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Low-Temperature Phases of Itinerant Fermions Interacting with Classical Phonons: The Static Holstein Model

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We consider models of independent itinerant fermions interacting with classical continuous or discrete variables (spins), the static Holstein model being a special case. We prove for all values of the fermion-spin coupling and a special value of the fermion chemical potential and classical magnetic field, at which the average fermion density is one-half and the average total spin is zero, that there are two degenerate ground states of period two with antiferromagnetic order for the spins and fermions. The existence of two corresponding low-temperature phases is proven for large coupling and dimension two or more by using a Peierls argument. This generalizes results of Kennedy and Lieb for the Falicov–Kimball model.

KEY WORDS: Itinerant fermions; low-temperature phases; antiferromagnetic ordering; static Holstein model; classical phonons.

1. INTRODUCTION

We study the equilibrium properties of a general class of lattice models of free itinerant fermions interacting with classical degrees of freedom. The fermions are described by creation and annihilation operators $c_x^\dagger$, c_x at lattice sites $x \in \Lambda$, Λ a finite subset of the d-dimensional cubic lattice $\mathbf{Z}^d$. They satisfy the canonical anticommutation relations $c_x^\dagger c_y + c_y^\dagger c_x = \delta_{xy}$, $x \in \Lambda$, $y \in \Lambda$. The classical degrees of freedom are described by a spin variable s_x, $x \in \Lambda$, which takes discrete or continuous values in $\mathbf{R}$. This is specified by

Dedicated to Philippe Choquard on the occasion of his 65th birthday.

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an *a priori* even spin measure $p(s_x)$ chosen according to the physical significance of the spin variables in the models considered. We follow the ideas of Kennedy and Lieb[18,19] on the Falicov–Kimball model which corresponds to s_x taking on only two values.

The Hamiltonian of the system is given by

$$H_\Lambda(\mu, h) = \sum_{x,y\in\Lambda} t_{xy} c_x^+ c_y + \lambda \sum_{x\in\Lambda} n_x s_x - h \sum_{x\in\Lambda} s_x - \mu \sum_{x\in\Lambda} n_x + \sum_{x\in\Lambda} f(s_x^2) \tag{1.1}$$

where the hopping matrix is $t_{xy} = -1$ for $|x-y| = 1$ and 0 otherwise, $n_x = c_x^+ c_x$, and h and μ are the magnetic field and chemical potential acting, respectively, on the classical and fermion degrees of freedom. The term $f(s_x^2)$ represents the energy associated to the classical degree of freedom.

The average value of a general observable $O(\{c_x^\dagger, c_x, s_x\})$ at inverse temperature β is given by

$$\langle O(\{c_x^\dagger, c_x, s_x\})\rangle_\Lambda (\beta, \mu, h) = \int \prod_{x\in\Lambda} ds_x \operatorname{Tr}[O(\{c_x^\dagger, c_x, s_x\})\, \rho_\Lambda(\beta, \mu, h)] \tag{1.2}$$

where ρ_Λ is the density matrix

$$\rho_\Lambda(\beta, \mu, h) = \frac{1}{Z_\Lambda} \prod_{x\in\Lambda} p(s_x) \exp[-\beta H_\Lambda(\mu, h)] \tag{1.3}$$

and Z_Λ is the partition function

$$Z_\Lambda = \int \prod_{x\in\Lambda} p(s_x)\, ds_x \operatorname{Tr} \exp[-\beta H_\Lambda(\mu, h)] \tag{1.4}$$

Since for specified values of the $\{s_x\}$ the fermions are not interacting, the average of observables which depend exclusively on the spin variables, for example, $S_A = \prod_{x\in A} s_x$, $A \subset \Lambda$, can be computed by first tracing out the fermions. This yields a classical (Gibbs) probability distribution for the spins such that

$$\langle S_A\rangle_\Lambda (\beta, \mu, h) = \frac{1}{Z_\Lambda} \int S_A \exp[-\beta F_\Lambda(\{s_x\}, \beta, \mu, h)] \prod_{x\in\Lambda} p(s_x)\, ds_x \tag{1.5}$$

where $F_\Lambda(\{s_x\}, \beta, \mu, h)$, the effective *interaction* energy between the spins, is given by the formula

$$F_\Lambda(\{s_x\}, \beta, \mu, h) = \beta^{-1} |\Lambda| \ln 2 + \frac{1}{2} \operatorname{tr}[H(\{s_x\}) - \mu] - \beta^{-1} \operatorname{tr}\left\{\ln \cosh \frac{\beta}{2} \sqrt{[H(\{s_x\}) - \mu]^2}\right\} - h \sum_{x \in \Lambda} s_x + \sum_{x \in \Lambda} f(s_x^2) \quad (1.6)$$

The one-fermion hamiltonian $H(\{s_x\})$ in (1.6) is a $|\Lambda| \times |\Lambda|$ matrix

$$H(\{s_x\}) = T + \lambda S \quad (1.7)$$

where $(T)_{xy} = t_{xy}$ and $(S)_{xy} = s_x \delta_{xy}$. [To get (1.6) one uses the identity $1 + e^{-x} = 2e^{-x/2} \cosh(\frac{1}{2}\sqrt{x^2})$].

It is possible to recover from the classical distribution (1.5) information about certain quantum observables by using the following type of formula (proved in Appendix A):

$$\langle n_x \rangle_\Lambda (\beta, \mu, h) = \frac{h}{\lambda} + \frac{2}{\lambda} \langle s_x f'(s_x^2) \rangle_\Lambda (\beta, \mu, h) \quad (1.8)$$

In various applications the second term on the right-hand side of (1.8) is in fact proportional to the order parameter of the effective classical model [defined by (1.5) and (1.6)] so that information about the fermion phases can be obtained from the classical phase diagram. We also discuss in the conclusion and Appendix A a formula connecting the spin–spin correlation to the imaginary-time displaced density–density correlation of the fermions (or Duhamel two-point function).

The ground-state energy of the fermions in a given classical configuration $\{s_x\}$ is defined by

$$E_\Lambda(\{s_x\}, \mu, h) = \lim_{\beta \to \infty} F_\Lambda(\{s_x\}, \beta, \mu, h) \quad (1.9)$$

From (1.6) one finds

$$E_\Lambda(\{s_x\}, \mu, h) = -\frac{1}{2} \operatorname{tr}\{[H(\{s_x\}) - \mu]^2\}^{1/2} + \sum_{x \in \Lambda} f(s_x^2) + \left(\frac{\lambda}{2} - h\right) \sum_{x \in \Lambda} s_x - \frac{\mu}{2} |\Lambda| \quad (1.10)$$

The ground states of the full system are found by minimizing this function over all possible spin configurations.

Results

In the present work we obtain rigorous results about the ground states and low-temperature phases for the special case where $h=\lambda/2$ and $\mu=0$. We call this point in the (μ, h) plane the symmetry point because the Gibbs factor in (1.5) is invariant under a global spin reversal $\{s_x\} \to \{-s_x\}$. To see this, let $(U)_{xy}=\varepsilon_x \delta_{xy}$, $\varepsilon_x=+1$ for x even and -1 for x odd, be a $|\Lambda| \times |\Lambda|$ matrix; then $U^\dagger T U=-T$ and $U^\dagger S U=S$. Thus $U^\dagger H(\{s_x\})^2 U = H(\{-s_x\})^2$, which together with the unitarity of U implies the invariance of the Gibbs factor at the symmetry point. At the level of the fermion operators the transformation $c_x^\dagger \to \varepsilon_x c_x$, $c_x \to \varepsilon_x c_x^\dagger$, exchanges particles into holes because $c_x^\dagger c_x \to 1 - c_x^\dagger c_x$. Moreover, since the transformation is unitary, one can check that $\langle c_x^\dagger c_x \rangle_\Lambda (\beta, 0, \lambda/2) = 1 - \langle c_x^\dagger c_x \rangle_\Lambda (\beta, 0, \lambda/2)$. Thus at the symmetry point the electron density is exactly 1/2 for any β.

In particular we prove that for a large class of functions $f(s_x^2)$ there are two ground-state configurations of the spins for all λ

$$s_x = \pm \varepsilon_x \sigma_0(\lambda) \tag{1.11}$$

where the amplitude of the spin $\sigma_0(\lambda)$ is the solution of an integral equation depending on the particular single spin measure. At low temperature and large λ we prove that there are, in $d \geqslant 2$, at least two phases corresponding to the two antiferromagnetic ground states.

The proof makes use of a Peierls–Dobrushin argument adapted to our situation. The application is made difficult by the fact that the effective energy (1.6) and (1.10) contains many-body interactions among the spins, whose structure is difficult to obtain. This prevents the straightforward application of methods of classical statistical mechanics to the spin probability distribution (1.5). Our analysis brings out the following features of $F_\Lambda(\{s_x\}, \beta, 0, \lambda/2)$: At low temperatures the dominant terms in the total effective energy are the sum of a one-body and two-body potential; n-body terms with $n>2$ are negligible. The one-body term consists of a double well with two minima at $\pm\sigma_0(\lambda)$. The two-body term has an Ising antiferromagnetic form if the spins have values close to the minima. The main difficulty we have to overcome in applying the Peierls argument is that the energy gain associated with a Peierls contour becomes very small either when the spins adjacent to the contour take values close to zero or when they take very large values. It turns out that the one-body contribution acts as an "effective chemical potential" which discourages too small or too large values of the spins.

We discuss more specifically three special models.

The Static Holstein Model

This model has the single spin measure $p(s_x) = 1$ and energy

$$f(s_x^2) = \tfrac{1}{2}s_x^2 \tag{1.12}$$

Physically the corresponding Hamiltonian describes an interacting electron–phonon system[15,23] where the phonons are treated as *classical* oscillators. Since the oscillators are classical one can integrate out their momentum variables and only the position variables remain (hence the name static, for quantum mechanical oscillators position and momenta do not decouple). Thus in this case s_x is to be interpreted as a position variable of a harmonic oscillator at site x. This model has recently been discussed extensively in refs. 1 and 2, where it is called the adiabatic Holstein model.

An application of the formula (1.8) to the Holstein model at the symmetry point gives the simple relation

$$\langle n_x \rangle_\Lambda \left(\beta, 0, \frac{\lambda}{2}\right) = \frac{1}{2} + \frac{1}{\lambda} \langle s_x \rangle_\Lambda \left(\beta, 0, \frac{\lambda}{2}\right)$$

The behavior of $\langle n_x \rangle$ is the same as that of $\langle s_x \rangle$. Our results for the ground state in any dimension and at low temperatures, in $d \geqslant 2$, thus prove that the electron density forms a "charge density wave" of period 2. This makes rigorous the theory of the Peierls instability for this model (for results in one-dimensional models see refs. 3 and 19). We can also prove that at high enough temperature $F_\Lambda(\{s_x\}, \beta, 0, \lambda/2)$ is a strictly convex function of $\{s_x\}$ with a unique minimum at $s_x = 0$ for all $x \in \Lambda$. The abscence of long-range order for $\beta\lambda^2 \ll 1$ then follows from an application of the Brascamp–Lieb inequalities.

One can also add anharmonic corrections to the energy of the oscillator,[5] e.g.,

$$f(s_x^2) = \tfrac{1}{2}s_x^2 + \alpha_4 s_x^4 + \cdots, \qquad \alpha_4 > 0 \tag{1.13}$$

without changing the main results. The only difference is that convexity does not hold for single spin energies without the quadratic term, for example, $f(s_x^2) = \alpha_4 s_x^4$. In fact we will show that when the quadratic term is absent the effective energy is minimized for all temperatures by the two antiferromagnetic spin configurations. There is, of course, still an absence of long-range order at high temperature, but it does not follow directly from Brascamp–Lieb inequalities.

The Falicov–Kimball (FK) Model

In this case one takes

$$p(s_x) = \tfrac{1}{2}[\delta(s_x - 1) + \delta(s_x + 1)] \tag{1.14}$$

In other words, one can consider the spin as a discrete variable taking values in $\{-1, +1\}$. Moreover the Hamiltonian (1.1) is defined without the term $\sum_x f(s_x^2)$, which would just be a constant in this case. The FK model has been analyzed extensively in the literature. In refs. 18 and 19 (but see also ref. 26) it was studied in detail at the symmetry point (density 1/2), where one has two degenerate antiferromagnetic ground states and two corresponding low-temperature phases in $d \geqslant 2$. These results were extended[22] for large λ to a strip of width $1/\lambda$ in the (μ, h) plane around the symmetry point, thereby allowing the density to be different from but close to 1/2. Results concerning the ground state for other rational densities can be found in refs. 7, 20, 11, 13, and 14 for the one-dimensional case and in ref. 17 for two dimensions.

One can obtain this model as the limit $\gamma \to \infty$ of a continuous spin model with

$$p_\gamma(s_x) = e^{-\gamma(s_x^2 - 1)^2} \left[\int ds_x \, e^{-\gamma(s_x^2 - 1)^2} \right]^{-1} \tag{1.15}$$

This enables us to apply (1.8) and obtain (see Appendix A)

$$\langle n_x \rangle_\Lambda \left(\beta, 0, \frac{\lambda}{2} \right) = \frac{1}{2} + \frac{\lambda}{2} g(\beta, \lambda) \langle s_x \rangle_\Lambda \left(\beta, 0, \frac{\lambda}{2} \right) \tag{1.16}$$

with $g(\beta, \lambda)$ given by (A.7). This relation, which is valid for any β and λ, is new to us. Since $g(\beta, \lambda)$ is analytic in β, the critical behavior of $\langle n_x \rangle$ is identical to that of $\langle s_x \rangle$, which is presumably of Ising type. The latter fact has been shown to hold in the limit of infinite dimensions.[25]

An Intermediate Model

A useful model which is intermediate between the Holstein and FK models has

$$p(s_x) = \tfrac{1}{3}[\delta(s_x) + \delta(s_x^2 - 1)] \tag{1.17}$$

In this case the spin takes the three values $+1$, 0, and -1, and the Hamiltonian is defined without the term $\sum_x f(s_x^2)$. This model already contains some essential features of the static Holstein model. For the sake of clarity we present the Peierls argument for this case and then indicate the necessary modification needed to treat the case of continuous unbounded spin.

The rest of the paper is organized as follows. In the next section we analyze the ground states for continuous spins according to the choice of $f(s_x^2)$. Section 3 is devoted to the study of the structure of the effective potential at positive temperatures. We prove there results about the minima of $F_\Lambda(\{s_x\}, \beta, 0, \lambda/2)$ for small and large β. The low-temperature behavior of the system is the subject of Section 4, where the Peierls argument is carried out. Section 5 contains a discussion of open problems. More technical material can be found in the appendices.

2. GROUND STATES

We consider the model on a cube $\Lambda \subset \mathbf{Z}^d$ containing $(2N)^d$ sites with periodic or free boundary conditions. We want to minimize the ground-state energy at the symmetry point $(\mu, h) = (0, \lambda/2)$,

$$E(\{s_x\}) = -\tfrac{1}{2}\operatorname{tr}\{[H(\{s_x\})]^2\}^{1/2} + \sum_{x \in \Lambda} f(s_x^2) \tag{2.1}$$

where, to keep the notation simple, we do not write the Λ and (μ, λ) dependence explicitly. The case of the Falicov–Kimball model has been treated in refs. 18 and 19 and the case where $p(s_x)$ is a uniform distribution on the interval $[-1, +1]$ and $f(s_x^2)$ is absent has been considered in ref. 21. For both situations $E(\{s_x\})$ attains its two unique minima for the antiferromagnetically ordered configuration $s_x = \pm\varepsilon_x$, all $x \in \Lambda$. When one has to take into account the energy $f(s_x^2)$ the amplitude of the minimizing spin configuration will be different from $+1$ and is determined by an integral equation.

Theorem 2.1. Let $f(t)$ be a positive convex function for $t \geqslant 0$, with $f'(t) > 0$ for t large enough. Then

(i) $E(\{s_x\})$ in (2.1) attains its global minimum for the antiferromagnetic spin configurations

$$s_x = \pm\varepsilon_x \sigma_0(\lambda) \tag{2.2}$$

where $\sigma_0^2(\lambda)$ is the solution of the equation in t

$$f'(t) = \frac{\lambda^2}{4}\frac{1}{|\Lambda|}\sum_{k_\alpha, \alpha = 1 \cdots d}\left[4\left(\sum_{\alpha=1}^{d}\cos k_\alpha\right)^2 + \lambda^2 t\right]^{-1/2} \tag{2.3}$$

and the sum is over the modes $k_\alpha = \pi n_\alpha/N$, $n_\alpha = -N, \ldots, +N$, $(2N)^d = |\Lambda|$.

(ii) These are the only two global minima.

Remarks. (a) This theorem makes rigorous the theory of the Peierls instability for this class of models. Here it is valid in any dimension due to the fact that there is no coupling between the phonons on different sites. Equation (2.3) is standard in the solid state literature.

(b) The theorem makes sense because a unique solution of (2.3) always exists (for all λ) as long as $|\Lambda|$ is large enough. This is also true in the thermodynamic limit. In the case of the Holstein model for large λ, $\sigma_0(\lambda) \sim \lambda/2$ and for small λ, $\sigma_0(\lambda) \sim \lambda^{-1} \exp(-4\lambda^{-2})$. These facts are proved in Appendix B.

(c) We could consider more general bipartite lattices, in which case the sum over cosines in (2.3) would have to be replaced by the appropriate dispersion relation $\sum_x t_{x0} \exp(ik \cdot x)$.

(d) Fermions with a spin one-half would give the same result with a factor of 2 multiplying the right-hand side of (2.3).

Proof of Theorem 2.1. The first step of the proof uses an idea of refs. 18 and 19, which we reproduce here for completeness. As noted in the introduction, $H(\{s_x\})^2$ and $H(\{-s_x\})^2$ are unitarily equivalent. Thus from (1.12) we have for $\mu = 0$ and $h = \lambda/2$

$$E(\{s_x\}) = \tfrac{1}{2}[E(\{s_x\}) + E(\{-s_x\})] \tag{2.4}$$

Using the fact that tr $\sqrt{X}$ is a concave function of the matrix X together with (2.4), one gets

$$\begin{aligned} E(\{s_x\}) &\geqslant -\tfrac{1}{2} \operatorname{tr}[H(\{s_x\})^2 + H(\{-s_x\})^2]^{1/2} + \sum_{x \in \Lambda} f(s_x^2) \\ &= -\tfrac{1}{2} \operatorname{tr}(T^2 + \lambda^2 S^2)^{1/2} + \sum_{x \in \Lambda} f(s_x^2) \end{aligned} \tag{2.5}$$

In (2.5) the equality is attained for configurations such that $TS + ST = 0$, i.e., $s_x + s_y = 0$ for all nearest neighbor pairs $x, y \in \Lambda$. The most general form of such configurations is $s_x = \pm \varepsilon_x \sigma$, where σ is any positive real number.

We will now show that there exists such a configuration which minimizes the lower bound in (2.5). Clearly this will also be a minimum of $E(\{s_x\})$. We set $S^2 = \Phi$, $(\Phi)_{xy} = \phi_x \delta_{xy}$. The lower bound is a function of $\{\phi_x\}$, namely

$$G(\{\phi_x\}) = -\tfrac{1}{2} \operatorname{tr}(T^2 + \lambda^2 \Phi)^{1/2} + \sum_{x \in \Lambda} f(\phi_x) \tag{2.6}$$

We have

$$\frac{\partial G}{\partial \phi_x} = f'(\phi_x) - \frac{\lambda^2}{4} \operatorname{tr}\left[\frac{\partial \Phi}{\partial \phi_x} (T^2 + \lambda^2 \Phi)^{-1/2}\right] \tag{2.7}$$

Since $\langle y|\, \partial\Phi/\partial\phi_x \,|z\rangle = \delta_{xy}\delta_{zx}$, any local minimum satisfies the set of equations

$$f'(\phi_x) = \frac{\lambda^2}{4} \langle x|\, (T^2 + \lambda^2\Phi)^{-1/2}\, |x\rangle, \qquad x \in \Lambda \tag{2.8}$$

For a solution of (2.8) we try the ansatz $\phi_x = \sigma^2$, σ a real constant independent of x. One obtains (2.3) by expressing the right-hand side of (2.8) by a sum over the wavenumbers of the first Brillouin zone. (See remarks after the theorem for the existence of a solution.) Thus we have found at least one local minimum of $G(\{\phi_x\})$. Obviously G is a convex function, so this must also be a global minimum of G and therefore of $E(\{s_x\})$ also.

It remains to prove statement (ii). In fact this follows from the unicity of the minimum of $G(\{\phi_x\})$, which we now prove by showing that for any $\{\phi_x\}$ the matrix $\partial^2 G/\partial\phi_u\, \partial\phi_v$ is strictly positive. From (2.7) we have

$$\frac{\partial^2 G}{\partial \phi_u\, \partial \phi_v} = f''(\phi_u)\, \delta_{uv} + M_{uv} \tag{2.9}$$

with

$$M_{uv} = -\frac{\lambda^2}{4} \langle v|\, \frac{\partial}{\partial \phi_u} (T^2 + \lambda^2\Phi)^{-1/2}\, |v\rangle \tag{2.10}$$

To compute the partial derivative with respect to ϕ_u in (2.10) we use the following representation of the square root[16]

$$(T^2 + \lambda^2\Phi)^{-1/2} = \frac{1}{\pi} \int_0^\infty \frac{dr}{\sqrt{r}} \frac{1}{r + (T^2 + \lambda^2\Phi)} \tag{2.11}$$

An application of the resolvent equation leads to

$$M_{uv} = \frac{\lambda^4}{2\pi} \int_0^\infty \frac{dr}{\sqrt{r}} \langle u|\, \frac{1}{r + (T^2 + \lambda^2\Phi)}\, |v\rangle\langle v|\, \frac{1}{r + (T^2 + \lambda^2\Phi)}\, |u\rangle \tag{2.12}$$

Since (2.12) is *real* and *symmetric* with respect to exchange of u and v, we only have to show that

$$P \equiv \sum_{u,v \in \Lambda} M_{uv} \psi_u \psi_v > 0 \tag{2.13}$$

for all *real-valued* nonzero functions ψ_x, $x \in \Lambda$. Denoting by ψ the self-adjoint multiplication operator by the real function ψ_x, we have from (2.12)

$$P \equiv \frac{\lambda^4}{2\pi} \int_0^\infty \frac{dr}{\sqrt{r}} \operatorname{tr}\left[\psi \frac{1}{r + (T^2 + \lambda^2 \Phi)} \psi \frac{1}{r + (T^2 + \lambda^2 \Phi)}\right] \tag{2.14}$$

Since $T^2 \leqslant 4d^2$ we get, using (2.14) and the cyclicity of the trace,

$$\begin{aligned} P &\geqslant \frac{\lambda^4}{2\pi} \int_0^\infty \frac{dr}{\sqrt{r}} \operatorname{tr}\left[\psi^2 \frac{1}{(r + 4d^2 + \lambda^2 \Phi)^2}\right] \\ &= \frac{\lambda^4}{2\pi} \int_0^\infty \frac{dr}{\sqrt{r}} \sum_{x \in \Lambda} \psi_x^2 \frac{1}{(r + 4d^2 + \lambda^2 \phi_x)^2} \end{aligned} \tag{2.15}$$

By hypothesis there exists at least one $x \in \Lambda$ for which $\psi_x \neq 0$; thus P is strictly positive. Since $f''(t) \geqslant 0$ $(t \geqslant 0)$, $\partial^2 G/\partial \phi_u \, \partial \phi_v$ is positive definite. This concudes the proof of the theorem.

3. STRUCTURE OF THE EFFECTIVE ENERGY

We are concerned with qualitative properties of the total effective energy depending on the particular class of functions $f(s_x^2)$. At the symmetry point $(\mu, h) = (0, \lambda/2)$ it takes the form

$$F(\{s_x\}) = -\beta^{-1} \operatorname{tr}\left[\ln \cosh \frac{\beta}{2} \{[H(\{s_x\})]^2\}^{1/2}\right] + \sum_{x \in \Lambda} f(s_x^2) \tag{3.1}$$

The main results of this section are the following.

Theorem 3.1. Let $f(t)$ be a positive convex polynomial $\sum_{j=1}^N a_j t^j$, with $a_N > 0$. We consider two cases:

(i) $a_1 = 0$. Then for any β and λ, $F(\{s_x\})$ attains its global minimum for the antiferromagnetic spin configurations

$$s_x = \pm \varepsilon_x \sigma_1(\lambda, \beta) \tag{3.2}$$

where $\sigma_1^2(\lambda, \beta)$ is the solution of the equation in t,

$$f'(t) = \frac{\lambda^2}{4} \frac{1}{|\Lambda|} \sum_{k_\alpha, \alpha = 1 \cdots d} [E(k)]^{-1} \tanh\left[\frac{\beta}{2} E(k)\right] \tag{3.3}$$

with

$$E(k)=\left[4\left(\sum_{\alpha=1}^{d}\cos k_\alpha\right)^2+\lambda^2 t\right]^{1/2} \tag{3.4}$$

Moreover, these are the only two minima.

(ii) $a_1>0$. Then, for a given λ, Eq. (3.3) has a solution only for β large enough and the only two global minima of $F(\{s_x\})$ are given by (3.2).

Theorem 3.2. Suppose that $f(t)$ is as in (ii) of Theorem 3.1 and all $a_j>0$. Then there exists a positive constant c such that for $\beta\lambda^2<c$, $F(\{s_x\})$ is a strictly convex function of $\{s_x\}$. Since it is even, it attains its unique minimum at $s_x=0$, all $x\in\Lambda$. For the Holstein model $a_1=1/2$ and one can take $c=2$.

These results show that when the quadratic term is absent in $f(s_x^2)$, the qualitative structure of $F(\{s_x\})$ is independent of β, but it can change with β when a quadratic term is present. In particular the static Holstein model falls in the second category. An interesting application of Theorem 3.2, which we defer to the end of this section, is a proof of the absence of long-range order in the Holstein model for $\beta\lambda^2\ll 1$.

Proof of Theorem 3.1. The same arguments which led us to (2.5) imply the lower bound

$$F(\{s_x\})\geqslant -\frac{1}{\beta}\operatorname{tr}\left[\ln\cosh\frac{\beta}{2}(T^2+\lambda^2 S^2)^{1/2}\right]+\sum_{x\in\Lambda} f(s_x^2) \tag{3.5}$$

In particular the equality is satisfied by any antiferromagnetic configuration (indepently of the spin amplitude). Now we look for the minima of the function

$$\tilde{G}(\{\phi_x\})=-\frac{1}{\beta}\operatorname{tr}\ln\cosh\frac{\beta}{2}(T^2+\lambda^2\Phi)^{1/2}+\sum_{x\in\Lambda} f(\phi_x) \tag{3.6}$$

The local minima are given by

$$f'(\phi_x)\doteq\frac{\lambda^2}{4}\langle x|\,(T^2+\lambda^2\Phi)^{-1/2}\tanh\frac{\beta}{2}(T^2+\lambda^2\Phi)^{1/2}\,|x\rangle \tag{3.7}$$

which leads to Eq. (3.3) if we express the right-hand side as a sum over the first Brillouin zone. The convexity of (3.6) is obvious by inspection, so that the solutions of (3.7) are global minima. The existence of solutions for $a_1 = 0$, all β and $a_1 > 0$, large β is discussed in Appendix B. It remains to prove that (3.6) is strictly convex. To compute the second derivative of (3.6) we use the representation

$$(T^2 + \lambda^2 \Phi)^{-1/2} \tanh \frac{\beta}{2} (T^2 + \lambda^2 \Phi)^{1/2} = \beta \sum_{k=0}^{\infty} \frac{1}{(k + \frac{1}{2})^2 \pi^2 + \frac{1}{4}\beta^2 (T^2 + \lambda^2 \Phi)} \tag{3.8}$$

which leads to

$$\frac{\partial^2 \tilde{G}}{\partial \phi_u \, \partial \phi_v} = f''(\phi_u) \, \delta_{uv} + \frac{\lambda^4 \beta^3}{16} \sum_{k=0}^{\infty} \langle u | \frac{1}{(k + \frac{1}{2})^2 \pi^2 + \frac{1}{4}\beta^2 (T^2 + \lambda^2 \Phi)} | v \rangle$$
$$\times \langle v | \frac{1}{(k + \frac{1}{2})^2 \pi^2 + \frac{1}{4}\beta^2 (T^2 + \lambda^2 \Phi)} | u \rangle \tag{3.9}$$

Using (3.9), one can easily prove the analog of (2.15) and conclude the proof.

Proof of Theorem 3.2. For simplicity we consider first the case where $f(s_x^2)$ is purely quadratic (Holstein model) and give the necessary modifications for the general case. Since $\cosh(x)$ is an even function we can write

$$F(\{s_x\}) = -\frac{1}{\beta} \operatorname{tr} \left[\ln \cosh \frac{\beta}{2} (T + \lambda S) \right] + \sum_{x \in \Lambda} \frac{1}{2} s_x^2 \tag{3.10}$$

The second derivative of $F(\{s_x\})$ is

$$\frac{\partial^2 F}{\partial s_x \, \partial s_y} = \delta_{xy} - \frac{\lambda}{2} \langle x | \frac{\partial}{\partial s_y} \tanh \frac{\beta}{2} (T + \lambda S) | x \rangle \tag{3.11}$$

To compute the partial derivative in the right-hand side of (3.11) we use a formula analogous to (3.8),

$$\tanh \frac{\beta}{2} (T + \lambda S) = \beta (T + \lambda S) \sum_{k=0}^{\infty} G_k(S) \tag{3.12}$$

where

$$G_k(S) = \frac{1}{(k + \frac{1}{2})^2 \pi^2 + \frac{1}{4}\beta^2 (T + \lambda S)^2} \tag{3.13}$$

One then finds

$$\frac{\partial}{\partial s_y}\left[\tanh\frac{\beta}{2}(T+\lambda S)\right]$$

$$=\beta\lambda\,|y\rangle\langle y|\sum_{k=0}^{\infty}G_k(S)+\frac{\beta^3\lambda}{4}(T+\lambda S)$$

$$\times\sum_{k=0}^{\infty}G_k(S)[(T+\lambda S)\,|y\rangle\langle y|+|y\rangle\langle y|\,(T+\lambda S)]\,G_k(S) \qquad (3.14)$$

Combining (3.14) and (3.11) gives

$$\frac{\partial^2 F}{\partial s_x\,\partial s_y}=\delta_{xy}-(A_{xy}+B_{xy}) \qquad (3.15)$$

with

$$A_{xy}=\delta_{xy}\frac{\beta\lambda^2}{2}\sum_{k=0}^{\infty}\langle x|\,G_k(S)\,|x\rangle \qquad (3.16)$$

and

$$B_{xy}=\frac{\beta^4\lambda^2}{8}\sum_{k=0}^{\infty}[\langle x|\,(T+\lambda S)\,G_k(S)(T+\lambda S)\,|y\rangle\langle y|\,G_k(S)\,|x\rangle$$

$$+\ \langle x|\,(T+\lambda S)\,G_k(S)\,|y\rangle\langle y|\,(T+\lambda S)\,G_k(S)\,|x\rangle] \qquad (3.17)$$

Since A_{xy} and B_{xy} are real symmetric kernels, it is sufficient to check that

$$\sum_{x,\,y\in\Lambda}\frac{\partial^2 F}{\partial s_x\,\partial s_y}\psi(x)\,\psi(y)>0 \qquad (3.18)$$

for real nonvanishing functions $\psi(x)$, $x\in\Lambda$. We prove lower bounds for the contributions of A_{xy} and B_{xy} to (3.18).

Contribution of A_{xy}. We have

$$\langle x|\,G_k(S)\,|x\rangle\leqslant\|G_k(S)\|\leqslant\frac{1}{(k+\frac{1}{2})^2\,\pi^2} \qquad (3.19)$$

Thus

$$\sum_{x,\,y\in\Lambda}A_{xy}\psi(x)\,\psi(y)\leqslant\frac{\beta\lambda^2}{2}\left[\sum_{k=0}^{\infty}\frac{1}{(k+\frac{1}{2})^2\,\pi^2}\right]\sum_{x\in\Lambda}|\psi(x)|^2 \qquad (3.20)$$

Contribution of B_{xy}. Let ψ denote the multiplication operator by the function $\psi(x)$. We have

$$\sum_{x,y\in\Lambda} B_{xy}\psi(x)\,\psi(y)=\frac{\beta^3\lambda^2}{8}\sum_{k=0}^{\infty}\{\mathrm{tr}[\psi(T+\lambda S)\,G_k(S)(T+\lambda S)\,\psi G_k(S)]$$
$$+\ \mathrm{tr}[\psi(T+\lambda S)\,G_k(S)\,\psi(T+\lambda S)\,G_k(S)]\} \qquad (3.21)$$

We notice that

$$\frac{\beta^2}{4}(T+\lambda S)^2\leqslant[G_k(S)]^{-1} \qquad (3.22)$$

Multiplying this inequality on both sides by $[G_k(S)]^{1/2}$ and using the commutivity of $G_k(S)$ and $(T+\lambda S)$, we obtain

$$\frac{\beta^2}{4}(T+\lambda S)\,G_k(S)(T+\lambda S)\leqslant 1 \qquad (3.23)$$

Using (3.23), (3.19), and the cyclicity of the trace, we obtain

$$\frac{\beta^2}{4}\mathrm{tr}[\psi(T+\lambda S)\,G_k(S)(T+\lambda S)\,\psi G_k(S)]\leqslant\left[\frac{1}{(k+\frac{1}{2})^2\,\pi^2}\right]\sum_{x\in\Lambda}\psi(x)^2 \quad (3.24)$$

For the second trace we first use the Schwartz inequality

$$\begin{aligned}&\mathrm{tr}[\psi(T+\lambda S)\,G_k(S)\,\psi(T+\lambda S)\,G_k(S)]\\&\quad\leqslant\mathrm{tr}[\psi(T+\lambda S)\,G_k(S)^2\,(T+\lambda S)\psi]\\&\quad=\mathrm{tr}\{\psi[G_k(S)]^{1/2}\,(T+\lambda S)\,G_k(S)(T+\lambda S)[G_k(S)]^{1/2}\,\psi\}\end{aligned} \qquad (3.25)$$

Then by (3.24) and (3.19) we get the same upper bound as in (3.23). Collecting these two estimates, we obtain

$$\sum_{x,y\in\Lambda} B_{xy}\psi(x)\,\psi(y)\leqslant\frac{\beta\lambda^2}{2}\left[\sum_{k=0}^{\infty}\frac{1}{(k+\frac{1}{2})^2\,\pi^2}\right]\sum_{x\in\Lambda}|\psi(x)|^2 \qquad (3.26)$$

Finally, using the estimates (3.26) and (3.20), we get from (3.15)

$$\sum_{x,y\in\Lambda}\frac{\partial^2 F}{\partial s_x\,\partial s_y}\psi(x)\,\psi(y)\geqslant\left(1-\beta\lambda^2\sum_{k=0}^{\infty}\frac{1}{(k+\frac{1}{2})^2\,\pi^2}\right)\sum_{x\in\Lambda}|\psi(x)|^2 \quad (3.27)$$

The sum over k in (3.27) is equal to 1/2. Thus (3.18) holds for all non-vanishing $\psi(x)$ if $\beta\lambda^2<2$.

In the general case where $f(s_x^2) = \sum_j a_j s_x^{2j}$ the same arguments lead to (3.27) with the term in parentheses replaced by $(a_1 - \beta\lambda^2/2)$ plus an extra term which is surely positive when all $a_j > 0$.

Absence of Long-Range Order for $\beta\lambda^2 < c$

We first recall an inequality of Brascamp and Lieb.[4] Let C be a positive $n \times n$ matrix, and $W(z)$, $z = (z_1, ..., z_n) \in \mathbf{R}^n$, a log-concave function. Consider the average of a function $N(z)$

$$\langle N \rangle_h = \frac{\int N(z)\, W(z)\, e^{-(z, Cz)/2}}{\int W(z)\, e^{-(z, Cz)/2}} \tag{3.28}$$

Then if C_W is the matrix with entries $(\langle z_i z_j \rangle_h - \langle z_i \rangle_h \langle z_j \rangle_h)$, $i, j = 1 \cdots n$, we have the matrix inequality

$$C_W \leqslant C_{W=1} = C^{-1} \tag{3.29}$$

For a fixed $a > 0$ sufficiently small let

$$F_a(\{s_x\}) = F(\{s_x\}) - a \sum_{x \in A} s_x^2 \tag{3.30}$$

By the same proof as that of Theorem 3.2, $F_a(\{s_x\})$ is strictly convex for $\beta\lambda^2 \ll 1$, uniformly in $\{s_x\}$. Thus $\exp[-\beta F_a(\{s_x\})]$ is a log-concave function. A straightforward application of (3.29) then gives

$$(\langle s_i s_j \rangle_A (\beta) - \langle s_i \rangle_A (\beta) \langle s_j \rangle_A (\beta))_{i,j=1 \cdots |A|} \leqslant \frac{1}{\sqrt{a}} (\delta_{ij})_{i,j=1 \cdots |A|} \tag{3.31}$$

as quadratic forms. With periodic boundary conditions we have $\langle s_i \rangle_A (\beta) = 0$ so that by (3.29) all eigenvalues of $(\langle s_i s_j \rangle_A (\beta))_{i,j=1 \cdots |A|}$ are bounded by $a^{-1/2}$. Consequently the Hilbert–Schmidt norm of this matrix is bounded by $a^{-1} |A|$, i.e.,

$$\frac{1}{|A|} \sum_{i=1}^{|A|} \sum_{j=1}^{|A|} |\langle s_i s_j \rangle_A (\beta)|^2 \leqslant \frac{1}{a} \tag{3.32}$$

Clearly this means that there is no long-range order for $\beta\lambda^2 \ll 1$.

4. LOW-TEMPERATURE PHASES

We expect that in dimensions greater than or equal to 2 there are two low-temperature phases corresponding to the ground states for all λ. Here we prove this fact for λ large. To make this statement precise we impose + or − boundary conditions on H_Λ in (1.1). These are defined, respectively, by $\varepsilon_x s_x = +\sigma_0(\lambda)$ and $\varepsilon_x s_x = -\sigma_0(\lambda)$ for $x \in \{u \in \Lambda \mid |u-v|=1, v \in \mathbf{Z}^d \backslash \Lambda\}$. This set consists of the sites of Λ which are at the boundary. The corresponding averages at the symmetry point $(\mu, h) = (0, \lambda/2)$ are denoted by $\langle - \rangle_\Lambda^+ (\beta)$ and $\langle - \rangle_\Lambda^- (\beta)$. For the static Holstein model we prove the following result.

Theorem 4.1. There exists a fixed number $\delta' > 0$ such that for λ and β/λ sufficiently large we have

$$\pm\sigma_0(\lambda) - \delta' \leqslant \langle \varepsilon_x s_x \rangle_\Lambda^\pm (\beta) \leqslant \pm\sigma_0(\lambda) + \delta' \tag{4.1}$$

We recall that $\sigma_0(\lambda)$, the solution of (2.3), behaves as $\lambda/2$ as $\lambda \to \infty$.

We first present the detailed Peierls argument for the case of discrete spins taking values $-1, 0, +1$ [the model with single spin measure (1.17)]. To do this we combine an idea used in ref. 12 with the technique of refs. 18 and 19 and prove the statement of Theorem 4.1 with $\sigma_0(\lambda)$ replaced by 1, and some $\delta' \ll 1$. The case of continuous spins introduces extra technical complications which we explain at the end of the section.

Peierls Argument for the Discrete Case. We adopt the following setup. Fix + boundary conditions, i.e., fix $s_u = \varepsilon_u$ for u a boundary site. Given a configuration $\{s_x\}$, we say that the site $y \in \Lambda$ is "correct" if $s_y = \varepsilon_y$, otherwise it is "wrong." Clearly all boundary sites are correct and all sites y with $s_y = 0$ are wrong. Now draw the Peierls contours by drawing a bond on the dual lattice whenever one of the adjacent sites is correct and the other wrong.[12] Let γ be an external contour, i.e., from any site adjacent to γ externally there is a path to the boundary not crossing any contour. All the adjacent external sites will then have $s_x = \varepsilon_x$, while the sites adjacent to γ from the inside will have either $s_x = -\varepsilon_x$ or $s_x = 0$. Let $l(\gamma)$ be the total number of sites adjacent to γ from the inside. We label by $\xi_1, \ldots, \xi_{k(\gamma)}$ the sites which are adjacent to γ from the inside which are not zero and by $\xi_{k(\gamma)+1}, \ldots, \xi_{l(\gamma)}$ the remaining sites adjacent to γ from the inside (they have zero spin). Suppose that the probability of a contour γ with specified $\xi_1, \ldots, \xi_{k(\gamma)}$ satisfies the estimate

$$P(\gamma; \xi_1, \ldots, \xi_{k(\gamma)}) \leqslant e^{-\beta J(\lambda)\, l(\gamma)} \tag{4.2}$$

for some positive function $J(\lambda)$. Then the probability of a contour γ can be estimated as

$$P(\gamma) = \sum_{k=0}^{l(\gamma)} \sum_{\xi_1,\dots,\xi_{k(\gamma)}} P(\gamma; \xi_1,\dots,\xi_{k(\gamma)})$$
$$\leqslant \sum_{k=0}^{l(\gamma)} \sum_{\xi_1,\dots,\xi_{k(\gamma)}} e^{-\beta J(\lambda)\, l(\gamma)}$$
$$\leqslant \sum_{k=0}^{l(\gamma)} \frac{l(\gamma)!}{k(\gamma)!\,[l(\gamma)-k(\gamma)]!} e^{-\beta J(\lambda)\, l(\gamma)} \leqslant 2^{l(\gamma)} e^{-\beta J(\lambda)\, l(\gamma)} \tag{4.3}$$

With (4.3) one can easily complete the Peierls argument. In order to get the estimate (4.2) on $P(\gamma; \xi_1,\dots,\xi_{k(\gamma)})$ it is sufficient to show that

$$F(\{s_x\}) - F(\{s_x^*\}) \geqslant J(\lambda)\, l(\gamma) \tag{4.4}$$

where $\{s_x^*\}$ is obtained from $\{s_x\}$ by flipping all the spins inside γ except for those at the sites $\xi_{k(\gamma)+1},\dots,\xi_{l(\gamma)}$, and replacing the latter ones by those corresponding to the correct phase. For specified $\xi_1,\dots,\xi_{k(\gamma)}$ this transformation is one to one and removes the contour γ: it can also modify the contours inside γ.

Integral Representation for (4.4). We have to decouple the contributions to (4.4) coming from the interior (int γ), exterior (ext γ), and boundary of γ, $\partial\gamma = \{u, v \text{ n.n} \mid u \in \text{int}\,\gamma, v \in \text{ext}\,\gamma\}$. To this end we introduce three orthogonal projectors: A_γ, which projects on the subspace of one-particle wave functions supported on the sites $\xi_{k(\gamma)+1},\dots,\xi_{l(\gamma)}$; P_γ, which projects on the subspace of wave functions supported on the remaining sites of int γ; and finally Q_γ, which projects on the wave functions supported on ext γ. Obviously we have $P_\gamma + Q_\gamma + A_\gamma = \mathbf{1}$ and $P_\gamma Q_\gamma = P_\gamma A_\gamma = Q_\gamma A_\gamma = 0$. Moreover the projectors commute with S. The square of the Hamiltonian can be decomposed as[22]

$$H(\{s_x\})^2 = X_\gamma(S) + Y_\gamma(S) \tag{4.5}$$

where

$$X_\gamma(S) = P_\gamma H(\{s_x\})^2 P_\gamma + Q_\gamma H(\{s_x\})^2 Q_\gamma + A_\gamma H(\{s_x\})^2 A_\gamma \tag{4.6}$$

and

$$Y_\gamma(S) = P_\gamma H(\{s_x\})^2 A_\gamma + A_\gamma H(\{s_x\})^2 P_\gamma + P_\gamma H(\{s_x\})^2 Q_\gamma + Q_\gamma H(\{s_x\})^2 P_\gamma + A_\gamma H(\{s_x\})^2 Q_\gamma + Q_\gamma H(\{s_x\})^2 A_\gamma \tag{4.7}$$

We set

$$Z_t(S) = X_\gamma(S) + t Y_\gamma(S) \tag{4.8}$$

for $0 \leqslant t \leqslant 1$ and

$$F(S, t) = -\frac{1}{\beta} \operatorname{tr} \left\{ \ln \cosh \frac{\beta}{2} [Z_t(S)]^{1/2} \right\} \tag{4.9}$$

It follows from the orthogonality of the three projectors that the derivative of $F(S, t)$ with respect to t satisfies $F'(S, 0) = 0$. An integration by parts gives

$$F(\{s_x\}) = F(S, 1) = F(S, 0) + \int_0^1 dt (1-t) \, F''(S, t) \tag{4.10}$$

The second derivative in (4.10) can be computed by using the formula (3.8) with $Z_t(S)$ replacing $T^2 + \lambda^2 \Phi$. This leads to the integral representation

$$F''(S, t) = \frac{\beta^3}{16} \sum_{k=0}^{\infty} f_k(S, t) \tag{4.11}$$

where

$$f_k(S, t) = \operatorname{tr}[Y_\gamma(S) \, G_k(S, t) \, Y_\gamma(S) \, G_k(S, t)] \tag{4.12}$$

and

$$G_k(S, t) = \left[\left(k + \frac{1}{2} \right)^2 \pi^2 + \frac{\beta^2}{4} Z_t(S) \right]^{-1} \tag{4.13}$$

[For the sake of simplicity we have not indicated explicitly the unit matrix multiplying $(k + 1/2)\pi^2$.] Using these formulas, we can represent (4.4) as a sum of two contributions

$$F(\{s_x\}) - F(\{s_x^*\}) = (\mathrm{I}) + (\mathrm{II}) \tag{4.14}$$

which are

$$(\mathrm{I}) = F(S, 0) - F(S^*, 0) \tag{4.15}$$

$$(\mathrm{II}) = \frac{\beta^3}{16} \sum_{k=0}^{\infty} [f_k(S, t) - f_k(S^*, t)] \tag{4.16}$$

Lower Bound for (I). We note that

$$\begin{aligned} F(S, 0) &= -\frac{1}{\beta} \operatorname{tr} \left\{ \ln \cosh \frac{\beta}{2} [X_\gamma(S)]^{1/2} \right\} \\ &= -\frac{1}{\beta} \left(\operatorname{tr} \left\{ P_\gamma \ln \cosh \frac{\beta}{2} [P_\gamma H(\{s_x\})^2 \, P_\gamma]^{1/2} \right\} \right. \\ &\quad + \operatorname{tr} \left\{ Q_\gamma \ln \cosh \frac{\beta}{2} [Q_\gamma H(\{s_x\})^2 \, Q_\gamma]^{1/2} \right\} \\ &\quad \left. + \operatorname{tr} \left\{ A_\gamma \ln \cosh \frac{\beta}{2} [A_\gamma H(\{s_x\})^2 \, A_\gamma]^{1/2} \right\} \right) \end{aligned} \tag{4.17}$$

Moreover the operators $P_\gamma H(\{s_x\})^2 P_\gamma$ and $P_\gamma H(\{s_x^*\})^2 P_\gamma$ are unitarily equivalent under multiplication by ε_x; $Q_\gamma H(\{s_x\})^2 Q_\gamma$ and $Q_\gamma H(\{s_x^*\})^2 Q_\gamma$ are equal. Consequently

$$(\mathrm{I}) = -\frac{1}{\beta}\left(\operatorname{tr}\left\{A_\gamma \ln\cosh\frac{\beta}{2}\,[A_\gamma H(\{s_x\})^2 A_\gamma]^{1/2}\right\}\right.$$
$$\left. - \operatorname{tr}\left\{A_\gamma \ln\cosh\frac{\beta}{2}\,[A_\gamma H(\{s_x^*\})^2 A_\gamma]^{1/2}\right\}\right) \tag{4.18}$$

We have the matrix inequality $-2d-\lambda\,|S| \leqslant T+\lambda S \leqslant 2d+\lambda\,|S|$, where d stands for d times the identity operator, and $|S|$ is the diagonal matrix with entries $|s_x|$. Thus

$$(T+\lambda S)^2 \leqslant (2d+\lambda\,|S|)^2 \tag{4.19}$$

Using (4.19) and $A_\gamma S^2 A_\gamma = 0$, we obtain the estimate

$$\operatorname{tr}\left\{A_\gamma \ln\cosh\frac{\beta}{2}\,[A_\gamma H(\{s_x\})^2 A_\gamma]^{1/2}\right\} \leqslant \operatorname{tr}[A_\gamma \ln\cosh(\beta d)]$$
$$= [l(\gamma)-k(\gamma)]\ln\cosh(\beta d) \tag{4.20}$$

Consider the configuration $\tilde{s}_x = s_x^*$ for $x = \xi_{k(\gamma)+1},\dots,\xi_{l(\gamma)}$ and $\tilde{s}_x = +1$ for $x \neq \xi_{k(\gamma)+1},\dots,\xi_{l(\gamma)}$. We have $A_\gamma \tilde{S} A_\gamma = A_\gamma S^* A_\gamma$. Therefore

$$A_\gamma (T+\lambda S^*)^2 A_\gamma = A_\gamma (T+\lambda\tilde{S})^2 A_\gamma \geqslant A_\gamma (2d-\lambda)^2 A_\gamma \tag{4.21}$$

The last inequality follows from the fact that $|\tilde{s}_x| = 1$. From (4.21) we obtain the lower bound

$$\operatorname{tr}\left\{A_\gamma \ln\cosh\frac{\beta}{2}\,[A_\gamma H(\{s_x^*\})^2 A_\gamma]^{1/2}\right\} \geqslant [l(\gamma)-k(\gamma)]\ln\cosh\frac{\beta}{2}\,|\lambda-2d| \tag{4.22}$$

Finally, (4.20) and (4.22) imply

$$(\mathrm{I}) \geqslant [l(\gamma)-k(\gamma)]\,\beta^{-1}\left(\ln\cosh\frac{\beta}{2}\,|\lambda-2d| - \ln\cosh\beta d\right)$$
$$\geqslant c_1 \lambda [l(\gamma)-k(\gamma)] \tag{4.23}$$

for some positive constant c_1. This last inequality expresses the fact that the measure (1.5) gives a low probability to having zero spins on the sites $\xi_{k(\gamma)+1},\dots,\xi_{l(\gamma)}$.

Lower Bound for (II). We need to obtain a lower bound $f_k(S, t)$ and an upper bound on $f_k(S^*, t)$. We start with the lower bound on $f_k(S, t)$.

From (4.19), the commutivity of the projectors P_γ, Q_γ, and A_γ with S and (4.6)

$$X_\gamma \leqslant (2d + \lambda\,|S|)^2 \tag{4.24}$$

Since

$$Z_t(S) = (1-t)\,X_\gamma(S) + tH(\{s_x\})^2 \tag{4.25}$$

(4.19) and (4.25) imply

$$G_k(S, t) \geqslant g_k(2d + \lambda\,|S|) \tag{4.26}$$

with the diagonal matrix

$$g_k(x) = \frac{1}{(k+\frac{1}{2})^2\,\pi^2 + \frac{1}{4}\beta^2 x^2}, \qquad x \geqslant 0 \tag{4.27}$$

Therefore

$$f_k(S, t) \geqslant \operatorname{tr}[Y_\gamma(S)\,g_k(2d+\lambda\,|S|)\,Y_\gamma(S)\,g_k(2d+\lambda\,|S|)] \tag{4.28}$$

Let us compute all the contributions to the right-hand side of (4.28) coming from the various terms in $Y_\gamma(S)$. $Y_\gamma(S)$ involves off-diagonal blocks of the matrix $H(\{s_x\})^2 = T^2 + \lambda^2 S^2 + \lambda(TS + ST)$. The cyclicity of the trace and the commutivity of the projectors with S imply that the contribution of S^2 to (4.28) vanishes. The same is true about the cross terms involving T^2 and S^2. Also the terms with T^2 are positive, so the inequality is preserved if we drop them. The cross terms involving T^2 and $TS + ST$ or S^2 and $TS + ST$ vanish because they are odd under $T \to -T$ (multiplication by ε_x is unitary and transforms $T \to -T$ and $S \to S$). Thus it is sufficient to keep only the term coming from $\lambda(TS + ST)$, i.e.,

$$\begin{aligned} f_k(S, t) \geqslant{}& 2\lambda^2 \operatorname{tr}[P_\gamma(TS+ST)\,Q_\gamma\,g_k(2d+\lambda\,|S|) \\ &\times Q_\gamma(TS+ST)\,P_\gamma\,g_k(2d+\lambda\,|S|)] & (4.29\text{a}) \\ &+ 2\lambda^2 \operatorname{tr}[P_\gamma(TS+ST)\,A_\gamma\,g_k(2d+\lambda\,|S|) \\ &\times A_\gamma(TS+ST)\,P_\gamma\,g_k(2d+\lambda\,|S|)] & (4.29\text{b}) \\ &+ 2\lambda^2 \operatorname{tr}[Q_\gamma(TS+ST)\,A_\gamma\,g_k(2d+\lambda\,|S|) \\ &\times A_\gamma(TS+ST)\,Q_\gamma\,g_k(2d+\lambda\,|S|)] & (4.29\text{c}) \end{aligned}$$

The term (4.29a) is estimated as

$$2\lambda^2 \sum_{\langle u,v\rangle \in \partial\gamma, u=\xi_1,\dots,\xi_{k(\gamma)}} (s_u+s_v)^2 \, g_k(2d+\lambda\,|s_u|)\, g_k(2d+\lambda\,|s_v|)$$

$$\geqslant 2\lambda^2[g_k(2d+\lambda)]^2 \sum_{\langle u,v\rangle \in \partial\gamma, u=\xi_1,\dots,\xi_{k(\gamma)}} (s_u+s_v)^2$$

$$= 8\lambda^2[g_k(2d+\lambda)]^2\, k(\gamma) \tag{4.30}$$

For the last equality we use the fact that for the sites u, v we have $s_u+s_v=\pm 2$. For the term (4.29b) we can only use the fact that it is not negative,

$$2\lambda^2 \sum_{\langle u,v\rangle, u=\xi_{k(\gamma)+1},\dots,\xi_{l(\gamma)}, v\in \operatorname{int}\gamma} (s_u+s_v)^2\, g_k(2d+\lambda\,|s_u|)\, g_k(2d+\lambda\,|s_v|) \geqslant 0 \tag{4.31}$$

since $s_u=0$ and s_v might also be zero. The term (4.29c) is estimated as

$$2\lambda^2 \sum_{\langle u,v\rangle \in \partial\gamma, u=\xi_{k(\gamma)+1},\dots,\xi_{l(\gamma)}} (s_u+s_v)^2\, g_k(2d+\lambda\,|s_u|)\, g_k(2d+\lambda\,|s_v|)$$

$$\geqslant 2\lambda^2[g_k(2d+\lambda)]^2\,[l(\gamma)-k(\gamma)] \tag{4.32}$$

since in (4.32), $s_u+s_v=\pm 1$. Summing these contributions, we get

$$f_k(S) \geqslant 8\lambda^2[g_k(2d+\lambda)]^2\, l(\gamma) - 6\lambda^2[g_k(2d+\lambda)]^2\,[l(\gamma)-k(\gamma)] \tag{4.33}$$

Performing the sum over k an a trivial integration over t leads to

$$\frac{\beta^3}{16}\sum_{k=0}^{\infty}\int_0^1 dt(1-t)\, f_k(S,t) \geqslant \frac{c_2}{\lambda}\, l(\gamma) - \frac{c_2'}{\lambda}\,[l(\gamma)-k(\gamma)] \tag{4.34}$$

with $0<c_2'<c_2$. The first term on the right-hand side of (4.34) is just the standard Ising type of energy contribution one would have with ± 1 spins. It is reduced by the second term coming from the fact that the spin can take zero value inside γ.

We now obtain an upper bound for $f_k(S^*,t)$. We notice that for the configuration S^* we have

$$P_\gamma(TS^*+S^*T)\,Q_\gamma = Q_\gamma(TS^*+S^*T)\,P_\gamma = 0 \tag{4.35}$$

$$Q_\gamma(TS^*+S^*T)\,A_\gamma = A_\gamma(TS^*+S^*T)\,Q_\gamma = 0 \tag{4.36}$$

Therefore

$$f_k(S^*,t) = f_{k,PQ}(S^*,t) + f_{k,PA}(S^*,t) + f_{k,QA}(S^*,t) \tag{4.37}$$

with

$$f_{k,PQ}(S^*,t)=2\,\mathrm{tr}[P_\gamma T^2 Q_\gamma G_k(S^*,t)\,Q_\gamma T^2 P_\gamma G_k(S^*,t)] \tag{4.38a}$$

$$f_{k,QA}(S^*,t)=2\,\mathrm{tr}[Q_\gamma T^2 A_\gamma G_k(S^*,t)\,A_\gamma T^2 P_\gamma G_k(S^*,t)] \tag{4.38b}$$

$$f_{k,PA}(S^*,t)=2\,\mathrm{tr}[P_\gamma (T+\lambda S^*)^2\,A_\gamma G_k(S^*,t)\,A_\gamma (T+\lambda S^*)^2\,P_\gamma G_k(S^*,t)] \tag{4.38c}$$

To get an upper bound on each of these contributions we use the pointwise estimate (C.10) (see Appendix C) on the kernel of $G_k(S^*, t)$. Since in the discrte case $\max_{x\in A} |s_x^{*2}| = 1$, a computation leads to

$$f_{k,PQ}(S^*,t)\leqslant c_3[g_k(c_3'\lambda)]^2\,k(\gamma) \tag{4.39}$$

$$f_{k,QA}(S^*,t)\leqslant c_3[g_k(c_3'\lambda)]^2\,[l(\gamma)-k(\gamma)] \tag{4.40}$$

for positive constants c_3 and c_3' independent of λ. For (4.38c) we have to develop $(T+\lambda S^*)^2$ and consider each term separately. The one coming from $\lambda(TS^*+S^*T)$ is bounded by

$$\lambda^2[g_k(c_3'\lambda)]^2 \sum_{\langle uv\rangle,\langle v'v''\rangle} (s_u^*+s_v^*)^2\,e^{-|v-v'|}(s_{v'}^*+s_{v''}^*)^2\,e^{-|v''-u|}$$
$$\leqslant C\lambda^2[g_k(c_3'\lambda)]^2\,[l(\gamma)-k(\gamma)] \tag{4.41}$$

In (4.41) the sum is over $u, v''=\xi_1,\ldots,\xi_{k(\gamma)}$ and $v, v'\in \mathrm{int}\,\gamma$. Similarly, the contribution coming from T^2 is bounded above by

$$c_3[g_k(c_3'\lambda)]^2\,[l(\gamma)-k(\gamma)] \tag{4.42}$$

Note that one gets the same constant c_3 as in (4.39) and (4.40). For the cross term involving T^2 and $\lambda(TS^*+S^*T)$ we get an upper bound of the form

$$C'\lambda[g_k(c_3'\lambda)]^2\,[l(\gamma)-k(\gamma)] \tag{4.43}$$

Thus $f_{k,PA}(S^*,t)$ is bounded above by the sum of (4.41)–(4.43).

Putting together this last estimate and (4.39), (4.40), performing the sum over k and the integration over t, we obtain the final bound (with $c_2''>0$, $c_2'''>0$, independent of λ)

$$\frac{\beta^3}{16}\sum_{k=0}^{\infty}\int_0^1 dt(1-t)\,f_k(S^*,t)\leqslant\frac{c_2''}{\lambda^3}\,l(\gamma)+\frac{c_2'''}{\lambda}\,[l(\gamma)-k(\gamma)] \tag{4.44}$$

The term c_2''/λ^3 comes from (4.39), (4.40), and (4.42), while the term c_2'''/λ comes from (4.41) and (4.43).

Proof of (4.4) for the Discrete Case. From (4.34) and (4.44) we get the lower bound for (II) in the form

$$(\mathrm{II}) \geqslant \left(\frac{c_2}{\lambda} - \frac{c_2''}{\lambda^3}\right) l(\gamma) - \frac{1}{\lambda}(c_2' + c_2''')[l(\gamma) - k(\gamma)] \tag{4.45}$$

The term proportional to $l(\gamma)$ on the right-hand side of this inequality is the Ising type of energy gain associated to the removal of γ for ± 1 spins. This is also the contribution one would obtain for the FK model. The negative contribution comes from the contribution of the zero spins adjacent to γ from the inside. This is canceled by the "effective chemical potential" (I). Combining (4.23) with (4.45) then yields, for λ large enough, the bound

$$(\mathrm{I}) + (\mathrm{II}) \geqslant \frac{c}{\lambda} l(\gamma) \tag{4.46}$$

with c a positive constant. Thus we have obtained (4.4) with $J(\lambda) = c/\lambda$.

Peierls Argument for Continuous Spins. We first define the contours. For δ a fixed positive number of $O(1)$ we consider the partition of $\mathbf{R} = \Delta_+ \cup \Delta_- \cup \Delta_0$, with $\Delta_\pm = [\pm\sigma_0(\lambda) - \sigma, \pm\sigma_0(\lambda) + \delta]$ and $\Delta_0 = \mathbf{R} \backslash (\Delta_+ \cup \Delta_-)$. We fix + boundary conditions by considering $\varepsilon_x s_x \in \Delta_+$ for all $x \in \{u \in \Lambda \mid |u - v| = 1, v \in \mathbf{Z}^d \backslash \Lambda\}$. For a given configuration $\{s_x\}$ we say that a site x is in a "0 state" if $s_x \in \Delta_0$, in a "+1 state" if $s_x \in \Delta_+$, and in a "−1 state" if $s_x \in \Delta_-$. With these definitions we can draw the contours in exactly the same way as in the discrete case. Let $\Sigma(\gamma, \xi_1, ..., \xi_{k(\gamma)})$ be the set of configurations $\{s_x\}$ which have a contour $(\gamma, \xi_1, ..., \xi_{k(\gamma)})$. The probability of a contour $(\gamma, \xi_1, ..., \xi_{k(\gamma)})$ is simply the measure of $\Sigma(\gamma, \xi_1, ..., \xi_{k(\gamma)})$ with respect to the distribution (1.5), i.e.,

$$P(\gamma, \xi_1, ..., \xi_{k(\gamma)}) = \frac{1}{Z_\Lambda} \int_{\Sigma(\gamma, \xi_1, ..., \xi_{k(\gamma)})} dS\, e^{-\beta F(S)} \tag{4.47}$$

where $F(S)$ is given at the symmetry point by (3.1) and $dS = \prod_{x \in \Lambda} ds_x$. To get an inequality like (4.2), so we can repeat the argument of (4.3), we consider the configuration S^* obtained from S in the following way:

$$s_x^* = s_x, \qquad x \in \operatorname{ext} \gamma \tag{4.48}$$

$$s_x^* = -s_x, \qquad x \in \operatorname{int} \gamma, \quad x \neq \xi_{k(\gamma)+1}, ..., \xi_{l(\gamma)} \tag{4.49}$$

$$s_x^* = \varepsilon_x(\sigma_0(\lambda) + \delta q(s_x)), \qquad x = \xi_{k(\gamma)+1}, ..., \xi_{l(\gamma)} \tag{4.50}$$

where the function $q(t)$ is a smooth, monotone increasing, odd map from $\mathbf{R}$ to $[-1, +1]$ such that $q(\pm\infty) = \pm 1$. The exact form of q does not matter but we need to have $|q'(t)| < C$ for some constant and $1 - q^2(t) \sim |t|^{-1}$ for large $|t|$. We remark that the transformation from S to S^* is one to one once $\xi_1,..., \xi_{k(\gamma)}$ are specified; thus by a change of variables

$$P(\gamma, \xi_1,..., \xi_{k(\gamma)}) = \frac{1}{Z_\Lambda} \int_{\Sigma^*(\gamma, \xi_1,..., \xi_{k(\gamma)})} dS^* \, |J(S)| \, e^{-\beta F(S^*)} e^{-\beta[F(S) - F(S^*)]} \tag{4.51}$$

where Σ^* is the transformed Σ and the Jacobian (which is absent in the discrete case) of the transformation is

$$|J(S)| = \prod_{x = \xi_{k(\gamma)+1},..., \xi_{l(\gamma)}} \delta^{-1}[q'(s_x)]^{-1} \tag{4.52}$$

Thus (4.3) will hold if we prove the inequality

$$[F(S) - F(S^*)] - \frac{1}{\beta} \ln |J(S)| \geqslant J(\lambda)\, l(\gamma) \tag{4.53}$$

for all $\{s_x\} \in \Sigma(\gamma, \xi_1,..., \xi_{k(\gamma)})$. From our hypothesis on $q(t)$ we see that $\beta^{-1} \ln |J(S)| \leqslant \beta^{-1}(\ln \delta + \ln C)[l(\gamma) - k(\gamma)]$. With the choice $\delta = O(1)$ this can be made arbitrarily small for low temperatures and turns out to be harmless at the end.

Remark. The inequality (4.53) is the analog of (4.4), and is proved for some given δ. Going through the Peierls argument leads to Theorem 4.1 with some $\delta' \geqslant \delta$.

We recall that now $F(S)$ includes the energy $\sum_x \frac{1}{2} s_x^2$. Here $F(S)$ has the same integral representation as in the discrete case and is equal to (I) + (II) given by (4.15) and (4.16).

Modification of the Estimates for Continuous Spins. First we find the lower bound for (I). Let $\{\xi_{k(\gamma)+1},..., \xi_{l(\gamma)}\} = A_1 \cup A_2$, where A_1 is the set of sites for which $|s_x| < \sigma_0(\lambda) - \delta$ and A_2 the sites for which $|s_x| > \sigma_0(\lambda) + \delta$.

By the inequality (4.19) we get

$$\operatorname{tr} \left\{ A_\gamma \ln \cosh \frac{\beta}{2} [A_\gamma H(\{s_x\})^2 A_\gamma]^{1/2} \right\} \geqslant \sum_{x = \xi_{k(\gamma)+1},..., \xi_{l(\gamma)}} \ln \cosh \frac{\beta}{2} (2d + \lambda\, |s_x|) \tag{4.54}$$

Moreover with $\tilde{s}_x = s_x^*$, $x = \xi_{k(\gamma)+1},..., \xi_{l(\gamma)}$, and $\tilde{s}_x = \sigma_0(\lambda)$ for the other sites we have $A_\gamma(T + \lambda \tilde{S})^2 A_\gamma \geqslant A_\gamma(\lambda |s_x^*| - 2d)^2 A_\gamma$. Thus

$$\operatorname{tr}\left\{A_\gamma \ln\cosh\frac{\beta}{2}\,[A_\gamma H(\{s_x\})^2 A_\gamma]^{1/2}\right\}$$

$$\leqslant \sum_{x=\xi_{k(\gamma)+1},\ldots,\xi_{l(\gamma)}} \ln\cosh\frac{\beta}{2}(\lambda\,|s_x^*|-2d) \tag{4.55}$$

Splitting the sums over the two sets A_1, A_2, we get two corresponding contributions for $(\mathrm{I})=I_1+I_2$. Extracting the assymptotic behavior of (4.54) and (4.55) for $\beta\to\infty$, we get ($\alpha=1,2$)

$$I_\alpha \geqslant \frac{\lambda}{2}\sum_{x\in A_\alpha}(|s_x^*|-|s_x|)+|A_\alpha|\,O(e^{-\beta d}) \tag{4.56}$$

For continuous spins we have to take into account the energy difference coming from the single-particle measure and add it to (I). We have

$$\tfrac{1}{2}\sum_{x\in A}(s_x^2-s_x^{*2})=\tfrac{1}{2}\sum_{x\in\xi_{k(\gamma)+1},\ldots,\xi_{l(\gamma)}}(s_x^2-s_x^{*2})\equiv S_1+S_2 \tag{4.57}$$

where S_1, S_2 correspond, respectively, to $x\in A_1, A_2$. For $\alpha=1,2$ we have

$$I_\alpha+S_\alpha \geqslant \frac{1}{2}\sum_{x\in A_\alpha}\left[\left(|s_x|-\frac{\lambda}{2}\right)^2-\left(|s_x^*|-\frac{\lambda}{2}\right)^2\right]+|A_\alpha|\,O(e^{-\beta d}) \tag{4.58}$$

For $x\in A_1$, $(|s_x|-\lambda/2)^2\geqslant\delta^2$ and $(|s_x^*|-\lambda/2)^2=\delta^2[q(s_x)]^2\leqslant\delta^2[q(\lambda/2+\delta)]^2$. Thus with our choice of $q(t)$, we have for λ large enough, $\delta=O(1)$ (c_4' a positive constant)

$$I_1+S_1\geqslant|A_1|\,\frac{\delta^2}{2}\left\{1-\left[q\left(\frac{\lambda}{2}+\delta\right)\right]^2\right\}+|A_1|\,O(e^{-\beta d})\geqslant\frac{c_4'}{\lambda}|A_1| \tag{4.59}$$

For $x\in A_2$ we split the sum further into two contributions $A_2=A_3\cup A_4$, with $x\in A_3$ if $|s_x|>\sigma_0(\lambda)+\delta+1$, and $x\in A_4$ if $\sigma_0(\lambda)+\delta<|s_x|<\sigma_0(\lambda)+\delta+1$. The sum with $x\in A_4$ gives the same result as (4.59). For the sum with $x\in A_3$ we simply note that $(|s_x|-\lambda/2)^2-(|s_x^*|-\lambda/2)^2\geqslant 1$, so that it is bounded below by $Cst\,|A_4|$.

The result of this analysis is

$$(\mathrm{I})+\frac{1}{2}\sum_{x\in A}(s_x^2-s_x^{*2})\geqslant\frac{c_4}{\lambda}[l(\gamma)-k(\gamma)] \tag{4.60}$$

We now indicate the modifications needed to estimate (II). The lower bounds (4.28)–(4.29) on $f_k(S,t)$ are unchanged. In (4.30) we have $|s_x|\leqslant$

$\sigma_0(\lambda)+\delta$, $x=u, v$. Moreover $|s_u+s_v|\geqslant 2[\sigma_0(\lambda)-\delta]$. Thus the lower bound in (4.30) becomes

$$8\lambda^2[\sigma_0(\lambda)-\delta]^2\,\{g_k(2d+\lambda[\sigma_0(\lambda)+\delta])\}^2\,k(\gamma) \tag{4.61}$$

For the terms (4.31) and (4.32) we simply use the fact that they are positive. Therefore the bound (4.34) becomes (c_5, c_5' positive constants)

$$\frac{\beta^3}{16}\sum_{k=0}^{\infty}\int_0^1 dt(1-t)\,f_k(S,t)\geqslant\frac{c_5'}{\lambda}\frac{[\sigma_0(\lambda)-\delta]^2}{[\sigma_0(\lambda)+\delta]^3}\,k(\gamma)$$
$$\geqslant\frac{c_5}{\lambda^2}\,l(\gamma)-\frac{c_5}{\lambda^2}\,[l(\gamma)-k(\gamma)] \tag{4.62}$$

where we have used that $\delta=O(1)$ and $\sigma_0(\lambda)=O(\lambda)$ for large λ.

In the continuous case the operators involved in (4.35) and (4.36) do not vanish. Therefore T^2 must be replaced by $(T+\lambda S^*)^2$ in (4.38a)–(4.38b) and we must consider the contributions from T^2, $\lambda(TS^*+S^*T)$, and the cross terms not included in (4.27). In doing this we will use the bounds

$$\|P_\gamma(TS^*+S^*T)\,Q_\gamma\|\leqslant 4d\delta \tag{4.63}$$

$$\|Q_\gamma(TS^*+S^*T)\,A_\gamma\|\leqslant 4d\delta \tag{4.64}$$

For the terms coming from T^2 we proceed as in the discrete case, except that now $\max_{x\in\Lambda}|s_x^{*2}|\geqslant[\sigma_0(\lambda)-\delta]^2$. This yields upper bounds like (4.39)–(4.40) with $[g_k(c_3'\lambda)]^2$ replaced by $\{g_k(c_3'\lambda[\sigma_0(\lambda)-\delta])\}^2$.

For the ones coming from $\lambda(TS^*+S^*T)$ we also use (4.64) and (4.65). So we find upper bounds proportional to $\delta^2\{g_k(c_3'\lambda[\sigma_0(\lambda)-\delta])\}^2\,k(\gamma)$ and $\delta^2\{g_k(c_3'\lambda[\sigma_0(\lambda)-\delta])\}^2\,[l(\gamma)-k(\gamma)]$.

For the cross terms we have the same upper bounds with δ replacing δ^2. Since we choose $\delta=O(1)$ we see that the estimated of $f_{k,PQ}(S^*,t)$ and $f_{K,QA}(S^*,t)$ are as in (4.39)–(4.40) with $g_k(c_3'\lambda)$ replaced by $g_k[c_3'\lambda\sigma_0(\lambda)]$ and c_3 changed to some other constant of $O(1)$. For (4.38c) the analysis is similar. Finally we find

$$\frac{\beta^3}{16}\sum_{k=0}^{\infty}\int_0^1 dt\,(1-t)\,f_k(S,t)$$
$$\leqslant\frac{c_6'}{\lambda^3[\sigma_0(\lambda)-\delta]^3}\,l(\gamma)+\frac{c_6'''}{\lambda[\sigma_0(\lambda)-\delta]^3}\,[l(\gamma)-k(\gamma)]$$
$$\leqslant\frac{c_6}{\lambda^6}\,l(\gamma)+\frac{c_6''}{\lambda^4}\,[l(\gamma)-k(\gamma)] \tag{4.65}$$

From (4.62) and (4.66) we get the lower bound for (II)

$$(\text{II}) \geq \left(\frac{c_5}{\lambda^2} - \frac{c_6}{\lambda^6}\right) l(\gamma) - \frac{c_7}{\lambda^2}\,[l(\gamma) - k(\gamma)] \tag{4.66}$$

Finally, from (4.60), (4.66), and the remarks about the Jacobian factor $|J(S)|$ we obtain (4.53) for β, λ, and β/λ large enough with $J(\lambda) = c/\lambda$ and $\delta = O(1)$. This completes the proof of Theorem 4.1.

5. CONCLUDING REMARKS

We have indicated in Eq. (1.16) and below (1.12) the relation between the one-point functions $\langle s_x \rangle_\Lambda$ and $\langle n_x \rangle_\Lambda$ for the FK and Holstein models. One can also relate the spin–spin correlation to the imaginary *time-displaced* density–density correlation of the fermions; see Appendix A. For the Holstein and FK models at the symmetry point with periodic boundary conditions it takes the form

$$\frac{1}{\beta}\int_0^\beta dt\,\langle n_x n_y(t)\rangle_\Lambda = \frac{1}{4} - \frac{2}{\lambda}\,g(\beta, \lambda)(\langle n_x s_y \rangle_\Lambda + \langle n_y s_x \rangle_\Lambda)$$
$$+ \frac{4}{\lambda^2}\,[g(\beta, \lambda)]^2\,\langle s_x s_y \rangle_\Lambda, \qquad x \neq y \tag{5.1}$$

where $n_y(t) = \exp[-tH_\Lambda(0, \lambda/2)]\,n_y \exp[+tH_\Lambda(0, \lambda/2)]$. For the Holstein model we have $g(\beta, \lambda) = 1$ and for the FK model $g(\beta, \lambda)$ is given by (A.7).

In the present work we have only considered the case of density 1/2 for the fermions. In this case the ground-state spin configuration becomes periodic with period 2 and therefore opens a gap in the one-fermion energy spectrum. (In other words, the system is an insulator because we have a filled band.) Numerical simulations in one dimension show that for irrational densities ρ of electrons (in the infinite-volume limit one can make the density irrational) and small coupling λ the minimizing spin configuration is a function $u_\lambda(\rho x + \alpha)$ with $u_\lambda(y)$ analytic in λ and periodic in y of period 1 (thus it is incommensurate with the lattice), and α is a phase the value of which is arbitrary. This is in contrast to the case $\rho = 1/2$, where the function describing the spin configuration has an essential singularity at $\lambda = 0$ and is commensurate with the lattice, and the phase is fixed. This situation is analogous to the one encountered in the Frenkel–Kontorova model and is reminiscent of KAM theory (see refs. 1 and 2 for a discussion of these points). A rigorous proof of these numerical results is still an open problem but may not be out of reach. A related question is whether a gap opens or not in the one-fermion energy spectrum for irrational densities and small λ.

Although the integration over the quantum degrees of freedom is valid for any λ, thereby reducing the problem to a classical one, it seems to us that it is appropriate only for large λ. In the case of the Holstein model one can easily perform the Gaussian integration over the classical degrees of freedom by going to a functional integral representation using Grassman variables for the fermions. The problem is then reduced to an itinerant fermion problem with a long-range interaction in the time direction (in the functional integral formalism). This point of view might be useful to treat the small-λ limit, and more specifically the problems mentioned above. It can also be used to obtain some rigorous results about the fully quantum Holstein model (where the phonons are treated quantum mechanically) in one dimension.[10] We hope to come back to these questions in a future work.

Finally, we mention that in ref. 24 the authors treat a kind of mean-field version of the quantum Holstein model in which there is only a single-frequency phonon model coupled to the fermions. An exact solution then displays the transition to periodic structure at low temperatures. Also, Freericks and Lieb[9] have recently proved in a very general setting that if there is an even number of electrons (with spin 1/2), the ground state is a singlet for all electron–phonon couplings.

APPENDIX A

We prove several relations between electronic and spin correlation functions discussed in the introduction and the conclusion. To simplify the notation we do not write the β, μ, h dependence of various quantities.

Proof of Formula (1.8). Differentiating the total energy (1.6)

$$F'_\Lambda(\{s_x\}) = -\frac{1}{\beta}\log \operatorname{Tr} e^{-\beta H'_\Lambda(\mu,h)} \tag{A.1}$$

with respect to s_u gives

$$\frac{\partial F'_\Lambda}{\partial s_u} = \lambda\,\frac{\operatorname{Tr} n_u e^{-\beta H'_\Lambda(\mu,h)}}{\operatorname{Tr} e^{-\beta H'_\Lambda(\mu,h)}} - h \tag{A.2}$$

where H' is defined as in (1.1) without the term $f(s_x^2)$ and $p(s_x) = e^{-\beta f(s_x^2)}$. Performing the average over the spin degrees of freedom, we obtain

$$\frac{1}{\beta}\frac{1}{Z_\Lambda}\int \prod_{x\in\Lambda} p(s_x)\,ds_x \left(\frac{\partial}{\partial s_u} e^{-\beta F'_\Lambda}\right) = \lambda\langle n_u\rangle_\Lambda - h \tag{A.3}$$

An integration by parts shows that the left-hand side of (A.3) is equal to $\langle d/ds_u f(s_u^2)\rangle + [\rho_\Lambda(s_u=\infty) - \rho_\Lambda(s_u=-\infty)]$, where $\rho_\Lambda(s_u)$ is the probability distribution of s_u. Obviously for finite volume $\rho_\Lambda(s_u = \pm\infty) = 0$. Therefore (1.8) follows from (A.3).

Proof of Formula (1.16). We denote by $\langle - \rangle_{\Lambda,\gamma}$ and $\langle - \rangle_{\Lambda,\mathrm{FK}}$ the averages for the models defined by (1.15) and (1.14), respectively. Applying (1.8), we have

$$\lambda \langle n_u \rangle_{\Lambda,\gamma} = h - 4\gamma \langle (s_u^2 - 1)\, s_u \rangle_{\Lambda,\gamma} \tag{A.4}$$

We now restrict ourselves to the symmetry point. As $\gamma \to \infty$, the single spin measure (1.15) goes over to that of the FK model and from Theorem 3.1 the $\{s_x\}$ will be approximately given by

$$2\gamma(s_x^2 - 1) \approx \frac{\lambda^2}{4} \sum_{k_\alpha, \alpha = 1 \cdots d} [E(k)]^{-1} \tanh\left[\frac{\beta}{2} E(k)\right] \tag{A.5}$$

with $E(k)$ given by (3.4). Thus we have

$$\lim_{\gamma \to \infty} 4\gamma \langle (s_u^2 - 1)\, s_u \rangle_{\Lambda,\gamma} = \frac{\lambda^2}{2}\, g(\beta, \lambda) \langle s_u \rangle_{\Lambda,\mathrm{FK}} \tag{A.6}$$

with

$$g(\beta, \lambda) = \sum_{k_\alpha, \alpha = 1 \cdots d} [E(k)]^{-1} \tanh\left[\frac{\beta}{2} E(k)\right] \tag{A.7}$$

Combining (A.4) and (A.6), we obtain (1.16).

Proof of Formula (5.1). From (A.2) we get for u, v fixed

$$\frac{\partial^2 F'_\Lambda}{\partial s_u\, \partial s_v} = \lambda \frac{\partial}{\partial s_v} \frac{\mathrm{Tr}\, n_u e^{-\beta H'_\Lambda(\mu, h)}}{\mathrm{Tr}\, e^{-\beta H'_\Lambda(\mu, h)}} \tag{A.8}$$

The partial derivative on the right-hand side of (A.8) can be computed by using first-order perturbation theory

$$\frac{\partial}{\partial s_v} \mathrm{Tr}\, n_u e^{-\beta H'_\Lambda(\mu, h)} = -\lambda \int_0^\beta dt\, \mathrm{Tr}\, n_u e^{-tH'_\Lambda(\mu, h)} (n_v - h)\, e^{-(\beta - t) H'_\Lambda(\mu, h)} \tag{A.9}$$

Replacing (A.9) in (A.8) and performing the average over the spin variables gives

$$\frac{1}{Z_\Lambda} \int \prod_{x \in \Lambda} p(s_x)\, ds_x \left(\frac{\partial^2 F'_\Lambda}{\partial s_u\, \partial s_v}\right) e^{-\beta F'_\Lambda}$$

$$= -\lambda^2 \int_0^\beta dt\, (\langle n_u n_v(t) \rangle - \langle n_u \rangle \langle n_v \rangle) \tag{A.10}$$

where for any matrix V

$$V(t) = e^{tH'_\Lambda(\mu,h)} V e^{-tH'_\Lambda(\mu,h)} \tag{A.11}$$

The left-hand side of (A.10) can be written as $(A_1 + A_2)$, with

$$A_1 = \beta \frac{1}{Z_\Lambda} \int \prod_{x \in \Lambda} p(s_x)\, ds_x \left(\frac{\partial F'_\Lambda}{\partial s_u} \frac{\partial F'_\Lambda}{\partial s_v} \right) e^{-\beta F_\Lambda} \tag{A.12}$$

$$A_2 = -\frac{1}{\beta} \frac{1}{Z_\Lambda} \int \prod_{x \in \Lambda} p(s_x)\, ds_x \frac{\partial^2}{\partial s_u\, \partial s_v} (e^{-\beta F'_\Lambda}) \tag{A.13}$$

Replacing (A.2) in (A.12) and making a double integration by parts in (A.13), we obtain from (A.10) the final formula

$$\begin{aligned} &\lambda^2 \int_0^\beta dt\, \langle n_u n_v(t) \rangle + \beta\lambda \{ \langle n_u [2s_v f'(s_v^2) - h] \rangle + \langle n_v [2s_u f'(s_u^2) - h] \rangle \} \\ &\quad + 4\beta \langle s_u s_v f'(s_u^2) f'(s_v^2) \rangle \\ &= \langle 2f'(s_u^2) + 4s_u^2 f''(s_u^2) \rangle\, \delta_{uv} \end{aligned} \tag{A.14}$$

In particular, for the static Holstein model at the symmetry point we get (5.1) by setting $f(s_x^2) = \frac{1}{2} s_x^2$. In the case of the FK model we get (5.1) by using the spin measure (1.15) and (A.5).

APPENDIX B

We discuss the existence and behavior of solutions of Eqs. (2.3) of Theorem 2.1 and (3.3) of Theorem 3.1. We set

$$K_\Lambda(t) = \frac{\lambda^2}{4} \frac{1}{|\Lambda|} \sum_{k_\alpha, \alpha = 1 \cdots d} \left[4 \left(\sum_{\alpha=1}^{d} \cos k_\alpha \right)^2 + \lambda^2 t \right]^{-1/2} \tag{B.1}$$

Equation (2.3) reduces to $f'(t) = K_\Lambda(t)$, $t \geq 0$. The function $f'(t)$, $t \geq 0$, is continuous and increasing [since $f''(t) \geq 0$]. On the other hand, $K_\Lambda(t)$ is continuous and decreasing, and $K_\Lambda(\infty) = 0$, $K_\Lambda(0) \to \infty$ as $\Lambda \to \mathbf{Z}^d$ because $|\sum_{\alpha=1}^{d} \cos k_\alpha|^{-1}$ has a logarithmic singularity for $k_\alpha = \pi/2$, $\alpha = 1 \cdots d$. Therefore for $|\Lambda|$ large enough Eq. (2.3) always has a unique solution. This is also the case for the corresponding equation in the thermodynamic limit.

Behavior of the Solutions of (2.3) for the Holstein Model. For λ large the right-hand side of (2.3) (with $t = \sigma^2$) behaves as $\lambda/4\sigma$. Thus as $\lambda \to \infty$, $\sigma_0(\lambda) \sim \lambda/2$. For small λ

$$(2\pi)^{-d} \int_{[-\pi,\pi]^d} dk \left[4 \left(\sum_{\alpha=1}^{d} \cos k_\alpha \right)^2 + \lambda^2 \sigma^2 \right]^{-1/2} \sim \frac{1}{2} \ln(\lambda\sigma)^{-1} \tag{B.2}$$

Therefore we get $\sigma_0(\lambda) \sim \lambda^{-1} e^{-4\lambda^{-2}}$ as $\lambda \to 0$.

Existence and Nonexistence of Solutions of (3.3). We set

$$K_{\Lambda,\beta}(t)=\frac{\lambda^2}{4}\frac{1}{|\Lambda|}\sum_{k_\alpha,\alpha=1\cdots d}[E(k)]^{-1}\tanh\left[\frac{\beta}{2}E(k)\right] \tag{B.3}$$

Equation (3.3) reduces to $f'(t)=K_{\Lambda,\beta}(t)$, which is a monotone decreasing function of t for any β with $K_{\Lambda,\beta}(\infty)=0$. For $\beta<\infty$, $K_{\Lambda,\beta}(0)$ remains bounded as $\Lambda\to\mathbf{Z}^d$ because

$$\left|\sum_{\alpha=1}^{d}\cos k_\alpha\right|^{-1}\tanh\frac{\beta}{2}\left|\sum_{\alpha=1}^{d}\cos k_\alpha\right|$$

is integrable. Two cases have to be considered. When f is a polynomial of degree greater than or equal to two [case (i) of Theorem 3.1] then $f'(0)=0$. Thus in this case (3.3) has a unique solution for all β. On the other hand, in case (ii) of Theorem 3.1, $f'(0)=1$. Therefore there is a unique solution if β is such that

$$K_{\Lambda,\beta}(0)\geqslant 1 \tag{B.4}$$

and no solution if

$$K_{\Lambda,\beta}(0)\leqslant 1 \tag{B.5}$$

The inequality (B.4) is obviously satisfied for β small enough, while (B.5) holds for β large enough. The critical value of β is unique since $K_{\Lambda,\beta}$ is a monotone increasing function of β.

APPENDIX C

We derive an upper bound on the kernel of $G_k(S^*,t)$, by using the Combes–Thomas method.[6] The argument was used already in refs. 18 and 19, but here it is slightly different, so we provide the details. What follows is valid for discrete as well as continuous spins.

Let Q be the matrix with elements $(Q)_{uv}=e^{m\cdot u}\delta_{uv}$ for a vector m to be conveniently chosen later. A computation yields

$$Q[G_k(S^*,t)]^{-1}Q^{-1}=[G_k(S^*,t)]^{-1}+\frac{\beta^2}{4}R(S^*) \tag{C.1}$$

with

$$\begin{aligned}R(S^*)&=(ET+TE+E^2)_D+t(ET+TE+E^2)_{ND}\\&\quad+\lambda(ES+SE)_D+t\lambda(ES+SE)_{ND}\end{aligned} \tag{C.2}$$

where $(E)_{uv} = t_{uv}(e^{m \cdot (u-v)} - 1)$ and for any matrix V, V_D and V_{ND} are the diagonal and nondiagonal blocks i.e.,

$$V_D = P_\gamma V P_\gamma + Q_\gamma V Q_\gamma + A_\gamma V A_\gamma \tag{C.3}$$

$$V_{ND} = P_\gamma V Q_\gamma + Q_\gamma V P_\gamma + P_\gamma V A_\gamma + A_\gamma V P_\gamma + Q_\gamma V A_\gamma + A_\gamma V Q_\gamma \tag{C.4}$$

Since the operator norm $\|S^*\| = \max_{x \in \Lambda} |s_x^*|$,

$$\|R(S^*)\| \leqslant 8d^2(e^{|m|} - 1) + 8d^2(e^{|m|} - 1)^2 + 8d\lambda(e^{|m|} - 1) \max_{x \in \Lambda} |s_x| \tag{C.5}$$

Moreover the operator norm of

$$[G_k(S^*, t)]^{-1} = \left(k + \frac{1}{2}\right)^2 \pi^2 + \frac{\beta^2}{4} [\lambda^2 S^{*2} + (T^2)_D + t(T^2)_{ND} + \lambda(TS^* + S^*T)_D + \lambda t(TS^* + S^*T)_{ND}] \tag{C.6}$$

is given by its maximal eigenvalue. Consequently it is certainly greater than

$$\|[G_k(S^*, t)]^{-1}\| \geqslant \left(k + \frac{1}{2}\right)^2 \pi^2 + \frac{\beta^2}{4} (\lambda^2 \max_{x \in \Lambda} |s_x^{*2}| - 8d^2 - 8d\lambda \max_{x \in \Lambda} |s_x^*|) \tag{C.7}$$

The configuration $\{s_x^*\}$ has $\max_{x \in \Lambda} |s_x^*| \geqslant 1$ (for discrete as well as continuous spins); therefore for λ large enough we have

$$\|[G_k(S^*, t)]^{-1}\| \geqslant \left(k + \frac{1}{2}\right)^2 \pi^2 + \frac{\beta^2}{4} c_3'' \lambda^2 \max_{x \in \Lambda} |s_x^{*2}| \tag{C.8}$$

with c_3'' a positive constant independent of λ. From (C.5) and (C.8) we see that by choosing $|m| = 1$ we have for some positive constant c_3' independent of λ

$$\|[G_k(S^*, t)]^{-1}\| - \frac{\beta^2}{4} \|R(S^*)\| \geqslant \left(k + \frac{1}{2}\right)^2 \pi^2 + \frac{\beta^2}{4} c_3' \lambda^2 \max_{x \in \Lambda} |s_x^{*2}| \tag{C.9}$$

Therefore, taking $m = -(u-v)\,|u-v|^{-1}$, we conclude from (C.1) and (C.9)

$$\langle u| \, G_k(S^*, t) \, |v\rangle \leqslant \frac{1}{(k + \frac{1}{2})^2 \pi^2 + \frac{1}{4}\beta^2 c_3' \lambda^2 \max_{x \in \Lambda} |s_x^{*2}|} e^{-|u-v|} \tag{C.10}$$

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