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Order–disorder transition in the spinless fermion model

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Abstract. The spinless fermion model used by some authors for a description of a metal–insulator transition is proven to develop a long-range order at sufficiently low temperatures if the dimension of the underlying simple cubic lattice $\nu \geqslant 2$. The Hamiltonian of the model consists of the lattice kinetic energy term and a nearest-neighbour repulsion term. The method used in the proof is that of Fröhlich and Lieb, which combines a Peierls argument with chessboard estimates. For $\nu \geqslant 3$ infrared bounds are applied to find a simple expression for the critical temperature lower bound.

1. Introduction

The spinless fermion model is the simplest non-trivial model one can construct for spinless fermions on a lattice, possessing kinetic energy. Its second-quantised Hamiltonian reads

$$H_\mu = -t \sum_{\langle i,j\rangle} (c_i^* c_j + c_j^* c_i) + W \sum_{\langle i,j\rangle} n_i n_j - \mu \sum_{i\in\Lambda} n_i, \tag{1}$$

where c_i^*, c_i stand for fermion creation and annihilation operators at a site i of a lattice Λ respectively, $n_i = c_i^* c_i$ and $\Sigma_{\langle i,j\rangle}$ denotes summation over nearest-neighbour pairs, each pair being counted once. If the chemical potential $\mu = \mu_0$, where $\mu_0 = zW/2$ and z is the number of nearest neighbours, Hamiltonian (1) is invariant under the following canonical transformation called the hole–particle transformation (HPT):

$$c_i^* \to (-1)^{|i|} c_i, \qquad i = (i^1, i^2, \ldots, i^\nu) \in \Lambda, \qquad |i| = |i^1 + i^2 + \ldots + i^\nu|. \tag{2}$$

Therefore in the case $\mu = \mu_0$, the mean number of particles per site $\rho = \langle |\Lambda|^{-1} \Sigma_{i\in\Lambda} n_i\rangle$, where $\langle \ldots \rangle$ is the Gibbs state corresponding to a system placed on a finite lattice Λ with number of sites $|\Lambda|$ whose energy is given by Hamiltonian (1), is equal to $\frac{1}{2}$ independently of temperature.

In the one-dimensional case, for $\mu = \mu_0$ the model has received considerable attention in the literature, mainly due to its thermodynamic equivalence to the anisotropic Heisenberg chain (Des Cloizeaux 1966, Wolf and Zittartz 1981, Lorenz 1980).

Kohn (1967) used the model for a description of a metal–insulator transition in the framework of a Hartree–Fock approximation. With the same purpose the model was studied by Cullen and Callen (1970, 1973) and Lorenz and Ihle (1972), in a Hartree–Fock approximation. Lorenz (1980) proposed the model for a study of an order–disorder transition in superionic conductors, using a two-site cluster approximation.

The common feature of the results of the last three quoted references is that in the case of the simple cubic lattice, for $W>0$ (repulsion of particles) and $\mu=\mu_0$, below some critical temperature the system is in the so-called charge-ordered phase, i.e. there is a non-zero difference between mean occupation of odd and even sublattices. According to Hartree–Fock type approximations the above transition to a charge-ordered phase occurs for any value of the ratio $|t/W|$, while cluster approximations predict that it vanishes if $|t/W|$ is larger than some critical value (Lorenz 1982).

The purpose of this paper is to prove that system (1), with $W>0$, $\mu=\mu_0$ and Λ the simple cubic lattice, undergoes an order–disorder transition at some critical temperature if the ratio $|t/W|$ is sufficiently small and dimensions $\nu\geqslant 2$. Specifically we prove that under the above conditions, at sufficiently low temperatures, there is long-range order corresponding to the charge ordering. The result is achieved with the help of a rigorous method developed by Fröhlich and Lieb (1978), which is based on a version of the Peierls argument and the notion of reflection positivity of the Gibbs state generated by the system's Hamiltonian.

Finally, in order to obtain simple expressions for lower bounds of the critical temperature and the critical value of the ratio $|t/W|$, we use the method of infrared bounds (Fröhlich *et al* 1978). These results hold in dimensions $\nu\geqslant 3$.

2. Some properties of the Hamiltonian, reflection positivity

First, we shall transform H_μ to an equivalent form, more convenient for our purposes,

$$H_{\mu_0}=\tfrac{1}{8}|W|H^{\pm}_{\mu_0}(\alpha)+\text{constant}, \tag{3}$$

$$H^{\pm}_{\mu_0}(\alpha)=-\alpha\sum_{\substack{\langle i,j\rangle\\ i\in\Lambda^0}}(c_i^*c_j+c_j^*c_i)+\sum_{\substack{\langle i,j\rangle\\ i\in\Lambda^0}}[(2n_i-1)\pm(2n_j-1)]^2, \tag{4}$$

where $\alpha=8t/|W|$, the + sign corresponds to repulsion and the − sign to attraction of particles, and Λ^0 denotes the odd sublattice of Λ, which is assumed to be the simple cubic lattice wrapped on a torus ($\nu=2$). We also assume that $t>0$; however, this is not a restriction, since there is a canonical transformation which changes the sign of the kinetic energy but leaves the interaction term unchanged, $c_x\to\exp(\mathrm{i}|x|\pi)c_x$, $x\in\Lambda$. In the following we shall study the case of repulsion, i.e. the system given by $H^+_{\mu_0}$. We apply to $H^+_{\mu_0}$ the HPT restricted to the even sublattice: $c_i^*\to c_i$, $i\in\Lambda^{\mathrm{e}}$, in order to get a unitarily equivalent Hamiltonian $\tilde H(\alpha)$:

$$\tilde H(\alpha)=-\alpha\sum_{\substack{\langle i,j\rangle\\ i\in\Lambda^0}}(c_i^*c_j^*+c_jc_i)+\sum_{\substack{\langle i,j\rangle\\ i\in\Lambda^0}}[(2n_i-1)-(2n_j-1)]^2. \tag{5}$$

The purpose of the rest of this section is to explain and prove the reflection positivity property of the Gibbs state generated by Hamiltonian (5). The proof is based on that by Fröhlich (Fröhlich *et al* 1980, model 5.6) and is presented here to make the paper more self-contained.

We shall assume that $\Lambda\subset\mathbb{Z}^2$ can be parametrised as follows:

$$\Lambda=\{\mathbb{Z}^2\ni(i^1,i^2)\colon 0\leqslant i^1\leqslant 4M-1, 0\leqslant i^2\leqslant 4M-1, M=1,2,\ldots\}. \tag{6}$$

Because of periodic boundary conditions coordinates are calculated modulo $4M$ onto the set $0,1,\ldots,4M-1$. Consider pairs of lines parallel to the second coordinate axis, bisecting the bonds between two adjacent lattice lines:

$$L_x^- = \{(x+\tfrac{1}{2}, y) \colon y \in R\},$$
$$L_x^+ = \{(x+2M+\tfrac{1}{2}, y) \colon y \in R\}, \qquad x = 0, 1, \ldots, 4M-1. \tag{7}$$

With each pair L_x^-, L_x^+ we associate a partition of Λ into two subsets Λ_x^+, Λ_x^-:

$$\Lambda_x^+ = \{\mathbb{Z}^2 \ni (i^1, i^2) \colon x+1 \leqslant i^1 \leqslant x+2M, 0 \leqslant i^2 \leqslant 4M-1\},$$
$$\Lambda_x^- = \{\mathbb{Z}^2 \ni (i^1, i^2) \colon i^1 \leqslant x \text{ or } i^1 \geqslant x+2M+1, 0 \leqslant i^2 \leqslant 4M-1\}, \tag{8}$$

and a reflection $R_x \colon \Lambda \to \Lambda$,

$$R_x(i_1, i_2) = (2x+1-i^1, i^2). \tag{9}$$

Clearly we have that

$$\Lambda_x^+ \cup \Lambda_x^- = \Lambda, \qquad \Lambda_x^+ \cap \Lambda_x^- = \varnothing, \qquad R_x \Lambda_x^- = \Lambda_x^+. \tag{10}$$

As is well known, operators c_i^*, c_i, $i \in \Lambda$ obeying canonical anticommutation relations $c_i^* c_j + c_j c_i^* = \delta_{i,j}$, $c_i c_j + c_j c_i = 0$ have a real matrix representation on $\mathbb{C}^M$, $M = 2^{|\Lambda|}$. In this representation matrices of unitary operators $(-1)^{n_j}$ are also real. The set $\{c_i^*, c_i \colon i \in \Lambda\}$ of matrices generates the real matrix algebra $\mathcal{U}$ of local observables. With each partition of Λ it is possible to associate a partition of $\mathcal{U}$ into two subalgebras $\mathcal{U}_x^+, \mathcal{U}_x^-$, such that $\mathcal{U} = \mathcal{U}_x^+ \cup \mathcal{U}_x^-$, $[\mathcal{U}_x^+, \mathcal{U}_x^-] = 0$ and a real morphism $\theta_x \colon \mathcal{U}_x^- \to \mathcal{U}_x^+$ such that $\theta_x \mathcal{U}_x^- = \mathcal{U}_x^+$. This is done in the following way. Let

$$a_i = c_i \qquad \text{if } i \in \Lambda_x^+,$$
$$a_i = (-1)^{N^+} c_i \qquad \text{if } i \in \Lambda_x^-, N^+ = \sum_{i \in \Lambda_x^+} n_i. \tag{11}$$

Then $\mathcal{U}_x^+$ is the algebra generated by a_i^*, a_i, $i \in \Lambda_x^+$ and $\mathcal{U}_x^-$ is the algebra generated by a_i^*, a_i, $i \in \Lambda_x^-$. The morphism θ_x is given by

$$\theta_x(a_i) = (-1)^{N^-} a_{Ri} \qquad \text{if } (-1)^{|i|} = 1,$$
$$\theta_x(a_i) = a_{Ri}(-1)^{N^-} \qquad \text{if } (-1)^{|i|} = -1. \tag{12}$$

Moreover

$$\operatorname{Tr} A\theta_x(A) \geqslant 0 \qquad \text{for } A \in \mathcal{U}_x^-, \tag{13}$$

where the trace is taken over $\mathbb{C}^M$ and $-\tilde{H}(\alpha)$ has the form

$$-\tilde{H}(\alpha) = B + \theta_x(B) + \sum_{i=1}^{k} C_i \theta_x(C_i), \qquad B, C_i \in \mathcal{U}_x^-. \tag{14}$$

Equations (13) and (14) imply that the Gibbs state $\langle \ldots \rangle_{\sim} = \operatorname{Tr}[\ldots \exp(-\beta \tilde{H}(\alpha))]/\operatorname{Tr}\exp(-\beta \tilde{H}(\alpha))$ has the reflection positivity property, i.e. $\langle A\theta_x(A)\rangle_{\sim} \geqslant 0$ for all $A \in \mathcal{U}_x^-$.

Obviously all the above reasoning can be repeated for pairs of lines parallel to the first coordinate axis. By the general theory of reflection positivity we can use in our considerations chessboard estimates as well as infrared bounds (Fröhlich *et al* 1978).

3. The problem and its solution

Here we shall specify the problem, recall for completeness the main steps of the method which we shall use, and find necessary estimates. Let

$$m_\Lambda = |\Lambda|^{-1} \sum_{i \in \Lambda} (-1)^{|i+1|} m_i, \qquad m_i = 2n_i - 1. \tag{15}$$

By invariance of H_{μ_0} under the HPT, $\langle m_\Lambda \rangle \equiv 0$. Our aim is to prove that in the thermodynamic limit, denoted $\lim_{\Lambda \uparrow \mathbb{Z}^2}$, the staggered long-range order $\lim_{\Lambda \uparrow \mathbb{Z}^2} \langle m_\Lambda^2 \rangle$ of the system $H^+_{\mu_0}$ is non-zero at sufficiently low temperatures. An equivalent statement is

$$\lim_{\Lambda \uparrow \mathbb{Z}^2} \langle \tilde{m}_\Lambda^2 \rangle_\sim > 0, \qquad \tilde{m}_\Lambda = |\Lambda|^{-1} \sum_{i \in \Lambda} m_i \tag{16}$$

for $\beta > \beta_c$, where β_c is the inverse critical temperature. (16) is implied by the inequality

$$\langle m_0 m_j \rangle_\sim \geq K, \qquad K > 0 \tag{17}$$

uniformly in j and Λ, for $\beta > \beta_c$. Let P_i^+, P_i^- denote spectral projections of m_i to the eigenvalues 1 and -1 respectively. Then $m_i = P_i^+ - P_i^-$ and

$$\langle m_0 m_j \rangle_\sim = 1 - 4\langle P_0^+ P_j^- \rangle_\sim . \tag{18}$$

Therefore we are left with proving that $\langle P_0^+ P_j^- \rangle_\sim < \frac{1}{4}$ uniformly in j and Λ for sufficiently large β.

In our reasoning we stick to the method of Fröhlich and Lieb (1978). An upper bound for $\langle P_0^+ P_j^- \rangle_\sim$ uniform in j and Λ is obtained in the following sequence of steps.

(a)
$$\langle P_m^+ P_n^- \rangle_\sim \leq \sum_\gamma \left\langle \prod_{\langle i,j \rangle \in \gamma} P_i^+ P_j^- \right\rangle , \tag{19}$$

where a contour γ is a family of nearest-neighbour pairs $\{\langle i_1, j_1 \rangle, \ldots, \langle i_k, j_k \rangle : k = 4, 6, \ldots\}$ which divides Λ into two disjoint subsets, $\Lambda_m(\gamma) \supset \{i_1, \ldots, i_k, m\}$ and $\Lambda_n(\gamma) \supset \Delta \{j_1, \ldots, j_k, n\}$, such that $\Lambda_m(\gamma) \cup \Lambda_n(\gamma) = \Lambda$.

(b) *A chessboard estimate*

$$\left\langle \prod_{\langle ij \rangle \in \gamma} P_i^+ P_j^- \right\rangle_\sim \leq \langle P_\Lambda \rangle_\sim^{|\gamma|/2|\Lambda|}, \tag{20}$$

where

$$P_\Lambda = \prod_{i^1=0}^{M-1} \left(\prod_{i^2=0}^{4M-1} P^+_{(4i^1,i^2)} P^-_{(4i^1+1,i^2)} P^-_{(4i^1+2,i^2)} P^+_{(4i^1+3,i^2)} \right) \tag{21}$$

and $|\gamma|$ is the length of γ, i.e. the number of nearest-neighbour pairs in γ. (20) is obtained by the repeated application of the Schwartz inequality: $\langle A\theta_x(B)\rangle_\sim^2 \leq \langle A\theta_x(A)\rangle_\sim \langle B\theta_x(B)\rangle_\sim$ for A, $B \in \mathcal{U}_x^-$, which follows from the reflection positivity property of the state $\langle \ldots \rangle_\sim$, for all θ_x described in § 2. Note that P_Λ is a spectral projector of $\tilde{H}(0) = \Sigma_{\langle i,j \rangle} [(2n_i - 1) - (2n_j - 1)]^2$ onto the one-dimensional eigensubspace whose eigenvalue $2|\Lambda|$ is greater than $e_0(0)$, the ground state energy of $\tilde{H}(0)$ ($e_0(0) = 0$).

(c) *Peierls argument.* If for large enough Λ, $\langle P_\Lambda \rangle^{1/|\Lambda|} < \frac{1}{9}$, then

$$\langle P_m^+ P_n^- \rangle_\sim \leq \sum_{k=2}^{\infty} 2k 3^{2k-2} (\langle P_\Lambda \rangle_\sim^{1/|\Lambda|})^k . \tag{22}$$

Hence $\langle P_m^+ P_n^- \rangle_\sim < \frac{1}{4}$ uniformly in m, n and Λ if $\langle P_\Lambda \rangle_\sim^{1/|\Lambda|}$ is sufficiently small uniformly in Λ.

(d) For any $\varepsilon > 0$ there exists $\theta < \alpha_c < 1$ and $\beta_c < \infty$ such that for $\alpha < \alpha_c$ and $\beta > \beta_c$, $\langle P_\Lambda \rangle_\sim^{1/|\Lambda|} < \varepsilon$ uniformly in Λ.

Let $\{e_i\}$ denote the set of eigenvalues of $\tilde{H}(\alpha)$ and choose some $\Delta > 0$; then

$$\langle P_\Lambda \rangle_\sim = Z^{-1}(\beta, \alpha) \sum_{e_i < e_0(0) + \Delta|\Lambda|} \exp(-\beta e_i) \langle e_i | P_\Lambda | e_i \rangle$$
$$+ Z^{-1}(\beta, \alpha) \sum_{e_i \geqslant e_0(0) + \Delta|\Lambda|} \exp(-\beta e_i) \langle e_i | P_\Lambda | e_i \rangle, \tag{23}$$

where $Z(\beta, \alpha) = \operatorname{Tr} \exp(-\beta \tilde{H}(\alpha))$ and $e_0(\alpha)$ denotes the ground state energy of $\tilde{H}(\alpha)$.

If α were zero we could make the first term of (23) vanish identically by choosing Δ sufficiently small, while the second term of (23) could be estimated as follows:

$$Z^{-1}(\beta, \alpha) \sum_{e_i \geqslant e_0(0) + \Delta|\Lambda|} \exp(-\beta e_i) \langle e_i | P_\Lambda | e_i \rangle$$
$$\leqslant Z^{-1}(\beta, \alpha) \exp[-\beta(e_0(0) + \Delta|\Lambda|)] \operatorname{Tr} \mathbb{1} \leqslant 2^{|\Lambda|} \exp(-\beta \Delta |\Lambda|). \tag{24}$$

In the case $\alpha \neq 0$, (24) holds as well, but the first term of (23) does not vanish identically since $[P_\Lambda, \tilde{H}(\alpha)] \neq 0$ so P_Λ can have non-zero matrix elements in any eigenstate of $\tilde{H}(\alpha)$. However, one can expect that if e_i are close to $e_0(0)$, then when $\alpha \tilde{T} = \tilde{H}(\alpha) - \tilde{H}(0)$ is small with respect to $\tilde{H}(0)$ in a suitable sense, the matrix elements $\langle e_i | P_\Lambda | e_i \rangle$ are small. This idea is made mathematically rigorous by the following theorem, called by Fröhlich and Lieb (1978) the principle of exponential localisation.

Theorem (*Fröhlich and Lieb*). Let A and B be self-adjoint operators on a Hilbert space $\mathscr{H}$ such that

(i) $$A \geqslant 0, \tag{25}$$

(ii) $$\pm B \leqslant \varepsilon A \qquad \text{with } 0 \leqslant \varepsilon < 1. \tag{26}$$

Let ψ be a normalised eigenvector of $A + B$:

$$(A + B)\psi = \lambda \psi. \tag{27}$$

Choose some $\rho > \lambda \geqslant 0$ such that $\sigma \equiv \varepsilon \rho (\rho - \lambda)^{-1} < 1$. Let $M_\rho \subset \mathscr{H}$ be the subspace of $\mathscr{H}$ generated by all eigenvectors of A corresponding to eigenvalues $e \geqslant \rho((A - \lambda)|_{M_\rho} > 0)$ and let P be the projector onto the subspace $M_P \subset M_\rho$ such that $\varphi \in M_P$ if and only if

(iii) $$[B(A - \lambda)^{-1}]^j \varphi \in M_\rho \tag{28}$$

for $j = 0, 1, \ldots, d-1$, with $d \geqslant 1$. Then

$$\langle \psi | P | \psi \rangle \leqslant \sigma^{2d}. \tag{29}$$

Now, according to (A1.4) (see appendix 1)

$$\tilde{H}(0) - e_0(1) \geqslant 0 \tag{30}$$

and by definition of $e_0(1)$

$$\tilde{T}+\tilde{H}(0)-e_0(1)\geqslant 0 \qquad \text{or} \qquad -\tilde{T}\leqslant \tilde{H}(0)-e_0(1). \tag{31}$$

Since there exists a unitary transformation under which $\tilde{T}\to -\tilde{T}$ we also have

$$-\tilde{T}+\tilde{H}(0)-e_0(1)\geqslant 0 \qquad \text{or} \qquad \tilde{T}\leqslant \tilde{H}(0)-e_0(1). \tag{32}$$

Therefore, by (30), $A=\tilde{H}(0)-e_0(1)\geqslant 0$ and $B=-\alpha\tilde{T}$ satisfies the inequality $\pm B\leqslant \varepsilon A$ with $\varepsilon=\alpha$ by (31) and (32), which implies that $A+B=\tilde{H}(\alpha)-e_0(1)\geqslant 0$ for $\alpha<1$. The first term of (23) can be estimated by a single matrix element of P_Λ:

$$\sum_{e_i<e_0(0)+\Delta|\Lambda|}\exp(-\beta e_i)\langle e_i|P_\Lambda|e_i\rangle \Big/ \sum_{e_i}\exp(-\beta e_i)$$
$$\leqslant \max_{e_i<e_0(0)+\Delta|\Lambda|}\langle e_i|P_\Lambda|e_i\rangle=\langle e_{i_0}|P_\Lambda|e_{i_0}\rangle \tag{33}$$

for some $e_{i_0}<e_0(0)+\Delta|\Lambda|$, i.e. we are interested in an upper bound for $\langle e_{i_0}|P_\Lambda|e_{i_0}\rangle$. This suggests the identification $\psi=|e_{i_0}\rangle$, $P=P_\Lambda$. Hence λ has to fulfil the inequality

$$\lambda\leqslant e_0(0)-e_0(1)+\Delta|\Lambda|=-e_0(1)+\Delta|\Lambda|. \tag{34}$$

So we choose $\rho=-e_0(1)+n\Delta|\Lambda|$ with $n>1$.

In appendix 2 we find the upper bound for σ

$$\sigma\leqslant\alpha(1+1/\eta+\mathrm{O}(\beta^{-\xi}))<1 \tag{35}$$

for sufficiently small α and the lower bound for d

$$d\geqslant E((1-\eta)|\Lambda|/4)\geqslant 1 \tag{36}$$

for sufficiently large Λ, where ξ, η are parameters which satisfy relations $0<\xi<1$, $0<\eta<1$, $\Delta=\beta^{-\xi}$, $n=2\eta\beta^{\xi}$. (24), (29), (33) imply that

$$\langle P_\Lambda\rangle_{\sim}^{1/|\Lambda|}\leqslant 2\exp(-\beta^{1-\xi})+\{\alpha[1+1/\eta+\mathrm{O}(\beta^{-\xi})]\}^{(1-\eta)/2} \tag{37}$$

for sufficiently small α and sufficiently large Λ. This proves statement (d) and ends the proof of the existence of long-range order in the system $H^{+}_{\mu_0}$.

Since the series (22) has the sum equal to $2q^2(2-q)/(1-q)^2$, where $q=9\langle P_\Lambda\rangle_{\sim}^{1/|\Lambda|}<1$, α_c and β_c can be estimated from the equation

$$\bar{q}^2(2-\bar{q})/(1-\bar{q})^2=\tfrac{1}{8}, \tag{38}$$

where $\bar{q}$ stands for the upper bound of q which follows from (37) by an optimisation of the choice of ξ and η. This perhaps can be achieved numerically.

The above proof can be generalised to higher dimensions, as usual in methods based on a Peierls argument. However, in dimensions $\nu\geqslant 3$ a simpler proof by the method of infrared bounds is available (Dyson *et al* 1978). It gives simple analytic expressions for lower bounds for the critical temperature and α_c; this is carried out in § 4.

4. Infrared bounds for $\nu \geqslant 3$

For a vector k in the first Brillouin zone of Λ, let

$$m(k) = |\Lambda|^{-1/2} \sum_{j \in \Lambda} m_j \exp \mathrm{i}kj. \tag{39}$$

Since $\langle \ldots \rangle_{\sim}$ has the reflection positivity property, the following infrared bound holds (Fröhlich *et al* 1978):

$$(m(k), m(-k)) \leqslant (2\beta E(k))^{-1}, \tag{40}$$

where $E(k) = \Sigma_{l=1}^{\nu} (1 - \cos k_l)$ (the lattice constant is assumed to be 1) and $(A, B) = \beta^{-1} \int_0^\beta \mathrm{d}s \langle \exp(s\tilde{H}(\alpha)) A \exp(-s\tilde{H}(\alpha)) B \rangle_{\Lambda}^{\sim}$ is the Duhamel two-point function (Dyson *et al* 1978). (40) implies the upper bound for the correlation function $\langle m(k) m(-k) \rangle_{\sim}$ (Falk and Bruch 1969):

$$\langle m(k) m(-k) \rangle_{\sim} \leqslant \tfrac{1}{2} (C_k B_k)^{1/2} \coth \tfrac{1}{2}\beta (C_k / B_k)^{1/2}, \tag{41}$$

where C_k and B_k are such that $\langle [m(-k), [\tilde{H}(\alpha), m(k)]] \rangle_{\sim} \leqslant C_k$ and $(m(k), m(-k)) \leqslant \beta^{-1} B_k$. One finds $B_k = (2E(k))^{-1}$ and $C_k = 32\alpha\nu$. Thus

$$\langle m(k) m(-k) \rangle_{\sim} \leqslant 2(\alpha\nu / E(k))^{1/2} \coth 4\beta (\alpha\nu E(k))^{1/2}. \tag{42}$$

and by the argument of Dyson *et al* (1978)

$$\lim_{|i-j| \to \infty} \langle m_i m_j \rangle_\infty \geqslant \langle m_0^2 \rangle_\infty^{\sim} - \frac{1}{(2\pi)^\nu} \int_{-\pi}^{\pi} \mathrm{d}^\nu k \; 2(\alpha\nu / E(k))^{1/2} \coth 4\beta (\alpha\nu E(k))^{1/2}, \tag{43}$$

where $\langle \ldots \rangle_\infty$ denotes the thermodynamic limit of states $\langle \ldots \rangle_{\sim}$, and $|i-j|$ is the distance between i and j. It is well known (Ruelle 1969) that if $\lim_{|i-j| \to \infty} \langle m_i m_j \rangle_\infty > 0$ or (15) holds, then the state $\langle \ldots \rangle_\infty$ does not have the cluster property and at least two pure phases exist. Since $\langle m_0^2 \rangle_{\sim} = 1$ and $\coth x \leqslant 1 + 1/x$, we find

$$\lim_{|i-j| \to \infty} \langle m_i m_j \rangle_\infty \geqslant 1 - 2(\alpha\nu)^{1/2} C_{1/2} - (2\beta)^{-1} C_1, \tag{44}$$

where $C_r = (2\pi)^{-\nu} \int_{-\pi}^{\pi} \mathrm{d}^\nu k \, E^{-r}(k)$, $r = 1, \frac{1}{2}$. (44) gives the following lower bound for α_c and upper bound for β_c:

$$\alpha_c \geqslant (4 C_{1/2}^2 \nu)^{-1}, \qquad \beta_c \leqslant \tfrac{1}{2} C_1 (1 - 2(\alpha\nu)^{1/2} C_{1/2})^{-1}. \tag{45}$$

Appendix 1. Upper and lower bounds for the ground state energy $e_0(\alpha)$ of $\tilde{H}(\alpha)$

By the Peierls–Bogolyubov inequality

$$\operatorname{Tr} \exp(-\beta \tilde{H}(\alpha)) \geqslant \sum_{|a\rangle} \exp(-\beta \langle a | \tilde{H}(\alpha) | a \rangle), \tag{A1.1}$$

where $\{|a\rangle\}$ stands for a set of orthonormal vectors of $\mathscr{H}$. Let $\{|a\rangle\}$ be all eigenvectors of the occupation number operators n_i, $i \in \Lambda$. Then

$$\begin{aligned} \sum_{|a\rangle} \exp(-\beta \langle a | \tilde{H}(\alpha) | a \rangle) &= \sum_{|a\rangle} \exp(-\beta \langle a | \tilde{H}(0) | a \rangle) \\ &= \operatorname{Tr} \exp(-\beta \tilde{H}(0)). \end{aligned} \tag{A1.2}$$

Hence

$$\operatorname{Tr}\exp(-\beta\tilde{H}(\alpha)) \geqslant \operatorname{Tr}\exp(-\beta\tilde{H}(0)). \tag{A1.3}$$

The last inequality implies the following upper bound for $e_0(\alpha)$:

$$e_0(\alpha) \leqslant e_0(0). \tag{A1.4}$$

Clearly $e_0(0) = 0$. To get a lower bound for $e_0(\alpha)$ note that

$$\langle -\tilde{H}(\alpha)\rangle_{\sim} \leqslant \alpha\langle\tilde{T}\rangle_{\sim} \leqslant \alpha|\langle\tilde{T}\rangle_{\sim}|, \tag{A1.5}$$

where

$$\tilde{T} = \sum_{\substack{\langle i,j\rangle \\ i\in\Lambda^{0}}} (c_i^* c_j^* + c_j c_i).$$

Thus

$$\langle\tilde{H}(\alpha)\rangle_{\sim} \geqslant -\alpha|\langle\tilde{T}\rangle_{\sim}| \geqslant -\alpha\nu|\Lambda| \tag{A1.6}$$

and

$$e_0(\alpha) \geqslant -\alpha\nu|\Lambda|, \tag{A1.7}$$

where we used the Schwartz inequality to estimate $|\langle\tilde{T}\rangle_{\sim}|$.

Appendix 2. Upper bound for σ and lower bound for d

From (34), (A1.7) and the definition of ρ we get the inequalities

$$\lambda \leqslant (2+\Delta)|\Lambda|, \qquad \rho \leqslant (2+n\Delta)|\Lambda| \tag{A2.1}$$

which imply the following upper bound for σ:

$$\sigma \equiv \alpha\frac{\rho}{\rho-\lambda} \leqslant \alpha\left(1+\frac{2+\Delta}{(n-1)\Delta}\right). \tag{A2.2}$$

In our case P_Λ is the projector onto a definite configuration, i.e. M_P is a one-dimensional subspace of $\mathscr{H}$ corresponding to the eigenvalue $2|\Lambda| - e_0(1)$ of A (each bond $+-$ or $-+$ contributes 4 and there are $|\Lambda|/2$ of such bonds). To ensure that $M_P \subset M_\rho$ we require that

$$2|\Lambda| - e_0(1) - \rho = (2-n\Delta)|\Lambda| > 0; \tag{A2.3}$$

hence we get the constraint

$$2 - n\Delta > 0. \tag{A2.4}$$

Next we have to find a lower bound for d. Since B is of the form $-\alpha\Sigma_{\langle ij\rangle}(c_i^* c_j^* + c_j c_i)$, each application of B to an eigenstate of A gives another eigenstate of A with two particles on nearest-neighbour sites more or less. If in the new state the number of nearest-neighbour sites such that one of them is occupied and the other is empty ($+-$ or $-+$ bonds) is smaller by one, its A-energy is smaller by 4. Therefore, finding a lower bound for d amounts to estimation of the minimal number of successive applications of B to a state from M_P, which lower the energy $2|\Lambda| - e_0(1)$ to the energy $\rho = -e_0(1) + n\Delta|\Lambda|$. In the index (i^1, i^2) in (21), let i^1 denote columns. Then it is clear that the number of steps in the above process is minimal if we remove $+-$, $-+$ horizontal bonds, for example by creation of particles at horizontal pairs of empty sites. Such a step lowers the A-energy by 8. Thus

$$d \geqslant E((2-n\Delta)|\Lambda|/8), \tag{A2.5}$$

where for a real x, $E(x)$ denotes the largest integer which does not exceed x. Finally if we set $\Delta = \beta^{-\xi}$, $n = 2\eta\beta^{\xi}$ for some $0<\xi<1$ and $0<\eta<1$ then all the constraints are satisfied:

$$\sigma \leqslant \alpha(1+1/\eta+\mathrm{O}(\beta^{-\xi}))<1 \tag{A2.6}$$

for sufficiently small α and

$$d \geqslant E((1-\eta)|\Lambda|/4) \geqslant 1 \tag{A2.7}$$

for sufficiently large Λ.

References

Cullen J R and Callen E 1970 *J. Appl. Phys.* **41** 879
—— 1973 *Phys. Rev.* B **7** 397
Des Cloizeaux J 1966 *J. Math. Phys.* **7** 2136
Dyson F J, Lieb E H and Simon B 1978 *J. Stat. Phys.* **18** 335
Falk H and Bruch L W 1969 *Phys. Rev.* **180** 442
Fröhlich J, Israel R, Lieb E H and Simon B 1978 *Commun. Math. Phys.* **62** 1
—— 1980 *J. Stat. Phys.* **22** 297
Fröhlich J and Lieb E H 1978 *Commun. Math. Phys.* **60** 233
Kohn W 1967 *Phys. Rev. Lett.* **19** 789
Lorenz B 1980 *Phys. Status Solidi* (b) **101** 297
—— 1982 *Phys. Status Solidi* (b) **112** K47
Lorenz B and Ihle D 1972 *Phys. Status Solidi* (b) **54** 463
Ruelle D 1969 *Statistical Mechanics* (New York: Benjamin)
Wolf D and Zittartz J 1981 *Z. Phys.* **B 43** 173