $X\subset\mathbb{Z}^d$ and all $\underline{\mu}\in\mathcal{O}$, $\phi^0_X(\underline{\mu})$ is diagonal in the tensor-product-basis

$$\{\otimes_{x\in X}e^x_{j_x}\}_{j_x\in I}\ .$$

In our examples the basis $\{e^x_{j_x}\}_{j_x\in I}$ is given by (4).

The set of configurations on Λ, Ω_Λ, is defined as the set of all assignments $\{j_x\}_{x\in\Lambda}$ with $j_x\in I$. A configuration ω_Λ is an element of Ω_Λ and, for $X\subset\Lambda$, ω_X denotes the restriction of ω_Λ to the subset X. To each configuration ω_X one can associate the state $\otimes_{x\in X}e^x_{j_x}$, with $\omega_X=\{j_x\}_{x\in X}$, which will be denoted e_{ω_X}. Since the interactions ϕ^0_X are uniquely determined by the matrix elements

$$\begin{aligned}\langle e_{\omega_\Lambda}|\phi^0_X(\underline{\mu})|e_{\omega_\Lambda}\rangle &= \langle e_{\omega_X}|\phi^0_X(\underline{\mu})|e_{\omega_X}\rangle\\ &:= \phi^0_X(\underline{\mu})(\omega_\Lambda),\end{aligned}$$

we may view ϕ^0_X as a function on the set of configurations. Given a configuration $\omega:=\omega_{\mathbb{Z}^\nu}$ of the infinite system $(\Lambda\nearrow\mathbb{Z}^\nu)$, we let $e(\underline{\mu})(\omega)$ denote the energy density of ω, defined by

$$e(\underline{\mu})(\omega)\ =\ \overline{\lim}_{\Lambda\nearrow\mathbb{Z}^\nu}\frac{1}{|\Lambda|}\sum_{X\subset\Lambda}\langle e_{\omega_\Lambda}|\phi^0_X(\underline{\mu})|e_{\omega_\Lambda}\rangle\ . \tag{6}$$

Note that the limit exists e.g. if ω is periodic. Let $\mathcal{K}$ be the set of all of periodic states $\{s_1=e_{\omega_1},\cdots s_P=e_{\omega_p}\}$ (where $\omega_1,\cdots,\omega_P$ are periodic configurations) with the property that, for every $j=1,\cdots,P$, s_j is a groundstate of $H_0(\underline{\mu})$, for some $\underline{\mu}\in\mathcal{O}$, in the sense that $e_j(\underline{\mu}):=e(\underline{\mu})(\omega_j)$ is a minimum of $e(\underline{\mu})(\omega)$, $\omega\in\Omega$.

- **H2. Peierls condition.**
  The set, $\mathcal{K}$, of periodic groundstates of $H_0(\underline{\mu})$, with $\underline{\mu}\in\mathcal{O}$, is finite and $H_0(\underline{\mu})$ satisfies the Peierls condition with a Peierls constant κ independent of $\underline{\mu}\in\mathcal{O}$.

The Peierls condition requires that there be a non-zero energy per unit interface ("contour") separating two periodic groundstates. A precise statement and a useful criterion (see [7]) are given in Appendix B. Note that the dimension of $\mathcal{O}$, $P-1$, is assumed to be one less than the number of groundstates.

For each value of $\underline{\mu}$, there is a set of periodic groundstates of $H_0(\underline{\mu})$

$$\mathcal{Q}^{(\infty,0)}(\underline{\mu})\ :=\ \{s_j\ :\ e_j(\underline{\mu})=\min_{1\le k\le P}\ e_k(\underline{\mu})\}.$$

The classical zero-temperature phase diagram is the family of manifolds

$$\mathcal{S}^{(\infty,0)}_{\{s_{p_1},\ldots,s_{p_k}\}}\ :=\ \{\underline{\mu}\in\mathcal{O}\ :\ \mathcal{Q}^{(\infty,0)}(\underline{\mu})=\{s_{p_1},\ldots,s_{p_k}\}\},$$

with $1\le k\le P$; $s_{p_1},\ldots,s_{p_k}\in\mathcal{K}$. These manifolds are called the *strata* of the phase diagram.

- **H3. Regularity of the phase diagram**. The phase diagram is *regular*, i.e., the map

$$\underline{\mu}\ \longmapsto\ \Big(e_1(\underline{\mu})-\min_k e_k(\underline{\mu})\,,\ \ldots\ ,\ e_P(\underline{\mu})-\min_k e_k(\underline{\mu})\Big)$$

  is a homeomorphism of $\mathcal{O}$ into the boundary of the positive octant in $\mathbb{R}^P$.

Note that this means that the stratum of maximum coexistence, $\mathcal{S}_{\mathcal{K}}^{(\infty,0)}$, is a single point (= the origin of the P-octant), the strata with $p-1$ groundstates are curves starting from it (= the coordinate halfaxes), ... , the strata with $P-k$ groundstates are k-dimensional manifolds bounded by the strata with $P-k+1$ ground states. (This geometry is also known as the *Gibbs phase rule*.)

- **H4. Smoothness properties**.
  The maps $\underline{\mu} \longmapsto \phi_X^0(\underline{\mu})$ are differentiable, and their derivatives have uniformly bounded norm on $\mathcal{O}$. Moreover the determinant of the matrix

$$\left(\frac{\partial}{\partial \mu_j}(e(\sigma_i) - e(\sigma_p))\right)_{1\le i,j\le p-1} \tag{7}$$

  is uniformly bounded away from zero throughout $\mathcal{O}$.

The perturbation Hamiltonian V is assumed to satisfy the following conditions.

- **V1. Exponential decay**.
  There exists $\varepsilon > 0$ and $\lambda < 1$ such that

$$\|V_B\| \le \varepsilon \lambda^{g(B)},$$

  where $g(B)$ is the cardinality of the smallest connected subset of the lattice containing B.

For fermionic systems V is assumed to be gauge-invariant. This property is crucial both in proving statistical independence of the weights of disjoint contours in a low-temperature expansion (see [1]), and in our perturbation scheme (see Appendix A and [2]).

The first part of the analysis in [1] yields a criterion to determine the *stable phases* of H, for a fixed value of $\underline{\mu}$, if $H_0(\underline{\mu})$ is in the symmetric regime. The Hamiltonian $H_0(\underline{\mu})$ is said to be in the symmetric regime if, in a neighbourhood of $\underline{\mu}$, H_0 has a single groundstate or, more generally, finitely many groundstates related by some symmetry operation.

For a periodic state $s_j \in \mathcal{K}$, and finite regions $\Gamma \supset \Lambda$, the Hamiltonian "with boundary condition" s_j is the operator

$$H_\Gamma^{s_j} = \sum_{X\cap\Lambda\neq\emptyset} P_{\Gamma\setminus\Lambda}^{s_j}(\Phi_X^0(\underline{\mu}) + V_X)P_{\Gamma\setminus\Lambda}^{s_j}\,, \tag{8}$$

where $P_{\Gamma\setminus\Lambda}^{s_j} := |s_{j\Gamma\setminus\Lambda}\rangle\langle s_{j\Gamma\setminus\Lambda}|$. The *Gibbs state* in the finite volume Λ and boundary condition s_j and inverse temperature β is the positive linear functional on $\mathcal{F}_\Lambda$ defined by

$$\mathcal{F}_\Lambda \ni A \mapsto \langle A\rangle_\Lambda^j = \lim_{\Gamma\nearrow\mathbb{Z}^d} \frac{\mathrm{tr} A \exp\left(-\beta H_\Gamma^{s_j}\right)}{\mathrm{tr}\exp\left(-\beta H_\Gamma^{s_j}\right)}\,.$$

The infinite-volume limits of these functionals determine the phase diagram of the system.

In [1, Theorem 2.2] the following theorem has been proven:

Theorem 1.1 *(Low-temperature expansion in the symmetric regime.)*
Assume that, for a fixed value of $\underline{\mu}$, $H_0(\underline{\mu})$ satisfies condition **H1***, is in the symmetric regime, and satisfies the Peierls condition* **H2***. Assume, further, that the perturbation V satisfies condition* **V1***.*

Then there are constants $\bar{\kappa} = \mathrm{O}(\kappa)$ and $\varepsilon_0 > 0$ such that, for each β, ε and λ in the region

$$\max\left(e^{-\beta\bar{\kappa}}, \frac{\varepsilon\lambda}{\kappa}\right) < \varepsilon_0,$$

there exists a family of functions $f_j(\underline{\mu})$, $1 \leq j \leq P$ (the truncated free energy densities), such that the following holds: If, for some $j \in \{1, \cdots, P\}$,

$$f_j(\underline{\mu}) \;=\; \min_{1\leq k\leq P} f_k(\underline{\mu}) \tag{9}$$

for some values of ε, β and λ, then

1. *$f_j(\underline{\mu})$ coincides with the true free energy of the system*

$$f_j(\underline{\mu}) \;=\; -\frac{1}{\beta} \lim_{\Lambda\nearrow\mathbb{Z}^\nu} \frac{1}{|\Lambda|} \log Z_\Lambda^j\,. \tag{10}$$

2. *The infinite-volume limit*

$$\langle A\rangle^j \;:=\; \lim_{\Lambda\nearrow\mathbb{Z}^\nu} \langle A\rangle_\Lambda^j, \tag{11}$$

exists for any local observable A.

3.

$$|\,\langle A\rangle^j \;-\; \langle s_j|A|s_j\rangle\,| \leq \|A\||X|O(\varepsilon_0)$$

for any operator A in $\mathcal{A}_X$.

Theorem 1.1 shows that the long-range order of the groundstate survives at finite temperature and under the addition of a sufficiently small quantum perturbation. This theorem, combined with a high temperature expansion (see [8]), permits to prove the existence, at finite temperature, of phase transitions between ordered phases and a disordered phase.

The second part of the analysis refers to the stability of the phase diagram as a whole. It extends Pirogov-Sinai theory [9, 10] to a certain class of quantum Hamiltonians.

The set of coexisting Gibbs states, $\mathcal{Q}^{(\beta,\lambda)}(\underline{\mu})$, is defined similarly to the set $\mathcal{Q}^{(\infty,0)}(\underline{\mu})$, replacing groundstate energy densities by truncated free energy densities (see [1]):

$$\mathcal{Q}^{(\beta,\lambda)}(\underline{\mu}) \;=\; \{s_j \;:\; f_j(\underline{\mu}) = \min_{1\leq k\leq P} f_k(\underline{\mu})\}.$$

One then defines

$$\mathcal{S}^{(\beta,\lambda)}_{\{s_{p_1},\ldots,s_{p_k}\}} \;:=\; \{\underline{\mu} \in \mathcal{O} \;:\; \mathcal{Q}^{(\beta,\lambda)}(\underline{\mu}) = \{s_{p_1},\ldots,s_{p_k}\}\}.$$

The following theorem is proven in [1, Theorem 2.3]:

Theorem 1.2 *(Pirogov-Sinai theory)*
Assume that the Hamiltonian $H_0(\underline{\mu}) + V$ satisfies conditions **H1** - **H4** *and* **V1**.

Then there are constants $\bar{\kappa} = \mathrm{O}(\kappa)$ and $\varepsilon_0 > 0$ such that, for each β, ε and λ in the region

$$\max\,(e^{-\beta\bar{\kappa}}, \frac{\varepsilon\lambda}{\kappa}) \;<\; \varepsilon_0,$$

there exists a non-empty open set $\mathcal{O}_{\beta,\lambda} \in \mathbb{R}^{P-1}$ such that:

- *The phase diagram defined by the strata $\mathcal{O}_{\beta,\lambda} \cap \mathcal{S}^{(\beta,\lambda)}_{\{s_{p_1},\ldots,s_{p_k}\}}$ is regular, and these strata are differentiable manifolds.*

- *As $\varepsilon_0 \to 0$, the strata $\mathcal{O}_{\beta,\lambda} \cap \mathcal{S}^{(\beta,\lambda)}_{\{s_{p_1},\dots,s_{p_k}\}}$ tends to the zero-temperature classical strata $\mathcal{O} \cap \mathcal{S}^{(\infty,0)}_{\{s_{p_1},\dots,s_{p_k}\}}$, pointwise in $\underline{\mu}$. In particular, the distance between the maximal-coexistence manifolds $\mathcal{S}^{(\beta,\lambda)}_{\mathcal{K}}$ and $\mathcal{S}^{(\infty,0)}_{\mathcal{K}}$ is* $\mathrm{O}(\varepsilon_0)$.

This theorem describes the first order phase transitions (coexistence of several phases), when the parameters $\underline{\mu}$ vary. It shows that the phase diagram of $H_0(\underline{\mu}) + V$, at low-temperature and for a sufficiently small perturbation V, is a smooth deformation of the phase diagram of $H_0(\underline{\mu})$ at zero temperature.

In [2] it is shown how to describe the low-temperature phase diagram of certain quantum lattice systems for which conditions **H2** and **H3** are *not*, a priori, satisfied. Indeed, it may happen that the groundstates of the Hamiltonian $H_0(\underline{\mu})$ are infinitely degenerate (in the thermodynamic limit), but that the perturbation reduces this degeneracy to a finite one. We consider Hamiltonians of the form

$$H(t) \;=\; H_0(\underline{\mu}) \;+\; tV\,,$$

t being a perturbation parameter. We assume that $H_0(\underline{\mu})$ satisfies conditions **H1** and **H4** and, in addition, we require the following hypotheses on $H_0(\underline{\mu})$ and V.

- **P1. M-potential.**
  $H_0(\underline{\mu})$ can be written as
  $$H_0(\underline{\mu}) \;=\; \sum_{M\subset\Lambda} \phi^0_M(\underline{\mu}), \tag{12}$$
  where $\{\phi^0_M(\underline{\mu})\}$ is a translation-invariant, finite-range m-potential (see [7]).

More explicitly, condition **P1** amounts to assuming the following property. There exists at least one configuration ω of the infinite system minimizing Φ^0_M, for all M, i.e.,

$$\Phi^0_M(\omega) = \min_{\omega'} \Phi^0_M(\omega'), \quad \text{for all } M \subset \mathbb{Z}^d \tag{13}$$

The set of all configurations for which (13) holds are groundstate configurations of $H_0(\underline{\mu})$. Condition **P1** allows us to define local groundstates of the restriction of $H_0(\underline{\mu})$ to a subset of the lattice.

We assume that the perturbation V satisfies, instead of **V1**, the following stronger condition.

- **P2. Finite-Range**
  V is a finite-range translation-invariant perturbation Hamiltonian.

In [2] we construct a unitary transformation, $U(t)$, such that the transformed Hamiltonian,

$$\widetilde{H}(t) \;=\; U(t)H(t)U(t)^{-1},$$

can be cast in the form

$$\widetilde{H}(t) \;=\; H_0(t) \;+\; V(t),$$

such that Pirogov-Sinai theory, see [1, 2], can be applied to the pair $(H_0(t)\,,\,V(t))$, with $H_0(t)$ playing the role of $H_0(\underline{\mu})$ and $V(t)$ playing the role of the quantum perturbation V. In our applications, $U(t)$ will have the form

$$U(t) \;=\; \exp{(tS)}\,,$$

with $S = -S^*$ independent of t. The construction of S is reviewed in Appendix A. This choice of $U(t)$ corresponds to second order perturbation theory. If the accidental degeneracy of the groundstates of $H_0(\underline{\mu})$ is lifted by the perturbation tV in some finite order of perturbation theory one may construct corresponding unitary transformations (see [2]).

In order to apply Theorem 1.1 one has to check that the Hamiltonian $H_0(t)$ satisfies conditions **H1**, **H2**. Condition **H1** requires that there be a tensor-product basis in which $H_0(t)$ is diagonal. Condition **H2** is equivalent to saying that the perturbation lifts the infinite degeneracy of the groundstates to a finite one and that the Peierls condition holds with a (t-dependent) Peierls constant κ. If these conditions hold the spectrum of $H_0(t)$ can be described as follows. Above the groundstate there are "low-energy" states whose energies are separated from the groundstate energy by a (t-dependent) gap κ and "high-energy" states whose energies are separated from the groundstate energy by a gap Δ of order 1.

In order to apply Pirogov-Sinai theory (Theorem 1.2) one has to further check condition **H3**. That the phase diagram of $H_0(\underline{\mu})$ is not regular may mean, for example, that, on the hypersurfaces of the phase diagram separating two regions with different sets of groundstates, there are, besides those of the adjacent regions, (infinitely) many other ones. We have to understand how the degeneracy is lifted by the perturbation: It may happen that the phase diagram of $H_0(t)$ becomes regular or that a new phase appears in a small domain surrounding the hypersurface in question (as in the t-J model treated below).

Concerning condition **V1** the following lemma is proven in [2].

Lemma 1.3 *Assume that the Hamiltonian $H_0(\underline{\mu}) + tV$ satisfies conditions* **H1**, **P1** *and* **P2**. *Then the unitary transformation $U(t)$ (see Appendix A) is such that, for sufficiently small t, the new perturbation $V(t)$ satisfies condition* **V1** *(exponential decay).*

For quantum lattice systems, the perturbation is usually not relatively bounded, and we cannot apply standard theorems of analytic perturbation theory (as in e.g. [11]). We prove that if the Hamiltonian satisfies conditions **P1** and **P2** then the unitary transformation $U(t)$ can be written in terms of *local* operators. The commutativity of operators localized in disjoint subsets of the lattice (see (3)) ensures the exponential decay of the interactions contributing to $\widetilde{H}(t)$.

Note that, when applying Theorems 1.1 or 1.2 to the Hamiltonian $\widetilde{H}(t)$, all relevant parameters κ, ε and λ depend on t.

In subsequent sections we analyze concrete models.

2 The balanced model

We consider the Hamiltonian

$$H_{bal}(t) \;=\; H_{bal}(0) \;+\; tK,$$

where

$$H_{bal}(0) \;=\; \sum_{\substack{\|x-y\|=1\\ \langle xy\rangle\subset\Lambda}} (J\sigma_x^{(3)}\sigma_y^{(3)})n_x n_y \;+\; \sum_{\substack{\|x-y\|=\sqrt{2}\\ \langle xy\rangle\subset\Lambda}} (J'\sigma_x^{(3)}\sigma_y^{(3)})n_x n_y \;+\; \sum_{x\in\Lambda} U n_{x\uparrow}n_{x\downarrow}, \tag{14}$$

and

$$K \;=\; \sum_{\substack{\|x-y\|=1,\\ \langle xy\rangle\subset\Lambda}} K_X \;=\; -\sum_{\substack{\|x-y\|=1,\\ \langle xy\rangle\subset\Lambda}} \;\sum_{\sigma\in\{\uparrow,\downarrow\}} \left(c^\dagger_{x\sigma}c_{y\sigma} \;+\; c^\dagger_{y\sigma}c_{y\sigma}\right)\;. \tag{15}$$

As announced in the introduction, we consider the antiferromagnetic case, i.e., $J > 0$ and $J' > 0$, with $J' = J/2$ and with a large on-site repulsive interaction, $U \gg J$.

The Hamiltonian is defined on any finite subset Λ of $\mathbb{Z}^2$. For convenience, we take Λ to be a large square. In the sequel, we consider the model at half-filling, i.e., the number of particles is equal to the number of sites, $N = \sum_x n_x = |\Lambda|$.

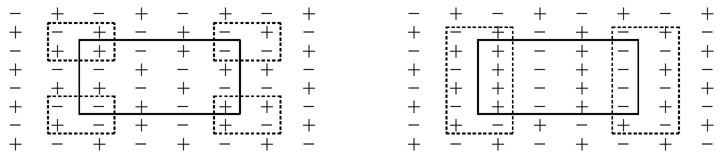

Figure 2: Examples of contours which do not satisfy the Peierls condition

The groundstates of $H_{bal}(0)$ are easily determined by regrouping the interactions so as to express them in terms of an m-potential:

$$H_{bal}(0) = \sum_B \phi^0_B,$$

where

$$\phi^0_B = \sum_{\substack{\|x-y\|=1 \\ <xy>\subset B}} (\frac{J}{2}\sigma^{(3)}_x\sigma^{(3)}_y)n_x n_y + \sum_{\substack{\|x-y\|=\sqrt{2} \\ <xy>\subset B}} (J'\sigma^{(3)}_x\sigma^{(3)}_y)n_x n_y + \sum_{x\in B}\frac{U}{4}n_{x\uparrow}n_{x\downarrow}$$

and B is a two-by-two block. One verifies that ϕ^0_B takes its minimal value for the following configurations (up to rotations by $\pi/2$ and global spin flips).

$$\begin{pmatrix} + & - \\ - & + \end{pmatrix} \quad \begin{pmatrix} + & - \\ + & - \end{pmatrix}$$

The groundstates are the configurations with the property that, on all two-by-two blocks, one encounters one of the above configurations. One can alternatively describe the groundstates as consecutive lines of Néel ordered spins where each line can be flipped independently of the other ones. Their degeneracy is infinite in the thermodynamic limit. The groundstate energy density is

$$e_{bal} = -J.$$

One can see that $H_{bal}(0)$ does not satisfy the Peierls condition: In Fig.2 we display two examples of configurations with one "island" of one groundstate in another groundstate for which the Peierls condition does not hold. The solid lines separate the regions with different groundstates and the dashed lines indicate the parts of the contour which contribute to the energy of the contour. The energy of the configuration shown on the left of Fig.2 does not depend on the length of the contour but only on the number of corners of the contour. The contour separating the two groundstates can be made arbitrarily long without changing its energy. The energy of the configuration shown on the right of Fig.2 is proportional to the vertical pieces of the contour. The length of the contour in the horizontal direction can be arbitrarily long without changing its energy.

Next, we consider the unitary transformation $\exp(tS)$ defined in Appendix A (see (46)). The operator S can be written as a sum of local operators

$$\begin{aligned} S &= \sum_{X=\langle xy\rangle} S_{B_X} \\ &= \sum_{X=\langle xy\rangle} \mathrm{ad}^{-1}\bar{H}_{0X}(K^{01}_{B_X}), \end{aligned}$$

where $X = \langle xy\rangle$ is a pair of nearest neighbours, and B_X, the support of the operator S_{B_X}, is the set of lattice sites at distance ≤ 1 from X (see (36)). The local operators $\bar{H}_{0X}$ are defined in (42), and

$$K^{01}_{B_X} = P^0_{B_X}K_X P^1_{B_X} + P^1_{B_X}K_X P^0_{B_X}$$

where K_X is given by (15) and $P^0_{B_X}$, $P^1_{B_X}$ are local projection operators with support B_X (see (37)). The operators $P^0_{B_X}$ are the projections onto the subspaces of states which, when restricted to B_X, are groundstates of $H_{bal}(0)$, and $P^1_{B_X}$ are the projections onto the subspaces of states which, when restricted to B_X, are excited states, the excitation being localized in X.

The transformed Hamiltonian reads (see (48))

$$\begin{aligned}\widetilde{H}_{bal}(t) &= \exp(tS)\, H_{bal}(t)\, \exp(-tS) \\ &= H_0(t) + V(t),\end{aligned}$$

with

$$H_0(t) = H_{bal}(0) + t \sum_{X=\langle xy\rangle} K^{00}_{B_X} + \frac{t^2}{2} \sum_{X=\langle xy\rangle} P^0_{B_X} \mathrm{ad} S_{1B_X}(K^{01}_{B_X}) P^0_{B_X} \ , \tag{16}$$

where $K^{00}_{B_X}$ is defined in (39), and $\mathrm{ad}A(B)$ denotes the commutator, $AB - BA$.

The second term of (16) vanishes and the third one gives a contribution to the groundstate energy given by

$$\begin{aligned}&\frac{t^2}{2} \sum_{X=\langle xy\rangle} [\mathrm{ad}^{-1} \bar{H}_{0X}(P^0_{B_X} K_X P^1_{B_X})\, P^1_{B_X} K_X P^0_{B_X} - P^0_{B_X} K_X P^1_{B_X}\, \mathrm{ad}^{-1} \bar{H}_{0X}(P^1_{B_X} K_X P^0_{B_X})] \\ &= \sum_{X=\langle xy\rangle} \frac{-t^2}{E_{1X} - E_0} P^0_{B_X} \ ,\end{aligned}$$

where $E_{1X} = 3J + U$ is the energy of the excitation caused by the hopping of a single particle, and E_0 is the groundstate energy of $H_{bal}(0)$.

It is easy to see that the groundstates of $H_0(t)$ are Néel states with an energy density

$$e_0(t) = -J - t^2 \frac{4}{2J + U},$$

and that the Peierls condition holds for $H_0(t)$ with a constant proportional to t^2. By Lemma 1.3 and Theorem 1.1, we have the following result

Proposition 2.1 *There exists a constant t_0 such that:*

1. *For any $0 < t < t_0$, the groundstates of $\widetilde{H}_{bal}(t)$ at half-filling are small perturbations of the Néel states.*

2. *There exists $\beta_0 = \beta_0(t) < \infty$ such that, for $0 < t < t_0$ and $\beta > \beta_0(t)$, the long-range order of the groundstates persists.*

Note that, in Proposition 2.1, t must be *strictly positive.*

3 The $t - J - \lambda - v - v'$ model

In this section, we study the $t - J - \lambda - v - v'$ model, i.e., the family of Hamiltonians

$$H_{t-J}(\lambda, t) = H_{t-J}(0,0) + \lambda V + tK \ ,$$

where

$$H_{t-J}(0,0) = \sum_{\substack{\|x-y\|=1 \\ \langle xy\rangle\subset\Lambda}} \frac{1}{2}\left(J\sigma_x^{(3)}\sigma_y^{(3)} + v\right) n_x n_y + \sum_{\substack{\|x-y\|=\sqrt{2} \\ \langle xy\rangle\subset\Lambda}} v' n_x n_y - \sum_{x\in\Lambda} \mu n_x \tag{17}$$

$$K = -\sum_{\substack{\|x-y\|=1 \\ \langle xy\rangle\subset\Lambda}} \sum_{\sigma\in\{\uparrow,\downarrow\}} \left(c_{x\sigma}^\dagger c_{y\sigma} + c_{y\sigma}^\dagger c_{x\sigma}\right) \tag{18}$$

$$V = \sum_{\substack{\|x-y\|=1 \\ \langle xy\rangle\subset\Lambda}} \left(\sigma_x^{(1)}\sigma_y^{(1)} + \sigma_x^{(2)}\sigma_y^{(2)}\right) n_x n_y. \tag{19}$$

The system described by this Hamiltonian is confined to an arbitrary finite subset Λ of $\mathbb{Z}^2$ which we take, for convenience, to be a large square.

This chapter is organized as follows. We first recall some results, derived by Gruber and Sütö [12], on the Hamiltonian $H_{t-J}(0,0)$. We then investigate the stable phases of $H_{t-J}(\lambda,t)$, for small t and λ. For the regions of the phase diagram where the groundstates of $H_{t-J}(0,0)$ are infinitely degenerate, we use the perturbation scheme of [2] (see Introduction and Appendix A) together with the low-temperature expansion of [1] (Theorem 1.1) to study the degeneracy breaking effect of the perturbation. We determine the low-energy spectrum of $H_{t-J}(\lambda,t)$ to leading order in t and λ, (i.e., to order t^2 and λ^2). We are able to determine all stable phases of the Hamiltonian $H_{t-J}(\lambda,t)$, except for one for which a higher order computation is needed. Finally, we investigate the regularity properties of the Hamiltonian $H_{t-J}(\lambda,t)$ for small t and λ. We have several kinds of results (some of them only at a heuristic level).

(i) For some parts of the phase diagram ($v < J$), it is straightforward to prove, with the help of our perturbation scheme, that the phase diagram of the "unperturbed part", $H_0(\lambda,t)$, of the unitarily equivalent Hamiltonian, $\widetilde{H}(\lambda,t)$, becomes regular. Thus we can apply Pirogov-Sinai theory (Theorem 1.2) and conclude the regularity of the phase diagram at low-temperature.

(ii) For other parts of the phase diagram, our computations indicate that the quantum perturbations induce new phases in a small region surrounding the non-regular part of the Hamiltonian $H_{t-J}(0,0)$. We are not able to predict anything about the stability of these phases because the "unperturbed" part $H_0(\lambda,t)$ does not satisfy condition **H1**: there is a basis in which $H_0(\lambda,t)$ is diagonal, but this is *not* a tensor-product basis. It is an interesting question to ask whether Theorems 1.1 and 1.2 still hold under this weaker condition. Nevertheless, we emphasize that our methods are able to detect the appearance of new quantum phases stabilized by the quantum perturbation in the vicinity of the non-regular part of the phase diagram of $H_{t-J}(0,0)$. If we only wish to prove that the groundstates we find are the true groundstates of $H_{t-J}(\lambda,t)$, we may use another method (the dressing transformation) developed by Albanese [13], as shown in [14].

(iii) On some lines of the phase diagram, the groundstates of $H_{t-J}(0,0)$ describe arbitrary configurations of holes in an antiferromagnetic background with an (extended) hardcore condition, (two holes cannot be nearest neighbours and/or next nearest neighbours), and with a constraint on the density of holes. In order to find the groundstates of the "unperturbed" part $H_0(\lambda,t)$ of the transformed Hamiltonian $\widetilde{H}(\lambda,t)$, we use the following idea (see [15]): the quantum perturbation induces (to a given finite order in the perturbation parameter) an effective finite-range interaction between holes in an antiferromagnetic background. One may hope to be able to derive an effective Hamiltonian that governs the arrangement of holes. An analogous method has been used by Gruber, Jedrzejewski and Lemberger [12], and Kennedy [17], to study the groundstates of the Falicov-Kimball model. It turns out that, for $\lambda > 0, t = 0$, one can derive an effective (Ising-type)

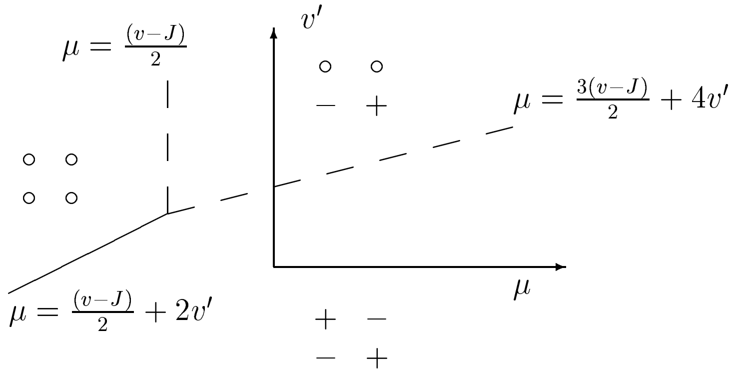

Figure 3: Zero-temperature phase diagram of $H_{t-J}(0,0)$ for $v < J$

Hamiltonian. For $t > 0$, the situation is more involved: for it can happen that the effective Hamiltonian is *not* of finite-range. In our model, we find a phenomenon that could be of some significance for superconductivity: We find that, for $v = J, v' > 0$, the effective Hamiltonian is not of Ising-type: there are terms describing hopping of two next-neighbour holes. Albanese and one of the authors have shown, [18], that the groundstates of two holes in an antiferromagnetic background describe a (delocalized) bound pair. We identify here the region of the phase diagram where such states might occur. This problem as well as related ones (see [19]) are, in our view, worth being further investigated.

3.1 The classical J-v-v' model

We first consider the classical limit of our Hamiltonian ($t = \lambda = 0$)

$$H_{t-J}(0,0) = \sum_{\substack{\|x-y\|=1 \\ (xy)\subset\Lambda}} \frac{1}{2}\left(J\sigma_x^{(3)}\sigma_y^{(3)} + v\right) n_x n_y + \sum_{\substack{\|x-y\|=\sqrt{2} \\ (xy)\subset\Lambda}} v' n_x n_y - \sum_{x\in\Lambda} \mu n_x .$$

This model is equivalent to a spin-1 model. Is has several physical interpretations, e.g., $He^3 - He^4$ mixtures, ternary mixtures, or diluted magnetic alloys. We recall some results, derived in [12], about the phase diagram of this model at low-temperature.

In order to find the groundstates, we regroup the interactions so as to express $H_{t-J}(0,0)$ in terms of an m-potential,

$$H_{t-J}(0,0) = \sum_B \phi_B^0 ,$$

where B is a square containing four lattice sites and

$$\phi_B^0 = \sum_{\substack{\|x-y\|=1 \\ <xy>\subset B}} \frac{1}{4}\left(J\sigma_x^{(3)}\sigma_y^{(3)} + v\right) n_x n_y + \sum_{\substack{\|x-y\|=\sqrt{2} \\ <xy>\subset B}} v' n_x n_y - \sum_{x\in B} \frac{1}{4}\mu n_x .$$

On a square B there are 3^4 possible configurations. Since we consider the case $J > 0$, we can exclude all configurations on the square B where one pair of nearest neighbour spins is parallel. This reduces the number of possible configurations to 35. The invariance of the Hamiltonian under rotations by $\pi/2$ and under spin flip splits these configurations into 6 groups listed below.

$$\omega_B \in \left\{ \begin{pmatrix} + & - \\ - & + \end{pmatrix} \begin{pmatrix} + & - \\ - & \circ \end{pmatrix} \begin{pmatrix} \circ & \circ \\ - & + \end{pmatrix} \begin{pmatrix} \circ & - \\ + & \circ \end{pmatrix} \begin{pmatrix} \circ & \circ \\ \circ & + \end{pmatrix} \begin{pmatrix} \circ & \circ \\ \circ & \circ \end{pmatrix} \right\}$$

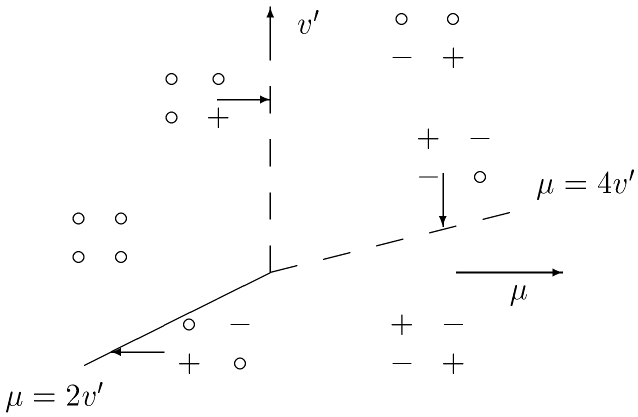

Figure 4: Zero-temperature phase diagram of $H_{t-J}(0,0)$ for $v = J$

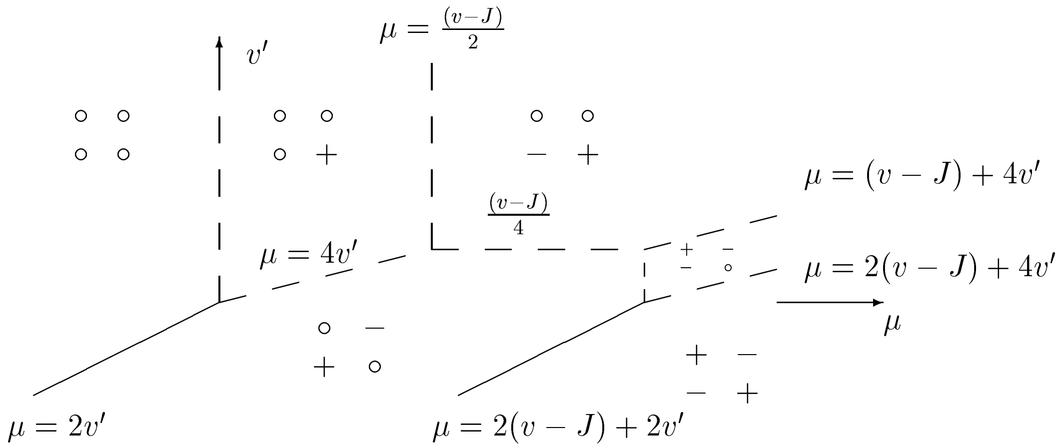

Figure 5: Zero-temperature phase diagram of $H_{t-J}(0,0)$ for $v > J$

The groundstates are obtained by constructing configurations which, when restricted to an arbitrary square B, are among those 35 allowed configurations. Note that the energy per site of any one of these configurations, ω, is equal to the value of $\phi_B(\omega)$. The zero-temperature phase diagram of $H_{t-J}(0,0)$ is shown in Figs. 3, 4 and 5 for different domains of the parameters. On the phase boundaries of the phase diagram, the allowed configurations on each square B are those allowed on both sides of the boundaries, except when $v = J$, where additional allowed configurations exist; see Fig.4.

On the solid lines, the groundstates are those of both regions adjacent to the line. Hence the phase diagram is regular on the solid lines. On the dashed lines, apart from the groundstates of both regions adjacent to the line, there are infinitely many other groundstates. The phase diagram is therefore not regular on the dashed lines.

The low-temperature phase diagram of this model has been studied by Gruber and Süto [12]. They show how to extend the usual Peierls argument and Pirogov-Sinai theory to some models with an infinite number of groundstates. Their key idea is to introduce an equivalence relation among groundstates and to replace the concept of groundstates by the concept of equivalence classes. Furthermore, they introduce some conditions replacing the Peierls condition. A necessary condition for their Peierls argument to apply is that the model has a residual entropy. They prove e.g. that the ordering of the groundstates described by $\begin{pmatrix} \circ & - \\ + & \circ \end{pmatrix}$ survives at finite temperature, and that there are coexistence lines between three or four phases which are small deformations of the solid lines shown in Fig.5.

3.2 The stable phases of the $t - J - \lambda - v - v'$ model

In this section, we discuss the stability of phases under perturbations in open domains of parameter space excluding the phase boundaries of $H_{t-J}(0,0)$. The phase boundaries are discussed in Sections 3.3 and 3.4.

For the region of the phase diagram where the groundstates of $H_{t-J}(0,0)$ are the Néel states or the empty lattice, one can directly apply the low-temperature expansion of [1] (Theorem 1.1) and prove the persistence of long-range order for small values of λ and t and for low enough temperatures.

For the other phases the degeneracy is infinite. An explicit description of the degeneracy in different regions of the phase diagram follows below. Then one has to apply the perturbation scheme described in Appendix A and compute the groundstates of $H_0(\lambda, t)$. The perturbations are given by

$$V = \sum_{X=\langle xy\rangle} V_X \,, \quad K = \sum_{X=\langle xy\rangle} K_X \,,$$

where $X = \langle xy\rangle$ is a pair of nearest neighbours, and V_X and K_X are given in eqs. (19) and (18). The unitary transformation is given by $U(\lambda,t) = \exp\left(tS^K + \lambda S^V\right)$, where

$$\begin{aligned} S^K &= \sum_X S^K_{B_X} = \sum_X \mathrm{ad}^{-1}\bar{H}_{0X}\left(K^{01}_{B_X}\right) && (20)\\ S^V &= \sum_X S^V_{B_X} = \sum_X \mathrm{ad}^{-1}\bar{H}_{0X}\left(V^{01}_{B_X}\right). && (21) \end{aligned}$$

Here B_X is the set of sites at distance ≤ 1 from X; the operators $\bar{H}_{0X}$, $K^{01}_{B_X}$ and $V^{01}_{B_X}$ are defined in Appendix A (see (40), (42) and (43)). The transformed Hamiltonian, $\widetilde{H}_{t-J}(\lambda,t)$, has the form

$$\begin{aligned} \widetilde{H}_{t-J}(\lambda,t) &= U(\lambda,t)H_{t-J}(\lambda,t)U(\lambda,t)^{-1} \,,\\ &= H_0(\lambda,t) + V(\lambda,t) \end{aligned}$$

where

$$\begin{aligned} H_0(\lambda,t) = {} & H_{t-J}(0,0) + t\sum_{X=\langle xy\rangle} K^{00}_{B_X} + \lambda \sum_{X=\langle xy\rangle} V^{00}_{B_X} \\ & +\frac{t^2}{2}\sum_{X=\langle xy\rangle} P^0_{B_X}\,\mathrm{ad}S^K_{B_X}(K^{01}_{B_X})P^0_{B_X} \\ & +\frac{\lambda^2}{2}\sum_{X=\langle xy\rangle} P^0_{B_X}\,\mathrm{ad}S^V_{B_X}(V^{01}_{B_X})P^0_{B_X} \\ & +\frac{\lambda t}{2}\sum_{X=\langle xy\rangle} P^0_{B_X}\left(\mathrm{ad}S^K_{B_X}(V^{01}_{B_X}) + \mathrm{ad}S^V_{B_X}(K^{01}_{B_X})\right)P^0_{B_X} \,, \qquad (22) \end{aligned}$$

$$
\begin{array}{cccccc}
- & + & - & + & - & + \\
+ & \circ & + & \circ & + & \circ \\
- & + & - & + & - & + \\
\circ & - & \circ & - & \circ & - \\
- & + & - & + & - & + \\
+ & \circ & + & \circ & + & \circ
\end{array}
\qquad\qquad
\begin{array}{cccccc}
- & + & - & + & - & + \\
+ & \circ & + & \circ & + & \circ \\
- & + & - & + & - & + \\
+ & \circ & + & \circ & + & \circ \\
- & + & - & + & - & + \\
+ & \circ & + & \circ & + & \circ
\end{array}
$$

Figure 6: Groundstates $(1/4_d)$ and $(1/4_v)$ of $H_0(\lambda, t)$, for hole density 1/4

and $K^{00}_{B_X}$ and $V^{00}_{B_X}$ are given by (39). The operator $V(\lambda, t)$ can be written as a sum of local terms, which, by Lemma 1.3, satisfy condition **V1** (see Appendix A).

Next, we compute the groundstates of $H_0(\lambda, t)$ for the different parts of the phase diagram. Note that $K^{00}_{B_X}$ and the last two terms of (22) vanish: there is no contribution of order t and of order λt. The other terms yield

$$
\begin{aligned}
\frac{t^2}{2} P^0_{B_X} \mathrm{ad} S^K_{B_X}(K^{01}_{B_X}) P^0_{B_X} &= -t^2 \sum_X \frac{1}{E^K_{1X} - E_0} P^0_{B_X} && (23) \\
\frac{\lambda^2}{2} P^0_{B_X} \mathrm{ad} S^V_{B_X}(V^{01}_{B_X}) P^0_{B_X} &= -\lambda^2 \sum_X \frac{1}{E^V_{1X} - E_0} P^0_{B_X} \ , && (24)
\end{aligned}
$$

where E_0 is the groundstate energy of $H_{t-J}(0,0)$, E^K_{1X} is the energy of the excitation caused by the hopping of a particle, and E^V_{1X} is the energy of the excitation caused by flipping a pair of nearest neighbour spins. We have the following results for the different regions of the phase diagram (see Figs.3, 4 and 5).

(i) $\omega_B \in \left\{ \begin{pmatrix} + & - \\ - & \circ \end{pmatrix} \right\}$.

The groundstates of $H_{t-J}(0,0)$ consist of lines of Néel-ordered spins alternating with lines with particle density 1/2. The degeneracy is infinite since the positions of the holes in each line are independent of the other lines. Both kinds of terms, the magnetic terms and the hopping terms, lift the degeneracy of the groundstates. The magnetic fluctuations favour the arrangement of holes $(1/4_d)$ shown on the left of Fig.6. The hopping terms favour the same arrangement, for $v' < (v-J)/4$, and the arrangement $(1/4_v)$ shown on the right of Fig.6, for $v' > (v-J)/4$. The corresponding groundstate energy densities are given by

$$
\begin{aligned}
e(1/4_d) &= \frac{(v-J)}{2} + v' - \frac{3\mu}{4} - \frac{7\lambda^2}{6J} - t^2 \left(\frac{1}{4v' + 6J} + \frac{1}{v + 5J} \right) \\
e(1/4_v) &= \frac{(v-J)}{2} + v' - \frac{3\mu}{4} - \frac{\lambda^2}{J} - t^2 \left(\frac{2}{v + 5J} \right) .
\end{aligned}
$$

(ii) $\omega_B \in \left\{ \begin{pmatrix} \circ & \circ \\ \circ & + \end{pmatrix} \right\}$.

The groundstates of $H_{t-J}(0,0)$ can be described as lines of holes alternating with lines with particle density 1/2. The degeneracy is infinite since the positions of the particles in one line are independent of the other lines and the orientations of the spins are arbitrary. The magnetic terms do not lift the degeneracy of the groundstates. The hopping terms favour antiferromagnetic ordering between spins at distance 2 within the lines. The hopping terms favour the groundstates

$$
\begin{array}{cccccc}
\circ & \circ & \circ & \circ & \circ & \circ \\
+ & \circ & - & \circ & + & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ \\
- & \circ & + & \circ & - & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ \\
+ & \circ & - & \circ & + & \circ
\end{array}
\qquad\qquad
\begin{array}{cccccc}
\circ & \circ & \circ & \circ & \circ & \circ \\
\circ & + & \circ & - & \circ & + \\
\circ & \circ & \circ & \circ & \circ & \circ \\
- & \circ & + & \circ & - & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ \\
\circ & + & \circ & - & \circ & +
\end{array}
$$

Figure 7: Groundstates $(3/4_v)$ and $(3/4_d)$ of $H_0(\lambda, t)$, for hole density 3/4

$$
\begin{array}{cccccc}
\circ & \circ & \circ & \circ & \circ & \circ \\
+ & - & + & - & + & - \\
\circ & \circ & \circ & \circ & \circ & \circ \\
- & + & - & + & - & + \\
\circ & \circ & \circ & \circ & \circ & \circ \\
+ & - & + & - & + & -
\end{array}
$$

Figure 8: Groundstates $(1/2_{af})$ of $H_0(\lambda, t)$, for hole density 1/2

$(3/4_v)$ shown on the left of Fig.7, for $v' > (v-J)/4$, and the groundstates $(3/4_d)$ shown on the right of Fig.7, for $v' < (v-J)/4$. The degeneracy of the groundstates $(3/4_d)$ is still infinite. (The spins in every line of density 1/2 can be flipped, independently in different lines.) We expect this degeneracy to be lifted only by the terms of order t^4 of the perturbation series. The corresponding groundstate energy densities are given by

$$
\begin{aligned}
e(3/4v) \quad &= \quad \frac{(v-J)}{2} + v' - \frac{1}{4}\mu - t^2\left(\frac{2}{v-J}\right) \\
e(3/4d) \quad &= \quad \frac{(v-J)}{2} + v' - \frac{1}{4}\mu - t^2\left(\frac{1}{v-J} + \frac{1}{2v'}\right).
\end{aligned}
$$

(iii) $\omega_B \in \left\{\left(\begin{smallmatrix} \circ & \circ \\ + & - \end{smallmatrix}\right)\right\}$.

The groundstates of $H_{t-J}(0,0)$ are lines of holes alternating with lines of Néel-ordered spins. The magnetic terms do not lift the degeneracy of the groundstates. The hopping terms do: they favour the antiferromagnetic ordering $(1/2_{af})$ of the spins at distance two (Fig.8). The groundstate energy density is given by

$$
e(1/2_{af}) = \frac{(v-J)}{4} - \frac{\mu}{2} - \frac{\lambda^2}{J} - \frac{2t^2}{8v' - (v-J)}.
$$

(iv) $\omega_B \in \left\{\left(\begin{smallmatrix} \circ & - \\ + & \circ \end{smallmatrix}\right)\right\}$.

In the groundstates of $H_{t-J}(0,0)$ the holes and the particles are arranged in a checkerboard configuration, the orientation of the spins is arbitrary. We discuss this case in [2]. It is shown there that, for $v' > 5J/3$, the degeneracy of the groundstates becomes finite in order t^4; the spins are aligned in one diagonal direction and Néel ordered in the other diagonal direction.

We now apply Theorem 1.1 (the low-temperature expansion) to the Hamiltonian

$$\widetilde{H}_{t-J}(\lambda, t) \;=\; H_0(\lambda, t) \;+\; V(\lambda, t),$$

in the region of parameters, where $H_0(\lambda, t)$ has a finite number of groundstates. Lemma 1.3 ensures that $V(\lambda, t)$ satisfies condition **V1**. Condition **H1** is clearly satisfied, since $H_0(\lambda, t)$ is diagonal in the same basis as H_0. To check the Peierls condition, we use the criterion of Holzstynsky and Slawny, (see [7] and Appendix B). We decompose the Hamiltonian as follows,

$$H_0(\lambda, t) = \sum_{M \subset \Lambda} \phi_M(\lambda, t),$$

where M is a four by four box containig 16 lattice sites, and

$$\begin{aligned}\phi_M(\lambda, t) = & \sum_{\substack{\|x-y\|=1 \\ \langle xy\rangle \subset M}} \frac{1}{24}\left(J\sigma_x^{(3)}\sigma_y^{(3)} + v\right) n_x n_y + \sum_{\substack{\|x-y\|=\sqrt{2} \\ \langle xy\rangle \subset M}} \frac{v'}{9} n_x n_y \\ & - \sum_x \frac{\mu}{16} n_x + \frac{1}{2} \sum_{\substack{X=\langle xy\rangle: \\ B_X \subset M}} P^0_{B_X}\left(\frac{\lambda^2}{2}\mathrm{ad}S^V_{1B_X}(V^{01}_{B_X}) + \frac{t^2}{2}\mathrm{ad}S^K_{1B_X}(K^{01}_{B_X})\right) P^0_{B_X}.\end{aligned}$$

Since the periodic groundstates found in this section (their degeneracy is finite) have all period 4, it is easily seen that the terms $\{\phi_M\}$ form an m-potential and hence, by the criterion quoted in Appendix B, $H_0(\lambda, t)$ satisfies the Peierls condition. Using Theorem 1.1 and Lemma 1.3, we obtain the following result.

Proposition 3.1 *For each choice of μ, $v - J$ and v' for which the groundstates of $H_0(\lambda, t)$ are $(1/4_d)$, $(1/4_v)$, $(3/4_v)$ or $(1/2_{af})$ (see Figs 6, 7 and 8) there are constants t_0 and λ_0 depending on μ, $v - J$ and v' such that*

1. *For $0 < \lambda < \lambda_0$ and $0 < t < t_0$, the groundstates of $\widetilde{H}_{t-J}(\lambda, t)$ are small perturbations of the groundstates of $H_0(\lambda, t)$.*
2. *For $0 < \lambda < \lambda_0$ and $0 < t < t_0$, and for low enough temperature (depending on t and λ), the long-range order of the groundstates of $\widetilde{H}_{t-J}(\lambda, t)$ persists.*

3.3 Regularity of the phase diagram (groundstates on the phase boundaries of $H_{t-J}(0, 0)$)

In this section we investigate the regularity properties of the phase diagram of the Hamiltonian $H_0(\lambda, t)$, i.e., we investigate how the perturbation Hamiltonians lift the infinite degeneracy of the non-regular part of the phase diagram of $H_{t-J}(0, 0)$ (the dashed lines of Figs. 3, 4 and 5).

(i) $v < J$, (see Fig.3).

- $\mu = (v - J)/2$, $\omega_B \in \left\{\begin{pmatrix} \circ & \circ \\ - & + \end{pmatrix}\begin{pmatrix} \circ & \circ \\ \circ & \circ \end{pmatrix}\right\}$.

  The groundstates of $H_{t-J}(0, 0)$ consist of lines of particles and lines of holes with the constraint that there not be two consecutive lines of particles. The magnetic (exchange) energy is minimized for the groundstates where lines of particles and lines of holes alternate. The hopping terms favour the same groundstates. In addition, in each line of alternating holes and particles, the kinetic energy is minimized if the spins of two consecutive particles (at distance 2) are anti-parallel (Fig.8). Hence the phase diagram of the classical part, $H_0(\lambda, t)$, of the unitarily equivalent Hamiltonian $\widetilde{H}_{t-J}(\lambda, t)$ becomes regular.

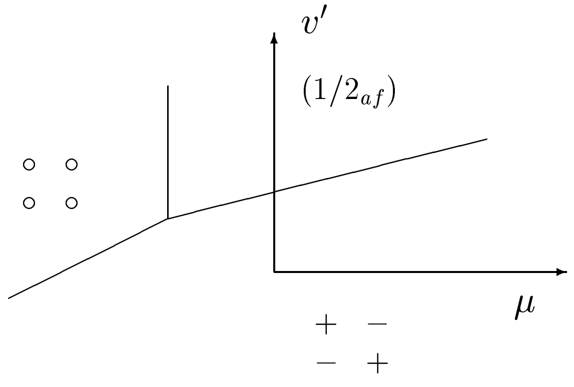

Figure 9: Zero-temperature phase diagram of $H_0(\lambda, t)$ for $v < J$

- $\mu = 3(v - J)/2 + 4v'$, $\omega_B \in \left\{ \begin{pmatrix} \circ & \circ \\ - & + \end{pmatrix} \begin{pmatrix} + & - \\ - & + \end{pmatrix} \right\}$.

  The groundstates of $H_{t-J}(0,0)$ consist of lines of holes and lines of particles without consecutive lines of holes. The magnetic perturbation favours the Néel states and the hopping terms the groundstates shown in Fig.8. Hence, the phase diagram of $H_0(\lambda, t)$ is regular.

The zero-temperature phase diagram of $H_0(\lambda, t)$, for $v < J$, is shown in Fig.9. With the results of Section 3.2 and Theorem 1.2, we obtain the following proposition:

Proposition 3.2 *There are constants t_0 and λ_0 such that, for $0 < t < t_0$, $0 < \lambda < \lambda_0$ and for $v < J$, the phase diagram of the Hamiltonian $\widetilde{H}_{t-J}(\lambda, t)$ is a smooth deformation of the zero-temperature phase diagram of $H_0(\lambda, t)$, provided the temperature is low enough (depending on t and λ).*

(ii) $v = J$, (see Fig.4).

- At the point $\mu = 0, v' = 0$,

$$\omega_B \in \left\{ \begin{pmatrix} + & - \\ - & + \end{pmatrix} \begin{pmatrix} + & - \\ - & \circ \end{pmatrix} \begin{pmatrix} \circ & \circ \\ - & + \end{pmatrix} \begin{pmatrix} \circ & - \\ + & \circ \end{pmatrix} \begin{pmatrix} \circ & \circ \\ \circ & + \end{pmatrix} \begin{pmatrix} \circ & \circ \\ \circ & \circ \end{pmatrix} \right\}.$$

  At this point of the phase diagram, any configuration of particles (with suitably ordered spins) and holes is a groundstate configuration of $H_{t-J}(0,0)$. It is not difficult to see that the magnetic perturbation favours the groundstates of spin singlet dimers with hole density 1/2 (see Fig.10), because these are the only configurations for which the terms $\lambda V_{B_X}^{00}$ in (22) yield a negative contribution to the energy. Their energy density is

$$e(1/2_d) = \frac{(v - J)}{8} + \frac{v'}{2} - \frac{\mu}{2} - \frac{\lambda}{2} + O(\lambda^2, t^2). \tag{25}$$

  Note that the Hamiltonian $H_0(\lambda, t)$ does not satisfy Condition **H1**, it is diagonal in a basis which is *not* a tensor-product basis. Nevertheless, given $\lambda > 0$, we conjecture that one can use low-temperature expansion methods to prove that, in a small neighbourhood of $\{J = v\,, v' = 0\,, \mu = 0\}$, and for low-enough temperatures, the ordering described on the left of Fig. 10 survives.

$$
\begin{array}{cccccc}
\circ & \circ & sdi & \circ & \circ \\
sdi & \circ & \circ & sdi \\
\circ & \circ & sdi & \circ & \circ \\
sdi & \circ & \circ & sdi \\
\circ & \circ & sdi & \circ & \circ \\
sdi & \circ & \circ & sdi
\end{array}
\qquad\qquad
\begin{array}{cccccc}
\circ & \circ & \circ & \circ & \circ & \circ \\
sdi & \circ & sdi & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ \\
sdi & \circ & sdi & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ \\
sdi & \circ & sdi & \circ
\end{array}
$$

$$sdi = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Figure 10: Dimer configurations with hole densities 1/2 and 2/3

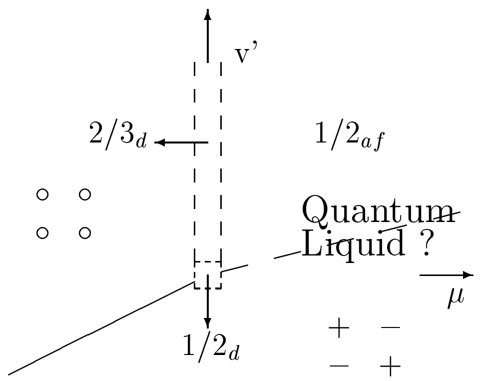

Figure 11: Zero-temperature phase diagram of $H_0(\lambda, t)$ for $v = J$

- $\mu = 0, v' > 0$, $\omega_B \in \left\{ \begin{pmatrix} \circ & \circ \\ - & + \end{pmatrix} \begin{pmatrix} \circ & \circ \\ \circ & + \end{pmatrix} \begin{pmatrix} \circ & \circ \\ \circ & \circ \end{pmatrix} \right\}$.

  The groundstates of $H_{t-J}(0,0)$ consist of segments of lines of particles of arbitrary length isolated by walls of holes. For $\lambda \ll v'$, the magnetic perturbation favours the phases of dimers with hole density 2/3 described in Fig.10, since these are the only states whose energy has a contribution proportional to λ. Their energy density is

$$e(2/3_d) = \frac{(v-J)}{12} - \frac{\mu}{3} - \frac{\lambda}{3} + O(\lambda^2, t^2). \tag{26}$$

  Note that the degeneracy of the groundstates remains infinite.

- The line $\mu = 4v'$ is discussed in Sect. 3.4.

(iii) $v > J$ (see Fig. 5).

- On the lines $\mu = 0$, ($\mu = 4v'$), $\omega_B \in \left\{ \begin{pmatrix} \circ & \circ \\ \circ & + \end{pmatrix} \begin{pmatrix} \circ & \circ \\ \circ & \circ \end{pmatrix} \right\}$ $\left(\left\{ \begin{pmatrix} \circ & - \\ + & \circ \end{pmatrix} \begin{pmatrix} \circ & \circ \\ \circ & + \end{pmatrix} \right\}, \text{resp.} \right)$.

  The groundstates of $H_{t-J}(0,0)$ consist of isolated particles with hardcore conditions. The magnetic perturbation does not lift the degeneracy of the groundstates. This is a domain of the phase diagram where we do not understand how the hopping perturbation lifts the degeneracy.

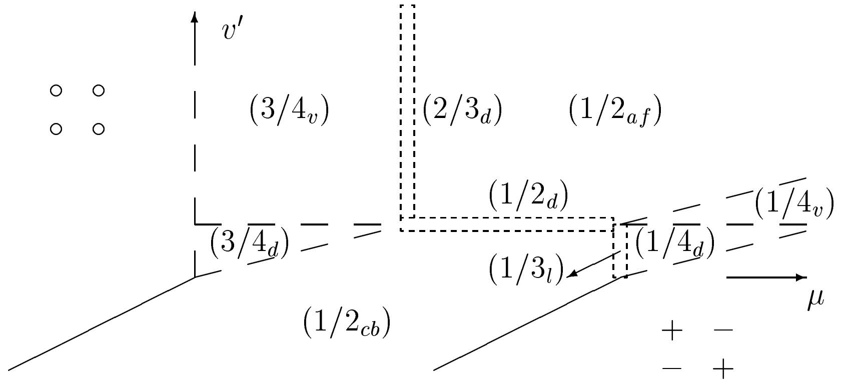

Figure 12: Zero-temperature phase diagram of $H_0(\lambda, t)$ for $v > J$

- $\mu = (v - J)$, $v' \geq (v - J)/4$, $\omega_B \in \left\{ \begin{pmatrix} \circ & \circ \\ - & + \end{pmatrix} \begin{pmatrix} \circ & \circ \\ \circ & + \end{pmatrix} \right\}$.

  The magnetic perturbation again favours the phase of dimers with hole density 2/3 shown on the right of Fig.10, with energy density given in (26).

- $v' = (v - J)/4$, $\omega_B \in \left\{ \begin{pmatrix} \circ & \circ \\ - & + \end{pmatrix} \begin{pmatrix} \circ & - \\ + & \circ \end{pmatrix} \right\}$.

  The groundstates of $H_{t-J}(0,0)$ consist of consecutive lines with hole density 1/2, the position of the holes in one line being independent of the position of the holes in the adjacent lines. It is not difficult to check that the magnetic perturbation favours the groundstate of dimers with hole density 1/2, shown on the left of Fig.10, with energy density given in (25).

3.4 Effective Hamiltonians for configurations of holes in an antiferromagnetic background

In this section, we investigate some non-regular parts of the phase diagrams shown in Figs.4 and 5, where the groundstates of $H_{t-J}(0,0)$ can be described as a "liquid" of holes. The positions of the holes are constrained by an extended hardcore condition, and the density of holes must belong to a certain interval.

1. For $v > J$, on the line $\mu = 2(v - J) + 4v'$, the groundstates correspond to arbitrary configurations of holes in the antiferromagnetic background without any pairs of nearest neighbour (n.n.) and next nearest neighbour (n.n.n.) holes, and the hole density is between 0 and 1/4.

2. For $v > J$, on the line $\mu = 2(v - J)$, the groundstates correspond to arbitrary configurations of holes without any pairs of n.n., and the hole density is between 0 and 1/2, for $v' = 0$, and between 1/4 and 1/2, for $v' > 0$.

3. For $v = J$ (resp. $v > J$), on the line $\mu = 4v'$ (resp. $\mu = (v - J) + 4v'$), the groundstates correspond to arbitrary configurations of holes without any pair of n.n.n., and the hole density is between 0 and 1/2, for $v = J$, (between 1/4 and 1/2, for $v > J$, respectively).

We shall consider only cases 1 and 2, for $\lambda > 0$, $t = 0$ (case 3 can be treated in a similar way), and case 3 for $t > 0$.

We first consider the case $\lambda > 0, t = 0$. In order to find the groundstates of $H_0(\lambda, 0)$, we work in the canonical ensemble, i.e., we fix the number of holes and compute their interaction by performing the unitary transformation (21). In a sense, we eliminate ("trace out") the spin degrees of freedom and obtain an effective (Ising-type) Hamiltonian governing the arrangement of holes in the antiferromagnetic background.

The energy, $E(\{x_1, \ldots, x_n\})$, of a configuration of holes at sites $x_1, \ldots, x_n$ is normalized by subtracting the energy of the half-filled lattice, $E_{h.f.} = |\Lambda| \left((v - J) + 2v' - 4\lambda^2/3J\right)$. We set

$$\begin{aligned} \varepsilon(\{x_1, \ldots, x_n\}) &= \varepsilon(x_1 - x_2, \ldots, x_1 - x_n) \\ &\equiv E(\{x_1, \ldots, x_n\}) - E_{h.f.}, \end{aligned}$$

and recursively define *N-body potentials*

$$\begin{aligned} &\mathcal{U}_N(\{x_1, \ldots, x_N\}) = \mathcal{U}_N(x_1 - x_2, \ldots, x_1 - x_N) \\ &= \varepsilon(\{x_1, \ldots, x_N\}) - \sum_{j=1}^{N-2} \sum_{\{i_1, \ldots, i_j\} \subset \{1, \ldots, N\}} \mathcal{U}_{N-j}(\{x_1, \ldots, x_N\} \backslash \{x_{i_1}, \ldots, x_{i_j}\}) - \sum_{i=1}^{N} \varepsilon(x_i). \end{aligned}$$

All the energies and N-body potentials are invariant under translations, rotations by $\pi/2$ and reflections.

It is now straightforward, but lengthy, to compute the effective Hamiltonians in different regimes. They have the following form

$$\begin{aligned} H_{eff} &= \sum_x \varepsilon(x) n_x + \sum_{xy} \mathcal{U}_2(x - y) n_x n_y + \sum_{xyz} \mathcal{U}_3(x - y, x - z) n_x n_y n_z \\ &\quad + \sum_{xyzw} \mathcal{U}_4(x - y, x - z, x - w) n_w n_x n_y n_z \end{aligned} \tag{27}$$

where $n_x = 0, 1$ is the hole number operator at site x. The hole selfenergy is given by

$$\varepsilon(x) \equiv \varepsilon = -2(v - J) - 4v' + \frac{16\lambda^2}{15J}. \tag{28}$$

The two-body potentials are given by

$$\mathcal{U}_2(e_1) = \frac{(v - J)}{2}, \tag{29}$$

$$\mathcal{U}_2(e_1 + e_2) = v' + \frac{4\lambda^2}{15J}, \tag{30}$$

$$\mathcal{U}_2(2e_1) = \frac{2\lambda^2}{15J}, \tag{31}$$

$$\mathcal{U}_2(2e_1 + e_2) = -\frac{3\lambda^2}{15J}, \tag{32}$$

$$\mathcal{U}_2(3e_1) = -\frac{1\lambda^2}{15J}, \tag{33}$$

where e_1 and e_2 are the unit vectors of the lattice $\mathbb{Z}^2$. The three-body and four-body potentials are considered below, for different regimes.

$$\begin{array}{ccc} \bullet & \circ & \bullet \\ \bullet & \bullet & \bullet \\ \circ & \bullet & \circ \end{array} \quad -\frac{\lambda^2}{15J}$$

Figure 13: Three-body potential in the presence of n.n. and n.n.n. hardcore condition

$$\begin{array}{cccccc} - & + & - & + & \circ & + \\ + & - & \circ & - & + & - \\ \circ & + & - & + & - & \circ \\ + & - & + & \circ & + & - \\ - & \circ & - & + & - & + \\ + & - & + & - & \circ & - \end{array} \qquad \begin{array}{cccccc} \circ & + & \circ & + & \circ & + \\ + & - & + & - & + & - \\ - & \circ & - & \circ & - & \circ \\ + & - & + & - & + & - \\ \circ & + & \circ & + & \circ & + \\ + & - & + & - & + & - \end{array}$$

Figure 14: Groundstates of H_{eff} with n.n. and n.n.n. hardcore conditions for densities $1/5$ and $1/4$

Finding the groundstates of such Ising-type Hamiltonians is, a priori, not easy. One way of finding them is to prove that one can express H_{eff} in terms of an m-potential. This is usually not possible. A more refined way, (see [17]), is to find a decomposition $H_{eff} = \sum_M \phi_M$ of the Hamiltonian and an auxiliary family of interactions K_M such that $\sum_M K_M = 0$. Then one has to find configurations minimizing $\phi_M + K_M$. We expect that this method would yield rigorous results on the groundstates of the Hamiltonians derived above, but we shall not prove such results in this paper.

For the case of a n.n and a n.n.n hardcore condition, the 2-body potentials are given by (31), (32) and (33). The only other non-vanishing many-body potential is the 3-body potential; see Fig.13. In Fig.14, we show the conjectured groundstates for hole density $1/5$ and $1/4$.

The corresponding energy densities are

$$e(1/5) = \frac{3(v-J)}{5} + \frac{6v'}{5} - \frac{4\mu}{5} - \frac{6\lambda^2}{5J} \tag{34}$$

$$e(1/4_d) = \frac{(v-J)}{2} + v' - \frac{3\mu}{4} - \frac{7\lambda^2}{6J}. \tag{35}$$

In the corresponding part of the phase diagram

$$v > J, \ \ \mu = 2(v-J) + 4v' - 2\lambda^2/3J,$$

it is easy to check that the Néel states, the groundstates with hole densities $1/4$ and $1/5$ (Fig.14) are degenerate. This leads to the following conjecture on the groundstates of $H_0(\lambda, 0)$: On the line $\mu = 2(v-J) + 4v' - 2\lambda^2/3J$ the groundstates consist of parallel lines of lattice sites which are either completely occupied by holes or completely occupied by particles, the slope of the lines with respect to the lattice is $(2,1)$, $(2,-1)$, $(1,2)$ or $(-1,2)$. The degeneracy is still infinite in this part of the phase diagram, and, to this order, the phase diagram is not regular.

For the case of a n.n. hardcore condition, the 2-body potentials are given by (30), (31), (32) and (33). The non-vanishing 3-body potentials are given by (3b.1), (3b.2) (3b.3)and (3b.4) in Fig.15,

$$\begin{array}{cccc} \bullet & \circ & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ \circ & \bullet & \circ & \bullet \end{array} \; -\tfrac{\lambda^2}{15J} \; (3b.1) \qquad \begin{array}{cccc} \bullet & \bullet & \bullet & \bullet \\ \bullet & \circ & \bullet & \bullet \\ \circ & \bullet & \circ & \bullet \end{array} \; +\tfrac{2\lambda^2}{15J} \; (3b.2) \qquad \begin{array}{cccc} \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \circ & \bullet \\ \circ & \bullet & \bullet & \circ \end{array} \; -\tfrac{\lambda^2}{15J} \; (3b.3)$$

$$\begin{array}{cccc} \bullet & \circ & \bullet & \bullet \\ \bullet & \bullet & \circ & \bullet \\ \circ & \bullet & \bullet & \bullet \end{array} \; -\tfrac{2\lambda^2}{15J} \; (3b.4)$$

$$\begin{array}{cccc} \bullet & \bullet & \circ & \bullet \\ \circ & \bullet & \bullet & \circ \\ \bullet & \circ & \bullet & \bullet \end{array} \; -\tfrac{2\lambda^2}{15J} \; (4b.1) \qquad \begin{array}{cccc} \bullet & \circ & \bullet & \bullet \\ \circ & \bullet & \circ & \bullet \\ \bullet & \circ & \bullet & \bullet \end{array} \; +\tfrac{4\lambda^2}{15J} \; (4b.2) \qquad \begin{array}{cccc} \bullet & \circ & \bullet & \bullet \\ \circ & \bullet & \bullet & \circ \\ \bullet & \circ & \bullet & \bullet \end{array} \; -\tfrac{2\lambda^2}{15J} \; (4b.3)$$

Figure 15: 3-body and 4-body potentials for n.n. hardcore condition

$$\begin{array}{cccccc} \circ & + & - & \circ & + & - \\ + & \circ & + & - & \circ & + \\ - & + & \circ & + & - & \circ \\ \circ & - & + & \circ & + & - \\ - & \circ & - & + & \circ & + \\ + & - & \circ & - & + & \circ \end{array}$$

Figure 16: Groundstates of H_{eff} with n.n. hardcore conditions for densities 1/3

and the non-vanishing 4-body potentials are given by (4b.1), (4b.2) and (4b.3) in Fig.15. We show, in Fig.16, the conjectured groundstates for density 1/3. The energy density is

$$e(1/3_l) = \frac{(v-J)}{3} + v' - \frac{2\mu}{3} - \frac{4\lambda^2}{3J}.$$

We conjecture that a new phase corresponding to the groundstates with density 1/3 (Fig.16) appears when μ belongs to the interval

$$\mu \in (2(v-J) - 8\lambda^2/J, 2(v-J) + \lambda^2/J),$$

around the line $\mu = 2(v-J)$. Since the groundstates are infinitely degenerate in this phase, one cannot predict anything about its stability.

Possible existence of a Fermi liquid of holes

For the case $t \neq 0$, the situation is more complicated. Then the effective Hamiltonian is, in general, *not* of finite range. Furthermore, for $v = J$ and $\mu = 4v'$, it is *not* of Ising-type: in order t^2, there are terms which correspond to the hopping of a pair of nearest neighbour holes: If $\langle xy \rangle$ denotes a pair nearest neighbour with $y = x + e_j$, $j = 1, 2$

$$T_{hopp} = \sum_{\langle xy \rangle} -\frac{t^2}{J}(c^\dagger_{x+e_j} c_x c^\dagger_{y+e_j} c_y + c^\dagger_{y-e_j} c_y c^\dagger_{x-e_j} c_x)$$

where c_x and $c_x^\dagger$ are the annihilation and creation operator for holes at site x obeying (spinless) fermion anticommutation relations.

This is a region of the phase diagram where we conjecture that the model is *not* a insulator (see [18] and [19] for related results). As one of the key results of this paper we regard this identification of regions in parameter space, where Fermi liquids of holes or superconductivity (see [18]) might appear.

3.5 Conclusions

The phase diagram of the $t-J-v-v'$ model, for small λ and t and at low temperature, shows a surprisingly rich stucture. The methods developed in [1] and [2] permit us to investigate the stability of finitely degenerate phases of $H_{t-J}(0,0)$ under small perturbations and the degeneracy-breaking effect of the perturbations (Proposition 3.1, Section 3.2). They enable us to show that the phase diagram of $H_{t-J}(\lambda,t)$ may be regular even in regions, where the phase diagram of $H_{t-J}(0,0)$ is not (Proposition 3.2, Section 3.3). They also suggest the appearance of several new phases, among them phases of dimers and, possibly, Fermi liquids or superconducting phases (Section 3.4).

A The Unitary conjugations

We consider Hamiltonians, $H(t)$, of the form H_0+tV satisfying conditions **H1**, **P1** and **P2** specified in the introduction. We briefly recall here the construction of the unitary transformation $U(t)$ used throughout the paper and refer to [2] for proofs and for extension of the methods to higher orders.

By condition **P1**, H_0 can be expressed in terms of finite-range, translation invariant m - potentials (see [7] and (12)). We define the set of groundstate configurations of H_0 associated with a subset Y of Λ as follows:

$$\Omega_Y^0 = \{\omega_Y : \Phi_X^0(\omega_Y) = \min_{\omega'_X} \Phi_X^0(\omega'_X) \text{ for any } X \subseteq Y\}$$

and let

$$\mathcal{H}_Y^0 := \{\psi \in \mathcal{H}_Y : \psi = \sum_{\omega_Y \in \Omega_Y^0} c_{\omega_Y} e_{\omega_Y}\}$$

be the subspace of $\mathcal{H}_Y$ spanned by the local groundstates in Y. We define P_Y^0 to be the projection operator onto the subspace $\mathcal{H}_Y^0$.

Let X be a finite subset of the lattice (which may be thought of as the support of an excitation). For $x \in X$, we define

$$\begin{aligned} W_x &:= \{y \in \Lambda : |y_i - x_i| \leq r, \text{ for } 1 \leq i \leq \nu\}, \\ B_X &:= \bigcup_{x\in X} W_x, \end{aligned} \tag{36}$$

r being the range of the m-potential, (eq.(5)).

We introduce some special projection operators on $\mathcal{H}_{B_X}$: Let $P_{B_X}^0$ be the orthogonal projection onto the subspace $\mathcal{H}_{B_X}^0$. Let $P_{B_X}^1$ be the orthogonal projection onto the space of states with excitations localized in $X \subset B_X$. It is defined as

$$P_{B_X}^1 := P_{B_X\setminus X}^0 - P_{B_X}^0. \tag{37}$$

Two excitations with support in X and X' are said to be connected if $X' \cap B_X \neq \emptyset$. If they are disconnected, our choice of B_X implies that their unperturbed energies are additive. We further define

$$P^2_{B_X} := \mathbf{1}_{B_X} - P^1_{B_X} - P^0_{B_X},$$

where $\mathbf{1}_{B_X}$ is the identity operator on $\mathcal{H}_{B_X}$.

We decompose the perturbation V with respect to the partition of unity

$$\mathbf{1}_{B_X} = P^0_{B_X} + P^1_{B_X} + P^2_{B_X}, \tag{38}$$

and since we restrict our attention to an analysis of the perturbation of the groundstates of H_0 by the term tV, it is convenient to write the perturbation $V = \sum_X V_X$ as

$$V = V^{00} + V^{01} + V^R,$$

where V^{00} is the operator defined by

$$V^{00} := \sum_X P^0_{B_X} V_X P^0_{B_X} := \sum_X V^{00}_{B_X}, \tag{39}$$

and V^{01} is the "off-diagonal" operator:

$$V^{01} := \sum_X P^0_{B_X} V_X P^1_{B_X} + P^1_{B_X} V_X P^0_{B_X} := \sum_X V^{01}_{B_X}. \tag{40}$$

Here $P^1_{B_X} V_X P^0_{B_X}$ is an operator in $\mathcal{A}_{B_X}$ that vanishes unless it acts on some local groundstate; every term in $V^{01}_{B_X}$ connects a local groundstate in $\mathcal{H}^0_{B_X}$ with an excited state localized in X. The operator V_R is given by

$$V^R := \sum_X (P^1_{B_X} V_X P^1_{B_X} + P^2_{B_X} V_X P^2_{B_X}) := \sum_X V^R_{B_X}. \tag{41}$$

We denote by $\mathrm{ad}A(B)$ the commutator $AB - BA$. We define

$$\mathcal{O}_{B_X} := \{A^{01}_{B_X} := P^0_{B_X} A_X P^1_{B_X} + P^1_{B_X} A_X P^0_{B_X} : A_X \in \mathcal{A}_X\}.$$

$\mathcal{O}_{B_X}$ contains only "off-diagonal" operators (with respect to the partition of unity (38)). We define

$$\bar{H}_{0X} \;=\; \sum_{M \cap X \neq \emptyset} \phi^0_M \;, \tag{42}$$

and, on $\mathcal{O}_{B_X}$, we define

$$\mathrm{ad}^{-1}\bar{H}_{0X}\left(A^{01}_{B_X}\right) \;=\; \int dP_E \frac{A^{01}_{B_X}}{E - E'} dP_{E'}, \tag{43}$$

where $\{P_E\}$ are the spectral projections of $\bar{H}_{0X}$. It is easy to see that

$$\mathrm{ad}\bar{H}_{0X}\left(\mathrm{ad}^{-1}\bar{H}_{0X}\left(A^{01}_{B_X}\right)\right) \;=\; A^{01}_{B_X}. \tag{44}$$

In [2] it is shown that, due to our choice of B_X, we have that

$$\mathrm{ad}H_0\left(\mathrm{ad}^{-1}\bar{H}_{0X}\left(A^{01}_{B_X}\right)\right) \;=\; A^{01}_{B_X}\;, \tag{45}$$

and that the operator norm of $\mathrm{ad}^{-1}\bar{H}_{0X}$ on $\mathcal{O}_{B_X}$ is bounded as follows:

$$||\mathrm{ad}^{-1}\bar{H}_{0X}\;|_{\mathcal{O}_{B_X}}\;|| \leq \frac{1}{\Delta}$$

where Δ is the gap between the groundstate energy of $\bar{H}_{0X}$ and the rest of its spectrum.

A unitary transformation, $U(t)$, is defined as

$$U(t)\;=\;e^{tS},$$

where

$$S = \sum_{X} S_{B_X}, \tag{46}$$

and

$$\begin{aligned} S_{B_X} &= \mathrm{ad}^{-1}\bar{H}_{0X}\left(V_{B_X}^{01}\right) \\ &= \mathrm{ad}^{-1}\bar{H}_{0X}\left(P_{B_X}^{0}V_X P_{B_X}^{1} + P_{B_X}^{1}V_X P_{B_X}^{0}\right). \end{aligned} \tag{47}$$

In [2] it is proven that the transformed Hamiltonian,

$$\widetilde{H}(t)\;=\;U(t)H(t)U(t)^{-1}$$

can be cast in the following form

$$\widetilde{H}(t)\;=\;H_0(t)+V(t),$$

where $H_0(t)$ is given by

$$H_0 + t\sum_{X} V_{B_X}^{00} + \frac{t^2}{2}\sum_{\substack{X,X':\\ X'\cap B_X\neq\emptyset}} P_{B_{X\cup X'}}^{0}\,\mathrm{ad}S_{B_X}(V_{B_{X'}}^{01})P_{B_{X\cup X'}}^{0}. \tag{48}$$

The proof is based on using the Lie-Schwinger series, the idendity (45) and the commutativity of operators with disjoint support (see (3)).

The new perturbation, $V(t)$, is given (see Lemma 1.3) by a sum of exponentially decaying interactions satisfying condition **V1**. *To order* t^2, the groundstate energy of $H(t)$, is given by the lowest eigenvalue of $H_0(t)$ and is obtained by diagonalizing $H_0(t)$.

One may apply Theorems 1.1 and 1.2 to the pair $(H_0(t), V(t))$, provided the new unperturbed part $H_0(t)$ satisfies Conditions **H1** - **H4** of the introduction.

B The Peierls condition

We assume that H_0 is a finite-range Hamiltonian satisfying condition **H1**,

$$H_0 = \sum_{Y\subset\Lambda} \Phi_{0Y}.$$

Let $\mathcal{K} := \{s_i\}_{i=1}^{k}$ be the set of periodic groundstate configurations of H_0. In order to state the Peierls condition, we introduce the notion of *contours*. We define sampling plaquettes $P(x)$ as

$$P(x) := \{y\in\Lambda :\mid x_i - y_i\mid\leq a \text{ for } 1\leq i\leq\nu\}.$$

The constant a is chosen to be larger than the period of each of the groundstate configurations of H_0 and the range of the interactions Φ_{0Y}. A contour is constructed from sampling plaquettes on which the configuration does not coincide with any of the groundstate configurations of H_0. The defect set, $\partial\omega$, of a configuration ω on the lattice Λ is defined as

$$\partial\omega = \bigcup_{x\in\Lambda} \{P(x) : \omega_{P(x)} \neq (s_i)_{P(x)}, \ \text{for all} \, 1 \leq i \leq k\} \, .$$

A contour of a configuration ω is a pair $\gamma = (M, \omega_M)$, where M is a maximally connected component of the defect set $\partial\omega$. The set M is the support of γ. Two contours γ, γ' are disjoint if no pair of plaquettes, $P \in \gamma$, $P' \in \gamma'$, intersect. Due to our choice of the size of the sampling plaquettes we have a one-to-one correspondence between configurations and families of contours. This is seen by associating to each configuration of the lattice, the corresponding set of disjoint contours, with the restriction that the interiors and exteriors of nested contours match. Families of contours corresponding to a configuration are said to be compatible. The energy of a configuration is then expressible in terms of contour energies. To each contour γ, there corresponds a unique configuration ω^γ that has γ as its only contour. The configuration in any connected component of the set $\Lambda \setminus M$ coincides with one of the groundstates. If the energy of the groundstate is normalized to zero then the energy of the configuration ω^γ is given by

$$\begin{aligned} H_0(\omega^\gamma) &= \sum_{Y\cap\Lambda\neq\emptyset} \frac{\mid Y \cap M \mid}{\mid Y \mid} \Phi_{0Y}(\omega^\gamma) \\ &=: E(\gamma). \end{aligned}$$

If a configuration ω corresponds to a family of compatible contours

$$\{\gamma_1, \ldots, \gamma_n\},$$

then its energy is given by the sum of the energies of its contours, i.e.,

$$H_0(\omega) \; = \sum_{i=1}^{n} E(\gamma_i)$$

because of our choice of the size of the sampling plaquettes. This allows us to rewrite the partition function $Z(\Lambda)$ of the system in Λ in terms of an ensemble of contours, with no other than excluded-volume interaction. and use cluster expansion methods to study the system at low-temperatures. The *Peierls condition* demands that the energy of a contour be proportional to the total number of lattice sites in the contour. More precisely, it requires that there exist a positive constant κ, such that the energy $E(\gamma)$, of a contour γ, satisfies

$$E(\gamma) > \kappa \mid \gamma \mid,$$

$\mid \gamma \mid$ being the number of sites in γ. A useful criterion for the Peierls condition to hold has been proven in [7].

CRITERION :*If the Hamiltonian H_0 is expressible in terms of a finite-range m-potential and has a finite number of groundstates then the groundstates are necessarily periodic, and the Peierls condition is satisfied.*

Acknowledgements

We thank C. Albanese, N. Datta and R. Fernandez for many useful discussions.

References

[1] N. Datta, R. Fernandez, J. Fröhlich. Low-temperature phase diagrams of quantum lattice systems. I. Stability for quantum perturbations of classical systems with finitely-many groundstates. To be published in *J. Stat. Phys.*

[2] N. Datta, R. Fernandez, J. Fröhlich, L. Rey-Bellet. Low-temperature phase diagrams of quantum lattice systems. II. Convergent perturbation expansions and stability in systems with infinite degeneracy. ETH-preprint.

[3] C. Borgs, R. Kotecky, D. Ueltschi. Low-temperature phase diagrams for quantum perturbations of classical spin systems. Preprint.

[4] B. Simon. *The Statistical Mechanics of Lattice Gases.* Princeton Univ. Press, Princeton, N.J., 1993.

[5] O. Bratteli and D. W. Robinson. *Operator Algebras and Quantum Statistical Mechanics I and II.* Springer-Verlag, New York-Heidelberg-Berlin, 1987.

[6] D. Ruelle. *Statistical Mechanics: Rigorous Results.* W. A. Benjamin Inc., New York, 1969.

[7] W. Holsztynsky, J. Slawny. Peierls condition and number of groundstates. *Comm. Math. Phys.* 61: 177, (1978)

[8] Y. M. Park. The cluster expansion for classical and quantum lattice systems. *J. Stat. Phys.*, 27:553, 1981.

[9] S. A. Pirogov, Ya. G. Sinai. Phase diagrams of classical lattice systems. *Theor. Math. Phys.*, 25:1185–1192, 1976; 26:39–49, 1976.

[10] C. Borgs, J.Z. Imbrie. A unified approach to phase diagrams in field theory and statistical mechanics. *Comm. Math. Phys.*, 123:305, 1989.

[11] T Kato: Perturbation theory for linear operators. Springer Verlag, 1966.

[12] C. Gruber, A. Sütö. Phase diagrams of lattice systems with residual entropy. *J. Stat. Phys.*, 52: 113, 1988.

[13] C. Albanese. On the spectrum of the Heisenberg Hamiltonian. *J. Stat.Phys.* 55: 297 (1989).

[14] L. Rey-Bellet. Diploma-Thesis. ETH 1994.

[15] S. A. Kivelson, V. J. Emery, H. P. Lin. Doped antiferromagnets in the weak-hopping limit. *Phys Rev. B.*, 42: 6523, 1990.

[16] C. Gruber, J. Jedrzejewski , P. Lemberger. Groundstates of the spinless Falicov-Kimball model. *J. Stat. Phys.*, 66: 913, 1991.

[17] T. Kennedy. Some rigorous results on the groundstates of the Falicov-Kimball model. Submitted to *Rev. Math. Phys.*

[18] C. Albanese, J. Fröhlich. Dynamical binding of holes in doped antiferromagnets. *Helv. Phys. Acta*, to appear.

[19] C. Albanese, N. Datta. Quantum criticality, Mott transition and sign problem for a model of lattice fermions. *Comm. Math. Phys.*, 167:571, 1995.