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Mott Transition and Sign Problem for a Model of Lattice Fermions

Claudio Albanese[1,2,★], **Nilanjana Datta**[1,3]

[1] Institut für Theoretische Physik, ETH-Hönggerberg, CH-8093, Zürich, Switzerland
[2] Department of Mathematics, Erindale College, University of Toronto, 3359 Mississagna Rd, Mississagna, Ontario L5L 1C6, Canada
[3] Paul Scherrer Institut, Badener Str. 569, CH-8048, Zürich, Switzerland

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Abstract: We consider a model of spinless fermions on the square lattice $\mathbb{Z}^2$ with an interaction potential of strength $U > 0$ at distance one and strength J at distance two, in the large U limit $|t|, |J| \ll U$, where t is the hopping amplitude. As the chemical potential μ is varied, if $t = T = 0$ we find three different phases corresponding to full, half and zero filling fractions. We study the system at low temperature $T \geqq 0$ by a method involving a canonical transformation and a functional integral representation. If $T = 0$ we locate the phase boundaries of the Mott metal-insulator transition for all $|J| \ll U$ with upper and lower bounds, show that mean field theory is valid if $J < 0$ but fails for $J = 0$ when also the Peierls condition is violated. This result is a quantum extension of the Pirogov–Sinai theory of phase transitions. If $T > 0$ we have only one sided bounds for the phase boundaries and we can't validate mean field theory in case $J < 0$. We introduce a new resummation scheme for low temperature expansions which yields finite and convergent perturbation series and permits us to study issues like the sign problem. Our algorithm gives an optimal canonical transformation for the functional integral such that the expectation of the sign observable S is $\geqq \exp(-c \cdot t \cdot V e^{-\frac{\beta}{2}})$, where V is the volume and $\beta = T^{-1}$.

1. Introduction

We consider a family of Hamiltonians describing a system of spin polarized lattice fermions with short range repulsive interactions:

$$\mathbb{H} = -t \sum_{\langle xy \rangle \subset \Lambda} (c_x^+ c_y + c_y^+ c_x) + U \sum_{\|x-y\|_1 = 1} \left(n_x n_y + \frac{1}{2} \right) + 2J \sum_{\|x-y\|_1 = 2} n_x n_y - \mu \sum_{x \in \Lambda} n_x \tag{1.1}$$

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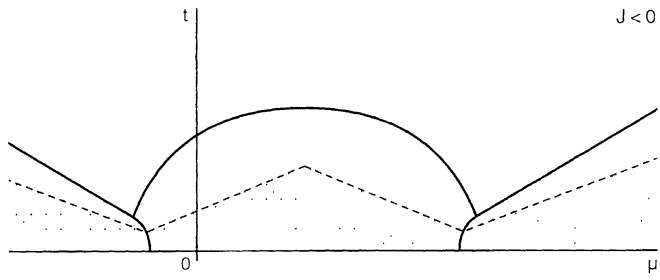

Fig. 1

in the strong coupling limit $t \ll U$. The next neighbour coupling J is assumed to be small in absolute value, i.e. such that $J \ll U$. Our system is defined on a finite square $\Lambda \subset \mathbb{Z}^2$ the length of whose side is an even integer. The dimension is chosen to be $d = 2$ just to fix ideas and do a few calculations explicitly, but our results extend to all other dimensions. Finally, c_x^+, c_x are the Fermi creation and annihilation operators for spin up electrons. We impose periodic boundary conditions. It is convenient to fix energy units so that $U = 2$ and to rewrite $\mathbb{H}$ as follows:

$$\mathbb{H} = \mathbb{H}_0 + (4 - \mu + 8J)\mathbb{N} , \tag{1.2}$$

where $\mathbb{N}$ is the number operator

$$\mathbb{N} = \sum_x n_x . \tag{1.3}$$

The Hamiltonian

$$\mathbb{H}_0 = -t \sum_{\|x-y\|_1 = 1} (c_x^+ c_y + c_y^+ c_x) + \sum_{\|x-y\|_1 = 1} \left[2\left(n_x - \frac{1}{2}\right)\left(n_y - \frac{1}{2}\right) + \frac{1}{2} \right] + \sum_{\|x-y\|_1 = 2} \left[2\left(n_x - \frac{1}{2}\right)\left(n_y - \frac{1}{2}\right) - \frac{1}{2} \right] \tag{1.4}$$

is a special case of $\mathbb{H}$ enjoying particle-hole symmetry. For a numerical study of this model, see [1]. [2] is a recent mathematical paper on the subject.

In the classical limit $t = 0$ and for μ in the interval $[8J, 8 + 8J]$ if $J < 0$ and in $[16J, 8]$ if $J > 0$, the Hamiltonian $\mathbb{H}$ has a "Néel ordered" ground state in which the filling fraction is one half and particles are arranged in a checkerboard configuration. A "ferromagnetic" phase takes over in case either $|\mu - 4 - 8J| > 4$ and $J < 0$, or $|\mu - 4 - 8J| > 4 + 8J$ and $J > 0$; in this phase, the ground state becomes either the eigenstate in which the filling fraction is one, or the one in which it is zero. For the special value of the chemical potential corresponding to the symmetric Hamiltonian $\mathbb{H}_0$, one can prove that there are two states at the bottom of the spectrum whose energy difference is $\approx |\Lambda|(c \cdot t)^{\frac{1}{2}|\Lambda|}$; imposing a parity condition with respect to global spin flips, one of these states Ψ_N is singled out. This wavefunction Ψ_N is in the sector with filling fraction one half, is separated by an energy gap of order 4 from the first excited band and in the infinite volume limit it exhibits off diagonal long range order of the Néel type. The two ferromagnetic states Ψ_{F0} and Ψ_{F1} with filling fraction 0 and 1, respectively, are eigenfunctions of $\mathbb{H}$ for all values of μ and they become the ground states when $|\mu - 4 - 8J|$ is large enough and t is small. The phase diagram is sketched in Figs. 1, 2, 3. The cluster

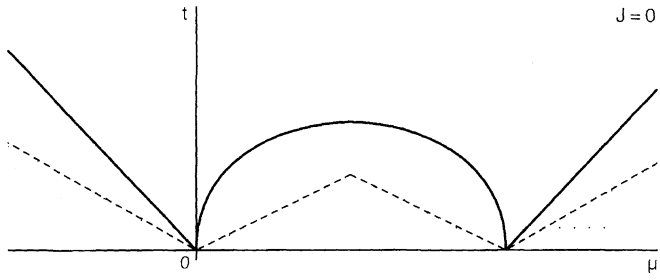

Fig. 2

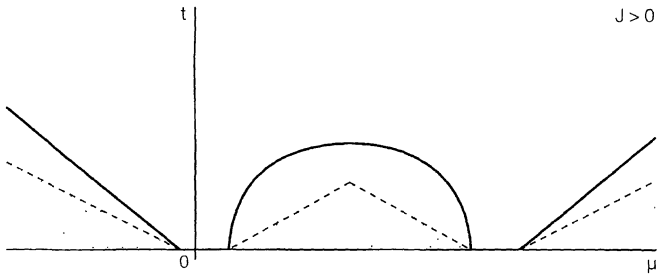

Fig. 3

expansion algorithm we use provides detailed information on the excited states and permits one to compute the coexistence line for $J < 0$ in a convergent small t expansion. This extends to the quantum case $T = 0, t > 0$ a celebrated result that Pirogov and Sinai [3] obtained in the classical case $T > 0, t = 0$. By using particle number symmetry, we also locate the phase boundaries beyond the tricritical point with upper and lower bounds. The lower bound is imprecise and can't be attached a precise physical meaning. On the other hand, the upper bound is made up of the three curves $g_N = 0$, $g_{F0} = 0$ and $g_{F1} = 0$ on which the gap of one quasiparticle excitations above one of the three perturbative ground states, vanishes. The idea of using particle number symmetry to find phase boundaries is also in a recent work by Freericks and Monien [6] on the Bose–Hubbard model.

Mott transitions [4] for an ordered system like the one we are considering can be first order [5]. Mathematically, these transitions are related to some kind of level crossing among ground state energies E_N corresponding to sectors with different particle number N. The typical situation is illustrated in Fig. 4, the first excited band of continuous spectrum in $\sigma(\mathbb{H})$ intersects the t axis at the critical value t_c. As we discuss later in this article, the occurrence of this intersection doesn't necessarily imply that the ground state wavefunction for $t < t_c$ looses analyticity ad $t = t_c$ or develops long range correlations. If $\mu \approx 0$, the quasiparticles with the smallest gap are quasiholes. In case the quasiholes don't form bound states, the higher order bands with $n = 2, 3, \ldots$ intersect the t axis at about $t = t_c$, up to finite volume corrections which vanish as if n is kept fixed and we take the thermodynamic limit $\Lambda \uparrow \mathbb{Z}^2$. Hence, for $t > t_c$ we obtain a liquid of quasiparticles interacting via an effective short range interacting potential of order $O(t)$ and with an

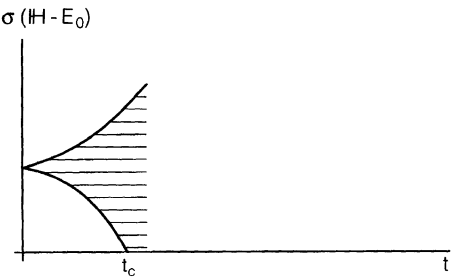

Fig. 4

effective chemical potential of order $c(t - t_c)$, where c is the slope of the lowest edge of the first spectral band at $t = t_c$. If the transition is towards a metallic phase, an important question is whether the density of holes has a first order jump at the phase transition or whether the transition is second order, see [4] and [5]. A different kind of first order phase transition which is also possible can be triggered by a charge density wave instability. In case the transition is first order, the gap of quasiparticle excitations doesn't close at the phase transition and, as a consequence, the upper bound computed by requiring the one quasiparticle gap to close, is not saturated and the transition occurs for smaller values of t. What one can say on the basis of the results in this paper is that, if $J < 0$, then on the part of the phase boundary of the Néel ordered phase which is closest to the tricritical point, the excitation spectrum for one quasiparticle states has a gap. Our cluster expansions might also be useful to compute the minimum metallic conductivity, analytically, because they provide a systematic way of renormalizing the bare strong coupling interaction to an effective weak coupling interaction among dressed quasiparticles near the Mott transition.

Our interest in this problem is also motivated by the desire of developing a practical algorithm for low temperature expansions for quantum spin systems. The convergent low temperature expansion given by Kennedy and Tasaki in [7] is based on a direct application of the Trotter product formula to the bare Hamiltonian and involves $(d + 1)$-dimensional polymers. This formalism is elegant and mathematically under control, but it is rather inconvenient for numerical applications. To overcome this difficulty, Gelfand, Singh and Huse [14] developed a different algorithm for zero temperature expansions which involves only d-dimensional polymers. For similar reasons, in this article, we develop an algorithm for low temperature expansions which can be implemented in a strictly d-dimensional setting.

The extension of the classical low temperature expansions to quantum spin systems within a d-dimensional formalism is a non-trivial problem. The difficulty can be seen as one attempts to compute the partition function

$$Z = \mathrm{Tr}\, e^{-\beta \mathbb{H}(t)} = \sum_{\gamma \subset \Lambda} z(t, \gamma) \tag{1.5}$$

as a sum over cluster $\gamma \subset \Lambda$ of activities $z(t, \gamma)$ such that

$$z(t, \gamma) = \langle \gamma | e^{-\beta \mathbb{H}(t)} | \gamma \rangle \,. \tag{1.6}$$

Although Z is a physical quantity whose value doesn't depend on the representation in which the operator $\mathbb{H}$ is expressed, the activities $z(\gamma)$ are representation dependent. The problem is that if one works in the natural Ising representation given in (1.1), then the coefficients $z_n(\gamma)$ of the expansion

$$z(t, \gamma) = \sum_{n=0}^{\infty} t^n z_n(\gamma) \tag{1.7}$$

are such that $|z_n(\gamma)| \to \infty$ as $\beta \to \infty$, for a large family of clusters γ, see for instance [2]. Due to this divergence, the numerical implementation of low temperature expansions is an ill conditioned problem. The expansion coefficients of physical quantities are computed as sums of terms of fluctuating signs. Each of these terms diverges as $\beta \to \infty$, but the physically meaningful coefficients are finite. It is hard to keep track correctly of many cancellations between very large quantities if finite precision arithmetics is used. Needless to say, the divergence of the activities is also problematic for the rigorous analysis of such models. Since the activities are clearly representation dependent, one can ask whether there is a constructive algorithm to pass to a new representation in which the activities $z_n(\gamma)$ are finite. In this article, we give a possible solution to this problem and prove that not only is the low temperature expansion we generate finite term by term, but it is also convergent as long as t and $e^{-\beta}$ are small enough.

By means of our expansion, we can also avoid the difficulties related to the sign problem of Fermi systems at low temperature. The sign problem is one of the factors that limits the precision of quantum Montecarlo simulations [8] and its understanding can help improving these numerical methods. Using functional integrals, one can map a quantum statistical model at finite temperature into a problem of classical statistical physics. This can be done in many different ways and the sign pathology is more or less severe depending on the set up. Typically, if fermions are involved, there is a *signed* measure $\mu(\sigma)$ giving the "probability" of the configuration σ. Since Montecarlo simulations require positive definite probability measures, one has to express the expectation of a local observable $\mathcal{O}(\sigma)$ as follows:

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O}S \rangle_{|\mu|}}{\langle S \rangle_{|\mu|}}, \tag{1.8}$$

where $|\mu|$ is the positive definite probability measure $|\mu(\sigma)|$ and $S(\sigma) = \text{sign } \mu(\sigma)$. Then one evaluates $\langle S \rangle_{|\mu|}$ and $\langle \mathcal{O} \rangle_{|\mu|}$ independently and computes the ratio. The problem with this approach is that both quantities $\langle S \rangle_{|\mu|}$ and $\langle \mathcal{O}S \rangle_{|\mu|}$ tend to zero as $\beta \to \infty$, the typical asymptotic behaviour being given by $e^{-c \cdot \beta |\Lambda|}$, where $|\Lambda|$ is the volume. Moreover, if $\mathcal{O}$ is a local observable, then $\mathcal{O}S$ is not local. In particular, only the ratio in (1.8) is independent of the volume, while $\langle \mathcal{O}S \rangle_{|\mu|}$ and $\langle S \rangle_{|\mu|}$ are very sensitive to the boundary conditions. The asymptotic behaviour of $\langle S \rangle$ is well known to depend on the particular canonical transformation on the Hamiltonian one performs before setting up the functional integral formalism. Hence, to solve the sign problem, one has to find a functional integral representation that maximizes $\langle S \rangle_{|\mu|}$. A hint of what is the right direction to go is contained in Hirsch's paper on the half filled Hubbard model [9]. The idea is that one should transform the Hamiltonian in such a way to lift the quantum fluctuations from the level of the wavefunctions to the level of the operators themselves. In this article, we show how to construct a canonical transformation for our model such that in the Néel ordered state we have $\langle S \rangle \geqq \exp(-s \cdot t \cdot |\Lambda| \cdot e^{-\frac{\beta}{2}})$. In case quasiparticles or

quasiholes are present, the sign problem is more severe. In this case, our algorithm can also be helpful as they give a systematic way of constructing the exact creation and annihilation operators for dressed quasiparticles; see for instance [10] for a discussion of how this knowledge can be helpful to enhance the Quantum Montecarlo signal.

Next, we give a precise statement of our results.

Theorem. *There are constants $J_0 > 0$ and $t_0 > 0$ such that if $|J| \leqq J_0$ and $|t| \leqq t_0$, then the following is true*:

(i) *The Hamiltonian $\mathbb{H}_0$ in* (1.2) *has a ground state wavefunction $\Psi_0(t, J)$ with long range order of the Néel type and whose energy is*

$$E_0(t, J) = |\Lambda|[-(3 - 8J)^{-1}t^2 + O((t^2 + J)^2)] . \tag{1.9}$$

The first excited eigenstate $\Psi'_o(t, J)$ has energy $E'_0(t, J)$ such that

$$E'_0(t, J) - E_0(t, J) \leqq |\Lambda|(c \cdot t)^{\frac{1}{2}|\Lambda|} . \tag{1.10}$$

Above these two states, the spectrum is arranged in bands in which the spectral density becomes absolutely continuous in the infinite volume limit. The first band is in the interval

$$I_1 = E_0(t, J) + 4 - 8J + [-2t^2, 2t^2] . \tag{1.11}$$

(ii) *The Hamiltonian in* (1.1) *admits the wave function $\Psi_0(t, J)$ as the ground state in a region of the form of the dotted domain in Fig.* 1, 2, 3. *Moreover, a phase transition line and a tricritical point lie within the shaded regions. The equations for the curves in this drawing are given in Sect.* 3 *and are analytic in t. In case $J < 0$, the one quasiparticle gap above the Neel ordered state doesn't close on the phase transition line in a neighborhood of the tricritical point.*

(iii) *There is a constant $T_0 > 0$ and a function $d(T)$ such that $d(T) \downarrow 0$ as $T \downarrow 0$ and for which the following holds: if the temperature $T \leqq T_0$ and if the point (t, μ) is inside the dotted region in Fig.* 1 *and at distance at least $d(T)$ from the boundary, then the model has off-diagonal long range order of the Néel type. Furthermore, in this region there exists a canonical transformation for the Hamiltonian $\mathbb{H}$ such that*

$$\langle S \rangle \geqq c \cdot \exp(-c \cdot t \cdot |\Lambda| \cdot e^{-\frac{\beta}{2}}) . \tag{1.12}$$

2. The Dressing Transformation

The Hilbert space $\mathscr{H}$ for our model of spin polarized fermions can be identified – though not in a canonical way – with the tensor product space $\bigotimes_{x \in \Lambda} \mathbb{C}^2_x$ being $|\uparrow\rangle_x$ and $|e\rangle_x$, where e stands for "empty." The identification $\mathscr{H} \approx \bigotimes_{x \in \Lambda} \mathbb{C}^2_x$ is not canonical because it depends on the choice of an order relation $\prec$ on Λ. To fix ideas, we choose the lexicographic ordering but any other ordering relation would work as well, as long as it is fixed once and for all. If $\Lambda_e \subset \Lambda$ is one of the two sublattices of Λ of period 2 and $\Lambda_o = \Lambda \setminus \Lambda_e$ is the other, let $|N\rangle$ and $|N'\rangle$ denote the two Néel states with the signs implied by the following ordered products:

$$|N\rangle = \prod_{x \in \Lambda_e}^{\prec} c_x^+ |0\rangle_{F0} , \tag{2.1}$$

$$|N'\rangle = \prod_{x \in \Lambda_o}^{\prec} c_x^+ |0\rangle_{F0} . \tag{2.2}$$

Since the Hamiltonian $\mathbb{H}_0$ in (1.3) has global particle-hole symmetry, we can restrict ourselves to the symmetric subspace $\mathscr{H}_S = \mathbb{P}_S \mathscr{H}$. Let $|0\rangle_N$ be the coherent superposition of $|N\rangle$ and $|N'\rangle$, i.e.

$$|0\rangle_N = \frac{1}{\sqrt{2}}(|N\rangle + |N'\rangle) . \tag{2.3}$$

We may also restrict the operator $\mathbb{H}_0$ to the antisymmetric subspace $\mathscr{H}_A = \mathbb{P}_A \mathscr{H}$ and our methods would work as well. In the antisymmetric sector, the ground state energy one obtains is slightly higher by an amount of order $O(|\Lambda|(c \cdot t)^{\frac{1}{2}|\Lambda|})$.

An excitation can be described either by a map $\gamma: \Lambda \to \{0, 1\}$ or by the support of this function, that we also denote by the same letter γ. Let $\partial\gamma$ be the boundary of γ, i.e. the set of the sites $x \in \gamma$ having a neighbour outside of γ. We denote with $|\gamma|$ and $|\partial\gamma|$ the volumes of these sets and with $d(\gamma)$ the number of bonds of the smallest connected set containing γ. Let us introduce the fermionic analog of Pauli matrices for hard core bosons, i.e. the operators

$$\begin{aligned} \bar{\sigma}_x^{(1)} &= c_x^+ + c_x , \\ \bar{\sigma}_x^{(2)} &= c_x^+ - c_x . \end{aligned} \tag{2.4}$$

If $x \neq y$, we have

$$\{\bar{\sigma}_x^{(1)}, \bar{\sigma}_y^{(1)}\} = \{\bar{\sigma}_x^{(1)}, i\bar{\sigma}_y^{(2)}\} = \{i\bar{\sigma}_x^{(2)}, i\bar{\sigma}_y^{(2)}\} = 0 . \tag{2.5}$$

We also have

$$\{\bar{\sigma}_x^{(1)}, i\bar{\sigma}_x^{(2)}\} = 0 , \tag{2.6}$$

$$\{\bar{\sigma}_x^{(1)}, \bar{\sigma}_x^{(1)}\} = -\{i\bar{\sigma}_x^{(2)}, i\bar{\sigma}_x^{(2)}\} = 2 . \tag{2.7}$$

Finally, let π_{xy} be the operator

$$\pi_{xy} = 2\left[\frac{1}{4} - \left(n_x - \frac{1}{2}\right)\left(n_y - \frac{1}{2}\right)\right] . \tag{2.8}$$

If γ is a connected excitation, we define τ_γ to be the operator

$$\tau_\gamma = \frac{1}{|\partial\gamma|} \sum_{\substack{\langle y_1 y_2 \rangle \\ y_1 \in \gamma,\, y_2 \notin \gamma}} \pi_{y_1 y_2} \prod_{x \in \gamma}^{\prec} \bar{\sigma}_x^{(1)} \tag{2.9}$$

in case $|\gamma|$ is even, and the operator

$$\tau_\gamma = \frac{1}{|\partial\gamma|} \sum_{\substack{\langle y_1 y_2 \rangle \\ y_1 \in \gamma,\, y_2 \notin \gamma}} i\bar{\sigma}_{y_1}^{(2)} \pi_{y_1 y_2} \prod_{x \in \gamma \setminus \{y\}}^{\prec} \bar{\sigma}_x^{(1)} \tag{2.10}$$

in case $|\gamma|$ is odd. If γ_1 and γ_2 are connected excitations such that $\partial\gamma_1 \cap \partial\gamma_2 = \emptyset$, we have

$$\tau_{\gamma_1}\tau_{\gamma_2} = (-1)^{|\gamma_1||\gamma_2|}\tau_{\gamma_2}\tau_{\gamma_1} . \tag{2.11}$$

If γ is the union of disjoint connected components $\gamma_1, \ldots, \gamma_k$, we set

$$\tau_\gamma = \prod_{j=1,\ldots,k}^{\prec} \tau_{\gamma_j} . \tag{2.12}$$

With this definition (2.11) extends to arbitrary excitations γ_1, γ_2 such that $\partial\gamma_1 \cap \partial\gamma_2 = \emptyset$. Thanks to the insertion of the factors $\pi_{y_1 y_2}$, we also have

$$\tau_\gamma |0\rangle_{F0} = \tau_\gamma |0\rangle_{F1} = 0 \,, \tag{2.13}$$

where $|0\rangle_{F0}$ and $|0\rangle_{F1}$ are the ferromagnetic eigenstates with filling fraction 0 and 1, respectively. As we discuss in the next section, this property is useful to study the coexistence line and the crossover region between the Néel and the ferromagnetic states.

Our perturbation expansion for the ground state wavefunction, generates a convergent sequence of approximate solutions belonging to the cyclic subspace

$$\mathscr{H}_0 = \mathrm{span}\{\mathbb{H}_0^n |0\rangle_N, n \geqq 0\} \,. \tag{2.14}$$

If γ is an excitation of odd volume, then due to particle number symmetry, we have $|\gamma\rangle \perp \mathscr{H}_0$. Hence, we can restrict the attention to the operators τ_γ for which γ is *admissible* in the sense that the volume $|\gamma|$ is even. If γ and γ' are two admissible excitations such that $\partial\gamma \cap \partial\gamma' = \emptyset$, then we have

$$[\tau_\gamma, \tau_{\gamma'}] = 0 \,. \tag{2.15}$$

Moreover, if we associate a state $|\gamma\rangle$ to the excitation γ so that

$$|\gamma\rangle = \prod_{x \in \gamma}^{\prec} \bar{\sigma}_x^{(1)} |0\rangle_N \,, \tag{2.16}$$

then, in case $|\gamma\rangle$ is admissible, we have

$$|\gamma\rangle = \tau_\gamma |0\rangle_N \,. \tag{2.17}$$

This is due to the fact that, if γ is admissible, then τ_γ contains an even number of operators $\bar{\sigma}_x^{(2)}$. This also implies that the operators τ_γ by means of which we express our dressing transformation, respect the global particle-hole symmetry of $\mathbb{H}_0$ and can thus be restricted to either $\mathscr{H}_S$ or $\mathscr{H}_A$.

If $\langle xy \rangle$ is a bound not intersecting the boundary γ, we also have

$$[c_x^+ c_y + c_y^+ c_x, \tau_\gamma] = \left[\left(n_x - \frac{1}{2} \right) \left(n_y - \frac{1}{2} \right), \tau_\gamma \right] = 0 \,. \tag{2.18}$$

The commutation relations above are weaker than the ones available in [12]. Also, since the operators τ_γ are not skewsymmetric, the resulting dressing transformation is not unitary. These inconveniences are related to the presence of a spontaneously broken symmetry and to the sign problem. However, in the following we show that one can still establish convergence of the resulting cluster expansion and that unitarity is neither necessary nor useful to derive low temperature expansions.

The dressing transformation we construct in this paper is given by a (nonunitary) operator of the form

$$\mathbb{A}(t) = \lim_{v \to \infty} e^{\mathbb{R}^2(t)} \ldots e^{\mathbb{R}^v(t)} \,, \tag{2.19}$$

which solves the conjugacy problem

$$\mathbb{A}(t)^{-1} \mathbb{H}_0 \mathbb{A}(t) |0\rangle = E_0(t) |0\rangle \,, \tag{2.20}$$

for some function $E_0(t)$. To simplify the notations, we assume that $J = 0$, although the case $J \neq 0$ can be treated with exactly the same methods, as long as $|J| \ll 1$. The operators $\mathbb{R}^v(t)$ are given by power series expansions in t

$$\mathbb{R}^v(t) = \sum_{n=v-1}^{\infty} t^n \mathbb{R}^v_n , \tag{2.21}$$

whose coefficients $\mathbb{R}^v_n$ have the form

$$\mathbb{R}^v_n = \sum_{|\partial\gamma|=v} r_{n\gamma}\tau_\gamma . \tag{2.22}$$

The coefficients $r_{n\gamma}$ are nonzero only if γ is an admissible excitation and $v \geqq (n+1)$. In this case, they are uniquely determined by the following recurrence relations:

$$\begin{aligned}
&\sum_v \mathbb{S}_0 \mathbb{R}^v_n |0\rangle_N \\
&= -\Bigg\{ \sum_{k\geqq 2} \sum_{\substack{v_1 \leqq \cdots \leqq v_k \\ i_1+\cdots+i_k=n}} \frac{1}{n(v_1,\ldots v_k)} [\,.\,.[\mathbb{S}_0, \mathbb{R}^{v_1}_{i_1}], \ldots \mathbb{R}^{v_k}_{i_k}] \\
&\quad + \sum_{k\geqq 0} \sum_{\substack{v_1 \leqq \cdots \leqq v_k \\ i_1+\cdots+i_k=n-1}} \frac{1}{n(v_1,\ldots v_k)} [\ldots [\mathbb{K}_0, \mathbb{R}^{v_1}_{i_1}], \ldots \mathbb{R}^{v_k}_{i_k}] \Bigg\} |0\rangle_N \\
&\quad + E_{0n}|0\rangle_N ,
\end{aligned} \tag{2.23}$$

where

$$n(v_1, \ldots, v_k) = \prod_{v=0}^{\infty} (\#\{i: v_i = v\})! , \tag{2.24}$$

$$\mathbb{S}_0 = \sum_{\langle xy\rangle} \left[2\left(n_x - \frac{1}{2}\right)\left(n_y - \frac{1}{2}\right) + \frac{1}{2} \right], \tag{2.25}$$

$$\mathbb{K}_0 = -\sum_{\langle xy\rangle} c_x^+ c_y + c_y^+ c_x . \tag{2.26}$$

To control the convergence of the series expansion for $\mathbb{A}(t)$, we introduce the following sequence:

$$r_n^* = \sup_{x\in\Lambda} \sum_{\partial\gamma\ni x} |\partial\gamma|\,|r_n(\gamma)| , \tag{2.27}$$

where $\varepsilon(\gamma)$ is the number of frustrated bonds in $|\gamma\rangle$. We have

$$r_1^* = 4 . \tag{2.28}$$

If $n \geqq 2$, we can proceed by iteration in k. Let us consider the first term in (2.23) and let $i_j, v_j, \gamma_j, j = 1, \ldots, k$, be sequences such that $i_1 + + \cdots + i_k = n$, $|\partial\gamma_j| = v_j$, $v_1 \leqq \cdots \leqq v_k$. Let $\langle xy\rangle$ be a bond, let $s_{xy} = [2(n_x - \frac{1}{2})(n_y - \frac{1}{2}) + \frac{1}{2}]$ and let $\bar\gamma_k$ be the excitation such that

$$[\,.\,.[s_{xy}, r_{i_1\gamma_1}\tau_{\gamma_1}], \ldots r_{i_k\gamma_k}\tau_{\gamma_k}]\,|0\rangle_N = f_{i_1\ldots i_k}(\langle xy\rangle, \gamma_1, \ldots \gamma_k)|\bar\gamma_k\rangle . \tag{2.29}$$

Making use of the translation invariance of $\mathbb{H}_0$, we find

$$\sup_{z\in\Lambda}\sum_{\langle xy\rangle}\sum_{\substack{|\partial\gamma_1|=v_1\ldots|\partial\gamma_k|=v_k:\\ z\in\partial\bar{\gamma}_k}}|f_{i_1\ldots i_k}(\langle xy\rangle,\gamma_1,\ldots\gamma_k)|$$

$$\leqq\sup_{\langle xy\rangle}\sum_{|\partial\gamma_1|=v_1,\ldots|\partial\gamma_k|=v_k}|\varepsilon(\bar{\gamma}_k)|\,|f_{i_1\ldots i_k}(\langle xy\rangle,\gamma_1,\ldots\gamma_k)|$$

$$\leqq\sup_{\langle xy\rangle}\sum_{|\partial\gamma_1|=v_1\ldots|\partial\gamma_{k-1}|=v_{k-1}}|\varepsilon(\bar{\gamma}_k)|\,|f_{i_1\ldots i_k}(\langle xy\rangle,\gamma_1,\ldots\gamma_{k-1})|\cdot 2|\partial\bar{\gamma}_{k-1}|$$

$$\cdot\sup_z\sum_{\substack{\partial\gamma_k\ni z\\ |\partial\gamma_k|=v_k}}|r_{i_k\gamma_k}|$$

$$\leqq\sup_{\langle xy\rangle}\left[\sum_{|\partial\gamma_1|=v_1\ldots|\partial\gamma_{k-1}|=v_{k-1}}|\varepsilon(\bar{\gamma}_{k-1})|\,|f_{i_1\ldots i_{k-1}}(\langle xy\rangle,\gamma_1,\ldots\gamma_{k-1})\right]$$

$$\cdot\sup_{z\in\Lambda}\sum_{\substack{\partial\gamma_k\ni z\\ |\partial\gamma_k|=v_k}}v_k|r_{i_k\gamma_k}|\,, \tag{2.30}$$

where

$$\bar{\gamma}_{k-1}=\langle xy\rangle\cup\gamma_1\cup\cdots\cup\gamma_{k-1}\,, \tag{2.31}$$

and we use the fact that volumes are ordered, so that

$$|\varepsilon(\bar{\gamma}_k)|\leqq(2+|\varepsilon(\gamma_1)|+\cdots+|\varepsilon(\gamma_k)|+1-k)\leqq|\varepsilon(\gamma_k)|\,. \tag{2.32}$$

The estimate in (2.30) can evidently be iterated, the final result being:

$$\sup_{z\in\Lambda}\sum_{\langle xy\rangle}\sum_{\substack{|\partial\gamma_1|=v_1\ldots|\partial\gamma_k|=v_k:\\ z\in\partial\bar{\gamma}_k}}|f_{i_1\ldots i_k}(\langle xy\rangle,\gamma_1,\ldots\gamma_k)|\leqq 2^k k!\prod_{j=1}^{k}v_k r^*_{i_k v_k}\,, \tag{2.33}$$

where

$$r^*_{i_k v_k}=\sup_{\langle xy\rangle}\sum_{\partial\gamma\ni x}|r_{i_k\gamma_k}|\,. \tag{2.34}$$

The contribution of the second term in (2.23) to r^*_n, which is evaluated analogously, is

$$\leqq 6.2^k k!\prod_{j=1}^{k}v_j r^*_{i_j v_j}\,. \tag{2.35}$$

The factor 6 is because each time a particle hops to a neighbouring site, under the action of the operator $\mathbb{K}_0$, six bonds become frustrated. Hence, summing the two contributions, we have

$$r^*_n\leqq 4+\left[\sum_{k\geqq 2}\sum_{\substack{v_1\leqq\cdots\leqq v_k\\ i_1\ldots i_k=n}}+6\cdot\sum_{k\geqq 1}\sum_{\substack{v_1\leqq\cdots\leqq v_k\\ i_1\ldots i_k=n-1}}\right]\frac{2^k.k!}{n(v_1\ldots v_k)}\prod_{j=1}^{k}v_j r^*_{i_j v_j}\,. \tag{2.36}$$

We define a formal power series

$$r^*(t)\approx\sum_{n=1}^{\infty}t^n r^*_n\,. \tag{2.37}$$

From (2.33) and (2.34), we find

$$\sum_{n=1}^{\infty} t^n r_n^* \leqq 4t + 6t \sum_{k \geqq 1} 2^k \prod_{j=1}^{k} \left(\sum_{i_j} t^{i_j} r_{i_j}^* \right) + \sum_{k \geqq 2} 2^k \prod_{j=1}^{k} \left(\sum_{i_j} t^{i_j} r_{i_j}^* \right) \tag{2.38}$$

or,

$$r^*(t) \leqq 4t + 6t[(1 - 2r^*(t))^{-1} - 1] + [(1 - 2r^*(t))^{-1} - 1 - 2r^*(t)] . \tag{2.39}$$

Let $a^*(t)$ be the function implicitly defined as the solution of the following equation:

$$a^*(t) = 4t + 4 \cdot (1 - 2a^*(t))^{-1} [3ta^*(t) + a^*(t)^2] . \tag{2.40}$$

By the implicit function theorem $a^*(t)$ is analytic for $|t| \leqq t_0$ for some constant $t_0 > 0$. Moreover since $a^*(t)$ majorizes the series (2.37). Hence, $r^*(t)$ also converges and hence $\mathbb{A}(t)$ is analytic in t for $|t| \leqq t_0$.

Next we pass to the proof that the operator

$$\mathbb{V}(t) \equiv \mathbb{A}(t)^{-1} \mathbb{H}_0 \mathbb{A}(t) - \mathbb{S}_0 - E_0(t) \tag{2.41}$$

is relatively bounded with respect to $\mathbb{S}$ in the sense that:

$$\| \mathbb{V} \mathbb{S}^{-1} u \|_2 \leqq c \cdot t \, \| u \|_2 \tag{2.42}$$

for all wavefunctions u which are orthogonal to $|0\rangle$ and are symmetric with respect to global spin flips. We have the following expression for $\mathbb{V}(\lambda)$:

$$\begin{aligned} \mathbb{V}(t) = \sum_{j=1}^{\infty} t^j \Bigg\{ & \sum_{k \geqq 1} \sum_{\substack{v_1 \leqq \cdots \leqq v_k \\ i_1 + \cdots + i_k = j}} \frac{1}{n(v_1, \ldots, v_k)} [\ldots [\mathbb{S}_0, \mathbb{R}_{i_1}^{v_1}], \ldots \mathbb{R}_{i_k}^{v_k}] \\ & + \sum_{k \geqq 0} \sum_{\substack{v_1 \leqq \cdots \leqq v_k \\ i_1 + \cdots + i_k = j-1}} \frac{1}{n(v_1, \ldots, v_k)} [\ldots [\mathbb{K}_0, \mathbb{R}_{i_1}^{v_1}], \ldots \mathbb{R}_{i_k}^{v_k}] \Bigg\} \\ & - E_0(t) . \end{aligned} \tag{2.43}$$

Expanding $\mathbb{V}(t)$ in a series of operators $v(\gamma)$ of support $\gamma \subset \Lambda$ and using the fact that $\mathbb{V}(t)|0\rangle = 0$, we see that

$$\mathbb{V}(t) = \sum_{\gamma \subset \Lambda} v(\gamma) = \sum_{\gamma \subset \Lambda} \operatorname{ad} v(\gamma) , \tag{2.44}$$

where $\operatorname{ad} v(\gamma)$ is the operator such that

$$\operatorname{ad} v(\gamma) |\gamma'\rangle = \operatorname{ad} v(\gamma) \tau_{\gamma'} |0\rangle = [v(\gamma), \tau_{\gamma'}] |0\rangle . \tag{2.45}$$

Let us fix a vector $|u\rangle \perp |0\rangle$ and let us expand it in the excitation basis

$$|u\rangle = \sum_{\gamma \neq \emptyset} u_\gamma |\gamma\rangle . \tag{2.46}$$

One then derives the following bounds:

$$
\begin{aligned}
|\langle u|\mathbb{V}(t)^+\mathbb{V}(t)|u\rangle| &\leqq \sum_{\gamma} |u_\gamma|^2 |\langle\gamma|\mathbb{V}(t)^+\mathbb{V}(t)|\gamma\rangle| \\
&\quad + 2 \sum_{\substack{\gamma' : |u_{\gamma'}| \leqq |u_\gamma| \\ \gamma' \neq \gamma}} |u_\gamma u_{\gamma'}| |\langle\gamma'|\mathbb{V}(t)^+\mathbb{V}(t)|\gamma\rangle| \\
&\leqq 2 \sum_{\gamma} |u_\gamma|^2 \sum_{\gamma'} |\langle\gamma'|\mathbb{V}(t)^+\mathbb{V}(t)|\gamma\rangle| \\
&\leqq 2 \sum_{\gamma} |u_\gamma|^2 \left(\sum_{\gamma' : x \in \gamma'} \| \operatorname{ad} v(\gamma') \|_1 \right)^2 . \qquad (2.47)
\end{aligned}
$$

The relative boundedness estimate in (2.42) follows from the inequality

$$
\sup_b \sum_{\gamma' : b \in \gamma'} \| \operatorname{ad} v(\gamma') \|_1 \leqq c \cdot t , \qquad (2.48)
$$

which is a direct consequence of the bounds on the operators $\mathbb{R}_n^v$ in the first part of the proof.

From the relative bound in (2.42), it follows that $|0\rangle$ is the ground state of $\mathbb{A}^{-1}\mathbb{H}\mathbb{A}$ in the even sector and that, in this sector, it separated by a gap of order $4 + O(t^2 + J)$ from the rest of the spectrum.

3. Phase Boundaries at Zero Temperature

In the preceding section, we construct a dressing operator $\mathbb{A}(t)$ which is analytic for $|t| < t_0$ for some $t_0 > 0$, and is such that the dressed Hamiltonian $\mathbb{A}(t)^{-1}\mathbb{H}_0\mathbb{A}(t)$ computed at $J = 0$, admits the free vacuum

$$
|0\rangle = \frac{1}{\sqrt{2}}(|N\rangle + |N'\rangle) \qquad (3.1)
$$

as the ground state. This result was obtained in the special case $J = 0$, but with the same methods one can construct a J-dependent dressing operator $\mathbb{A}(t, J)$ analytic for $|t| < t_0$ and $|J| < J_0$, for some $t_0, J_0 > 0$. This dressing transformation computed for $\mathbb{H}_0$, can then be applied to the operator in (1.1) and yields the dressed Hamiltonian

$$
\mathbb{H}_D = \mathbb{A}(t, J)^{-1}\mathbb{H}\mathbb{A}(t, J) . \qquad (3.2)
$$

Due to particle number symmetry, it suffices to consider the case $\mu \leqq 4 + 8J$. Thanks to particle number symmetry, $|0\rangle_N$ is also an eigenstate of $\mathbb{H}_D$ and we have that

$$
\mathbb{H}_D|0\rangle_N = E_N|0\rangle_N , \qquad (3.3)
$$

where

$$
\varepsilon_N \equiv |\Lambda|^{-1}E_N = -(3 - 8J)^{-1}t^2 + \left(2 - \frac{1}{2}\mu + 4J\right) + O((t^2 + J)^2) . \qquad (3.4)
$$

Also the vector

$$|0'\rangle_N = \frac{1}{\sqrt{2}}(|N\rangle - |N'\rangle) \tag{3.5}$$

is an eigenstate of $\mathbb{H}_D$ and satisfies the equation

$$\mathbb{H}_D|0'\rangle_D = E'_N|0'\rangle_N\,, \tag{3.6}$$

where $E'_N = E_N + O(|\Lambda|(c\cdot t)^{\frac{1}{2}|\Lambda|})$. This follows from the fact that the operators τ_γ in Sect. 2 treat the two Néel states in a symmetric way. Finally, we have that

$$\mathbb{H}_D|0\rangle_{F0} = E_{F0}|0\rangle_{F0}\,, \tag{3.7}$$

where

$$\varepsilon_{F0} = |\Lambda|^{-1}E_{F0} = 2\,. \tag{3.8}$$

Let us consider the case $J < 0$ first. The coexistence line $\mu = \mu_{cx}(t)$ is determined by the equation $E_N = E_{F0}$. We find

$$\mu_{cx}(t) = 8J - \frac{2}{3}t^2 + O((t^2 + J)^2)\,. \tag{3.9}$$

The operator $\mathbb{H}_D$ can be split as follows:

$$\mathbb{H}_D = \mathbb{S} + \mathbb{V} + E\,, \tag{3.10}$$

where, if $\mu < \mu_{cx}(t)$, we set $E = E_{F0}$ and

$$\begin{aligned}\mathbb{S} = &\sum_{\langle xy\rangle}\left[2\left(n_x - \frac{1}{2}\right)\left(n_y - \frac{1}{2}\right) - \frac{1}{2}\right] \\ &+ J\sum_{\|x-y\|_1 = 2}\left[2\left(n_x - \frac{1}{2}\right)\left(n_y - \frac{1}{2}\right) - \frac{1}{2}\right] + (4 - \mu + 8J)\sum_x n_x\,,\end{aligned} \tag{3.11}$$

while if $\mu_{cx}(t) \leqq \mu \leqq 4 + 8J$, we see $E = E_N$ and

$$\begin{aligned}\mathbb{S} = &\sum_{\langle xy\rangle}\left[2\left(n_x - \frac{1}{2}\right)\left(n_y - \frac{1}{2}\right) - \frac{1}{2}\right] \\ &+ J\sum_{\|x-y\|_1 = 2}\left[2\left(n_x - \frac{1}{2}\right)\left(n_y - \frac{1}{2}\right) - \frac{1}{2}\right] + (4 - \mu + 8J)\sum_x\left(n_x - \frac{1}{2}\right),\end{aligned} \tag{3.12}$$

To control the spectral gap near the coexistence line, we need to use the "Peierls condition," i.e. the lower bound

$$\mathbb{S} \geqq c\cdot J\cdot \mathbb{S}_P\,. \tag{3.13}$$

Here c is a constant > 0 and $\mathbb{S}_P$ is the diagonal operator defined as follows: If γ is an excitation, let $\mathscr{P}(\gamma)$ be the set of Peierls contours Γ in Λ separating connected regions in which the state $|\gamma\rangle$ coincides with either one of the Néel states, or with the Fock vacuum $|0\rangle_{F0}$. We define $\mathbb{S}_P$ on $|\gamma\rangle$ to be the operator of multipalication by

$$s_P(\gamma) = \inf_{\Gamma\in\mathscr{P}(\gamma)}\{|\Gamma|\}\,. \tag{3.14}$$

The operators τ_γ defined in (2.12) contain the projections π_{xy} which annihilate the states in which both sites x and y are empty. If $\mathbb{V} = \sum_{\gamma_0 \subset \Lambda} v(\gamma_0)$ is the decomposition of $\mathbb{V}$ into operators $v(\gamma_0)$ built out of operators τ_γ covering the set γ_0 and if γ is an excitation such that $n_x|\gamma\rangle = 0$ for all $x \in \gamma_0$, then we have $v(\gamma_0)|\gamma\rangle = 0$. Hence

$$\|\mathbb{V}|\gamma\rangle\|_1 \leqq c \cdot |t| s_P(\gamma) . \tag{3.15}$$

Proceeding as in the previous section, we find the following relative bounds:

$$\langle u|\mathbb{V}^+\mathbb{V}|u\rangle \leqq ct^2\langle u|\mathbb{S}_P^2|u\rangle \leqq ct^2 J^{-2}\langle u|\mathbb{S}^2|u\rangle ,$$

and

$$\|\mathbb{V}\mathbb{S}^{-1}u\|_2 \leqq c \cdot |t| J^{-1}\|u\|_2 \tag{3.16}$$

for all functions u which are orthogonal to $|0\rangle_N$, $|0'\rangle_N$, and $|F0\rangle$. We thus conclude that if $t < c \cdot |J|$, then the wavefunction

$$|0\rangle \equiv \begin{cases} |0\rangle_{F0} & \text{if } \mu < \mu_{cx}(t) \\ |0\rangle_N & \text{if } \mu_{cx}(t) \leqq \mu < 4 + 8J \end{cases} \tag{3.17}$$

is the ground state of $\mathbb{H}$ for $\mu \neq \mu_{cx}(t)$. If $\mu = \mu_{cx}(t)$, the ground state is doubly degenerate and is a mixture of the states $|0\rangle_{F0}$ and $|0\rangle_N$.

More accurate lower bounds can be obtained for values of μ away from $\mu_{cx}(t)$. In fact, we have

$$\mathbb{S} \geqq \begin{cases} (8J - \mu)\mathbb{S}_{F0} & \text{if } \mu \leqq 8J \\ (\frac{1}{4}\mu - 2J)\mathbb{S}_N & \text{if } 8J \leqq \mu \leqq 4 + 8J , \end{cases} \tag{3.18}$$

where we still suppose that $J < 0$ and we set

$$\mathbb{S}_{F0} = \sum_x n_x , \tag{3.19}$$

$$\mathbb{S}_N = \sum_{\langle xy \rangle} 2\left(n_x - \frac{1}{2}\right)\left(n_y - \frac{1}{2}\right) + \frac{1}{2} . \tag{3.20}$$

Since

$$\mathbb{V}|0\rangle_N = \mathbb{V}|0\rangle_{F0} = 0 , \tag{3.21}$$

if $|\gamma\rangle_N \neq |0\rangle_{F0}$ we have

$$\|u\|_2 \|\mathbb{V}\mathbb{S}^{-1}u\|_2 \leqq \begin{cases} ct(8J - \mu)^{-1} & \text{if } \mu \leqq 8J \\ ct(\frac{1}{4}\mu - 2J)^{-1} & \text{if } 8J \leqq \mu \leqq 4 + 8J \end{cases} \tag{3.22}$$

for all functions $|u\rangle \perp \text{span}(|0\rangle, |0'\rangle, |F0\rangle)$. We thus conclude that the wavefunction above in (3.17) is the ground state if $\mu < \mu_{cx}(t) - 8J$ and $t \leqq l_{F0}(\mu)$, where

$$l_{F0}(\mu) = c(8J - \mu) . \tag{3.23}$$

In case $\mu > \mu_{cx}(t) - 8J$, the lower bound is given by the curve

$$l_{F0}(\mu) = c\left(\frac{1}{4}\mu - 2J\right) . \tag{3.24}$$

This result extends by continuity to the case $J = 0$. If $J > 0$, then the lower bounds on the operator $\mathbb{S}$ are

$$\mathbb{S} \geqq \begin{cases} -\mu \mathbb{S}_{F0} & \text{if } \mu \leqq 0 \\ (\frac{1}{4}\mu - 4J)\mathbb{S}_N & \text{if } 16J \leqq \mu \leqq 4 - 8J \,. \end{cases} \tag{3.25}$$

Lower bounds to the phase transition lines, are given by the curves

$$l_N(\mu)) = e\left(\frac{1}{4}\mu - 4J\right), \quad \mu \geqq 16J \,, \tag{3.26}$$

and

$$l_{F0}(\mu) = -c \cdot \mu \,, \quad \mu < 0 \tag{3.27}$$

and the ground state of $\mathbb{H}_D$ is $|0\rangle_{F0}$ for $\mu \leqq l_{F0}(t)$ and $|0\rangle_N$ if $\mu \geqq l_N(t)$.

To find the upper bounds on the phase transition lines one has to study the excitation spectrum. In the case of the operator $\mathbb{H}_0$, i.e. for $\mu = 4 - 8J$, the eigenprojection corresponding to the first excited band is given by the operator

$$\mathbb{P}_1 = \oint_{\mathscr{C}_1} \frac{dz}{2\pi i} \frac{1}{z - \mathbb{S}_0 - \mathbb{V}(t)} \,, \tag{3.28}$$

where $\mathscr{C}_1 = \{z \in \mathbb{C} : |z - (4 - 8J)| < \frac{1}{2}\}$ and $\mathbb{S}_0$ is given in (2.25). Let $\mathbb{P}_{1h} = \bar{\mathbb{P}}_{\frac{1}{2}|\Lambda|-1} \mathbb{P}_1$, where $\bar{\mathbb{P}}_N$ is the orthogonal projection on the sector with N particles. To compute the spectrum of $\mathbb{P}_{1h}\mathbb{H}_0\mathbb{P}_{1h}$ to the lowest orders in t and J, it is convenient to redefine the operators τ_γ in such a way to generate as few diagrams as possible. The choice below is the best we know to compute with.

Let $|N\rangle$ be the Néel state in which the even sublattice Λ_e is occupied while the odd sublattice is empty. If $\gamma \subset \Lambda$, we set

$$\tau_\gamma = \prod_{x \in \Lambda_o} c_x^+ \prod_{y \in \Lambda_e} c_y \,. \tag{3.29}$$

The convergence of the dressing transformation constructed with such operators is hard to control because the τ_γ's don't respect Peierls contours and the resulting $\mathbb{V}(t)$ annihilates $|N\rangle$ but not $|N'\rangle$. This behaviour is at the original of some technical difficulties. In fact, the bad large order behaviour related to configurations with large bubbles of the opposite Néel phase invalidates both the proof of convergence and the discussion above of the coexistence line. However a different choice of the operator τ_γ doesn't affect the end result as far as the expansion coefficient of physically meaningful, i.e. representation independent, quantities are concerned. Since convergence is already established, it is legitimate to carry out the calculation of the lowest order coefficients by means of the new operators. The eigenspace $\mathbb{P}_{1h}\mathscr{H}$ is spanned by the states

$$\begin{aligned} \mathbb{P}_{1h}|y\rangle = &\left(1 - \frac{t^2}{4}\right)|y\rangle + \frac{t}{12} \sum_{\substack{\|x_1 - y\|_1 = 1 \\ \|y_1 - x\|_1 = 1}} c_{x_1}^+ c_{y_1} |y\rangle \\ &+ \frac{t^2}{24} \sum_{\|y - y_1\|_2 = \sqrt{2}} |y_1\rangle + \frac{t^2}{48} \sum_{\|y - y_1\|_2 = 2} |y_1\rangle \end{aligned} \tag{3.30}$$

with $y \in \Lambda_e$. Since

$$\langle y' | \mathbb{P}_{1h}^{+} \mathbb{P}_{1h} | y \rangle = \left[1 - \frac{5t^2}{12} \right] \delta_{yy'} + \frac{5t^2}{72} \sum_{\| y - y_1 \|_2 = \sqrt{2}} \delta_{yy'} + \frac{5t^2}{144} \sum_{\| y - y_1 \|_2 = 2} \delta_{y' y_1} , \tag{3.31}$$

an orthonormal basis for $\mathbb{P}_{1h}\mathscr{H}$ is given by the vectors

$$|\psi(y)\rangle = \left(1 - \frac{t^2}{24}\right) |y\rangle + \frac{t}{12} \sum_{\substack{\| x_1 - y \|_1 = 1 \\ \| y_1 - x \|_1 = 1}} c_{x_1}^{+} c_y |y\rangle$$

$$+ \frac{t^2}{144} \sum_{\| y - y_1 \|_2 = \sqrt{2}} |y_1\rangle + \frac{t^2}{288} \sum_{\| y - y_1 \|_2 = 2} |y_1\rangle \tag{3.32}$$

with $y \in \Lambda_e$. Hence, the reduced Hamiltonian is

$$\langle \psi(y') | \mathbb{H}_0 | \psi(y) \rangle = (4 - 8J - t^2) \delta_{yy'} + \frac{t^2}{2} \sum_{\| y_2 - y \|_2 = \sqrt{2}} \delta_{y_2 y'} + \frac{t^2}{4} \sum_{\| y_2 - y \|_2 = 2} \delta_{y_2 y'} , \tag{3.33}$$

and the dispersion law for holes is

$$\varepsilon_h^{(0)}(k) = (4 - 8J - t^2) + \frac{t^2}{2} \sum_{\| y \|_2 = \sqrt{2}} e^{ik \cdot y} + \frac{t^2}{4} \sum_{\| y \|_2 = 2} e^{ik \cdot y} . \tag{3.34}$$

As μ varies, thanks to particle nuber symmetry, $\mathbb{P}_{1h}\mathscr{H}$ remains an eigenspace of $\mathbb{H}_D$. The corresponding dispersion law is simply shifted by $(\mu - 4 - 8J)$, i.e. it becomes

$$\varepsilon_h(k) = \varepsilon_h^{(0)}(k) + (\mu - 4 - 8J)$$

$$= \mu - 16J - 2t^2 + t^2 (\cos k_1 + \cos k_2)^2 . \tag{3.35}$$

The bottom of the band is

$$\inf_h \varepsilon_h(k) = \inf_k \varepsilon_h(k) = \mu - 16J - 2t^2 . \tag{3.36}$$

Hence, along the line

$$t = u_N(\mu) = \frac{1}{2} \sqrt{\mu - 16J} \tag{3.37}$$

the one quasiparticle gap closes. The curve $u_N(\mu)$ provides an upper bound to the phase transition line.

A second upper bound can be obtained by considering the quasiparticles over the ferromagnetic vacuum $|F0\rangle$. In this case, we find the line

$$t = u_{F0}(\mu) = -\frac{\mu}{4} . \tag{3.38}$$

4. Finite Temperature Expansions

To extend the expansions in the previous section to finite temperature $T = \beta^{-1} > 0$, we need to evaluate traces of the form

$$\langle \mathcal{O} \rangle = Z^{-1} \operatorname{Tr}(\mathcal{O} e^{-\beta \mathbb{H}}) , \tag{4.1}$$

where $\mathcal{O}$ is a local observable and Z is the partition function

$$Z = \operatorname{Tr}(e^{-\beta \mathbb{H}}) . \tag{4.2}$$

Due to the cyclic property of traces, i.e. $\operatorname{Tr}(AB) = \operatorname{Tr}(BA)$, and to the fact that the excitation basis $\{|\gamma\rangle\}$ is orthonormal, we have

$$\begin{aligned} \operatorname{Tr}(\mathcal{O} e^{-\beta \mathbb{H}}) &= \operatorname{Tr}(\mathbb{A}^{-1} \mathcal{O} e^{-\beta \mathbb{H}} \mathbb{A}) \\ &= \operatorname{Tr}(\mathcal{O}_D e^{-\beta \mathbb{H}_D}) = \sum_{\gamma} \langle \gamma | \mathcal{O}_D e^{-\beta \mathbb{H}_D} | \gamma \rangle , \end{aligned} \tag{4.3}$$

where $\mathbb{H}_D$ is the dressed Hamiltonian in (3.1) and

$$\mathcal{O}_D = \mathbb{A}^{-1} \mathcal{O} \mathbb{A} . \tag{4.4}$$

For simplicity, we consider here the special value $\mu = 4 + 8J$ for which $\mathbb{H} = \mathbb{H}_0$. However, the arguments below apply as well to the whole interior of the Néel ordered phases, see Figs. 1, 2, 3, as long as the relative bound of the operator $\mathbb{V}(t)$ with respect to the operator $\mathbb{S}_N$ in (3.20) is much larger than $T = \beta^{-1}$.

Let us call (simple) polymer a map $\bar{\gamma}(\tau)$ defined for $\tau \in [0, \beta]$ with periodic boundary conditions $\bar{\gamma}(0) = \bar{\gamma}(\beta)$ and whose values are subsets of Λ. We assume that the range of values of a polymer $\bar{\gamma}$ consists of a finite number $n(\bar{\gamma})$ of different subsets of Λ. We also assume that $\bar{\gamma}(\tau)$ is upper semicontinuous so that if $\tau_0, \ldots, \tau_{n(\bar{\gamma})}$ are the points of discontinuity of the function $\bar{\gamma}$, then $\bar{\gamma}(\tau)$ is constant on the intervals $[\tau_i, \tau_{i+1}]$, $i = 0, \ldots n(\bar{\gamma}) - 1$. The support of $\bar{\gamma}$ is the set $\operatorname{supp} \bar{\gamma} = \bigcup_{i=0}^{n(\bar{\gamma})-1} \bar{\gamma}(\tau_i)$. Adopting the notations and the terminology of Glimm and Jaffe, see [11], we denote with $\mathscr{P}_1$ the set of (simple) polymers and with $\mathscr{P}_k$ the set of k-polymers, i.e. the k-fold product $\mathscr{P}_k = \mathscr{P}_1 \times \cdots \times \mathscr{P}_1$. We also need a notion of intersection bertween two polymers $\bar{\gamma}_1$ and $\bar{\gamma}_2$. We say that $\bar{\gamma}_1$ and $\bar{\gamma}_2$ are *disjoint* and write $\bar{\gamma}_1 \cap \bar{\gamma}_2 = \emptyset$ if $\operatorname{supp} \bar{\gamma}_1 \cap \operatorname{supp} \bar{\gamma}_2 = \emptyset$. This notion is appropriate for fermion systems because activities corresponding to families of paths whose supports are mutually disjoint but which wind around each other an odd number of times, do not factorize. Bosonic systems are slightly simpler in this respect because they require only the condition $\bar{\gamma}_1(\tau) \cap \bar{\gamma}_2(\tau) = \emptyset$ to be satisfied for all $\tau \in [0, \beta]$ in order to be declared as disjoint. If two polymers are not disjoint we say that they *intersect* and write $\bar{\gamma}_1 \cap \bar{\gamma}_2 \neq \emptyset$. Following [11], les us denote with $\mathscr{D}_k \subset \mathscr{P}_k$ and with $\mathscr{C}_k \subset \mathscr{P}_k$ the sets of the disjoint and of the connected k-polymers, respectively.

The partition function is given by

$$Z = \sum_{j=0}^{\infty} \frac{1}{J!} \int_{\mathscr{D}_j} [d\bar{\gamma}_1] \ldots [d\bar{\gamma}_j] z(\bar{\gamma}_1) \ldots z(\bar{\gamma}_j) , \tag{4.5}$$

where

$$\int_{\mathscr{D}_j} [d\bar{\gamma}_1] \dots [d\bar{\gamma}_j] z(\bar{\gamma}_1) \dots z(\bar{\gamma}_j)$$

$$= \sum_{(\bar{\gamma} \dots \bar{\gamma}) \in \mathscr{D}_j} \int_0^\beta d\tau_N \dots \int_0^{\tau_2} d\tau_1 \, T \prod_{k=1}^{j} z(\bar{\gamma}_{k1}, \dots \bar{\gamma}_{k,n(\gamma_k)-1}; \tau_{m(k,1)}, \dots \tau_{m(k,n(\bar{\gamma}_k)-1)}), \tag{4.6}$$

where T is the time ordering operator, $N = \sum_{k=1}^{j} (n(\bar{\gamma}_k) - 1)$, $m(k, n) = n + \sum_{k'=1}^{k-1} (n(\bar{\gamma}_k) - 1)$ and

$$z(\gamma_0, \dots \gamma_n; \tau_1 \dots \tau_n) = (-1)^n \langle \gamma_0 | e^{(\tau_n - \beta)\mathbb{S}} \operatorname{ad} \mathbb{V} | \gamma_n \rangle \langle \gamma_n | \dots \dots | \gamma_1 \rangle$$

$$\times \langle \gamma_1 | e^{(\tau_1 - \tau_2)\mathbb{S}} \operatorname{ad} \mathbb{V} | \gamma_0 \rangle. \tag{4.7}$$

The combinatorial factor $\frac{1}{j!}$ in (4.7) is due to the fact that $\mathscr{D}_j$ is the set of unordered j-tuples $(\bar{\gamma}_1, \dots \bar{\gamma}_j)$.

The linked cluster theorem in [11] gives

$$\ln Z = \sum_{j=0}^{\infty} \frac{1}{j!} \int_{\mathscr{C}_j} [d\bar{\gamma}_1] \dots [d\bar{\gamma}_j] n(\bar{\gamma}_1, \dots, \bar{\gamma}_j) z(\bar{\gamma}_1) \dots z(\bar{\gamma}_j) , \tag{4.8}$$

where $n(\bar{\gamma}_1, \dots \bar{\gamma}_j)$ is the index of the graph $\{\bar{\gamma}_1, \dots \bar{\gamma}_j\} \in \mathscr{C}_j$.

If γ_1 and $\gamma_2 \subset \Lambda$, let their distance $d(\gamma_1, \gamma_2)$ be defined as follows:

$$d(\gamma_1, \gamma_2) = \{\inf |\Gamma|, \Gamma \subset \Lambda \text{ such that } \forall x \in \gamma_1 \backslash \gamma_2 \text{ (resp. } \gamma_2 \backslash \gamma_1)$$

$$\text{there is a path in } \Gamma \text{ joining it to } \gamma_2 \text{ (resp. } \gamma_1)\} . \tag{4.9}$$

Lemma. *If $x \in \Lambda$ and $\gamma_0 \subset \Lambda$, $e^{-\beta} \leqq t$. Then, we have*

$$\sup_{x \in \Lambda} \int_{\mathscr{P}_{\gamma_0}(d_0)} [d\bar{\gamma}] |z(\bar{\gamma})| \leqq (ct)^{\frac{1}{4} d_0} [e^{-\frac{1}{4}\beta |\partial \gamma_0|} + e^{-\frac{1}{2}\beta} (ct)^{\frac{1}{4} |\partial \gamma_0|}] , \tag{4.10}$$

where $\mathscr{P}_{\gamma_0}(d_0)$ is the set of simple polymers $\bar{\gamma}$ for which we have $\bar{\gamma}(0) = \gamma_0$ and $d_0 = d(\partial\bar{\gamma}(0), \operatorname{supp} \bar{\gamma})$.

Proof. If $\mathbb{V}_m$, $m \geqq 1$, are the operators such that

$$\mathbb{V}(t) = \sum_{m=1}^{\infty} t^m \mathbb{V}_m , \tag{4.11}$$

we have that

$$\sum_{\gamma_1 \dots \gamma_n} \int_0^\beta d\tau_n \dots \int_0^\beta d\tau_1 \, |z(\gamma_0, \dots \gamma_n; \tau_1, \dots \tau_n)|$$

$$\leqq \beta^n \Bigg(\sum_{\substack{\gamma_1 \dots \gamma_n \\ |\partial\gamma_i| \geqq \frac{1}{2}|\partial\gamma_0|}} + \sum_{\substack{\gamma_1 \dots \gamma_n \\ |\partial\gamma_i| < \frac{1}{2}|\partial\gamma_0| \, \exists i}} \Bigg) \int_0^1 d\tau_n \dots \int_0^{\tau_2} d\tau_1 \sum_{m_0 + \dots + m_n \geqq d_0}$$

$$\times t^{m_0 + \dots + m_n} |\langle \gamma_0 | e^{\beta(\tau_n - 1)\mathbb{S}} \operatorname{ad} \mathbb{V}_{m_n} | \gamma_n \rangle| \dots .$$

$$|\langle \gamma_n | e^{\beta(\tau_1 - \tau_2)\mathbb{S}} \operatorname{ad} \mathbb{V}_{m_0} e^{-\beta\tau_1 \mathbb{S}} | \gamma_0 \rangle|$$

$$\leqq 2^n \Bigg(\sum_{\substack{\gamma_1, \ldots, \gamma_n: \\ |\partial \gamma_i| \geqq \frac{1}{2}|\partial \gamma_0|}} e^{-\frac{\beta}{4}|\partial \gamma_0|} + \sum_{\substack{\gamma_1, \ldots, \gamma_n: \\ |\partial \gamma_i| < \frac{1}{2}|\partial \gamma_0| \exists i}} e^{-\frac{\beta}{4}} t^{\frac{1}{4}|\partial \gamma_0|} \Bigg)$$

$$\times \sum_{m_0 + \cdots + m_n \geqq d_0} t^{\frac{1}{2}(m_0 + \cdots + m_n)} |\langle \gamma_0|$$

$$\times \operatorname{ad} \mathbb{V}_{m_n} \mathbb{S}^{-1} |\gamma_n\rangle| \ldots . |\langle \gamma_1| \operatorname{ad} \mathbb{V}_{m_0} \mathbb{S}^{-1} |\gamma_0\rangle|$$

$$\leqq (e^{-\frac{\beta}{4}|\partial \gamma_0|} + e^{-\frac{\beta}{4}} t^{\frac{1}{4}|\partial \gamma_0|}) \sum_{m_0 + \cdots + m_n \geqq d_0} (c \cdot t)^{\frac{1}{2}(m_0 + \cdots + m_n)}$$

$$\leqq (c \cdot t)^{\frac{1}{2} d_0} (e^{-\frac{\beta}{4}|\partial \gamma_0|} + e^{-\frac{\beta}{4}} t^{\frac{1}{4}|\partial \gamma_0|}) \,. \tag{4.12}$$

The geometrical meaning of this derivation is quite remarkable and is illustrated in Fig. 5. In the classical regime $e^{-\beta} \gg t$ the $(2+1)$-dimensional polymers that dominate in the expansion are the fat polymers in Fig. 5a, i.e. the polymers in which the size of the boundary of the excitation never shrinks below $\frac{1}{2}|\partial \gamma_0|$. On the other hand, in the regime dominated by quantum fluctuations, i.e. $e^{-\beta} \ll t$, the slim polymers of Fig. 5b are the most important ones.

The proof of convergence can now be completed by projecting the cluster expansion onto coordinate space, using (4.11) and following the method in [11]. Namely, we have that

$$\left| \frac{1}{k!} \int_{\mathscr{C}_k} [d\bar{\gamma}_1] \ldots [d\bar{\gamma}_k] n(\bar{\gamma}_1, \ldots \bar{\gamma}_k) z(\bar{\gamma}_1) \ldots z(\bar{\gamma}_k) \right|$$

$$\leqq \frac{1}{k!} \sum_{v_1 \ldots v_k} \sum_{d_1 \ldots d_k = 1} \frac{(k-)!}{\prod_i (d_i - 1)!} \int_{\mathscr{C}_k(v_1 \ldots v_k, d_1 \ldots d_k)}$$

$$\times [d\bar{\gamma}_1] \ldots [d\bar{\gamma}_k] |z(\bar{\gamma}_1) \ldots z(\bar{\gamma}_k)|, \tag{4.13}$$

where $\mathscr{C}_k(v_1, \ldots v_k; d_1, \ldots d_k)$ is the set of connected k-polymers $(\bar{\gamma}_1, \ldots \bar{\gamma}_k)$ such that for all $i = 1, \ldots k$, we have $|\partial \bar{\gamma}_i(0)| = v_i$ and

$$\# \{ j = 1, \ldots k, j \neq i : \bar{\gamma}_i \cap \bar{\gamma}_j \neq \emptyset \} = d_i \,. \tag{4.14}$$

Fixed a spanning tree with coordination numbers d_i for the graph $(\bar{\gamma}_1, \ldots \bar{\gamma}_k)$, one can use the lemma above to eliminate all vertices with $d_i = 1$, iteratively. We find

$$\int_{\mathscr{C}_k(v_1 \ldots v_k; d_1 \ldots d_k)} [d\bar{\gamma}_1] \ldots . [d\bar{\gamma}_k] |z(\bar{\gamma}_1) \ldots z(\bar{\gamma}_k)| \leqq c^k |\Lambda|$$

$$\prod_{i=1}^{k} v_i^{d_i} (e^{-\frac{1}{4}\beta v_i} + e^{-\frac{\beta}{2}} (c \cdot t)^{\frac{1}{4} v_i}) \,. \tag{4.15}$$

The point to underline here is that, thanks to the lemma above, to estimate this integral one can choose base points in coordinate space, i.e. on the sets $\bar{\gamma}_i(0)$. Since

$$\frac{1}{(d-1)!} \sum_{v \geqq 4} v^d (e^{-\frac{1}{4}\beta v} + e^{-\frac{1}{2}\beta} (ct)^{\frac{1}{4} v}) \leqq c \cdot d^{-2} e^{-\frac{1}{2}\beta} \,, \tag{4.16}$$

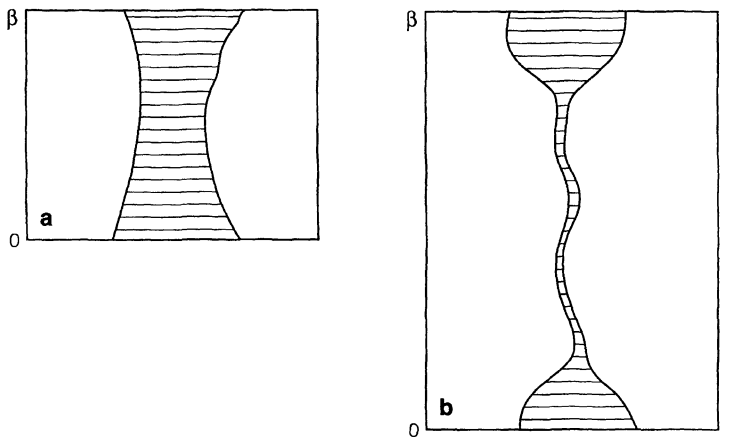

Fig. 5a, b

we have

$$\left|\frac{1}{|\Lambda|}\sum_{k=2}^{\infty}\frac{1}{k!}\int_{\mathscr{C}_k}[d\bar{\gamma}_1]\ldots.[\bar{\gamma}_k]n(\bar{\gamma}_1,\ldots.\bar{\gamma}_k)z(\bar{\gamma}_1)\ldots.z(\bar{\gamma}_k)\right|$$

$$\leqq c e^{\frac{1}{2}\beta}\sum_{k=2}^{\infty}\frac{1}{k(k-1)}\leqq c\cdot e^{\frac{1}{2}\beta}\,. \tag{4.17}$$

Finally, let us discuss the lower bound on the expectation of the sign observable S defined after (1.8). Using the linked cluster theorem above, we find

$$\langle S\rangle=\exp\left(\sum_{j=0}^{\infty}\int_{\mathscr{C}_j}d[\bar{\gamma}_1]\ldots.d[\bar{\gamma}_k]n(\bar{\gamma}_1,\ldots.\bar{\gamma}_j)\min(0,z(\bar{\gamma}_1)\ldots.z(\bar{\gamma}_j))\right) \tag{4.18}$$

Thanks to the lemma above, we find the lower bound

$$\langle S\rangle\geqq\exp(-c\cdot t\cdot|\Lambda|\cdot e^{-\frac{\beta}{2}})\,. \tag{4.19}$$

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