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Planar and lamellar antiferromagnetism in Hubbard models

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Abstract. The Hubbard model with extended hoppings on a cubic lattice is shown to have antiferromagnetic phases displaying long-range order, when the temperature is small and the repulsive Coulomb potential is sufficiently strong. Our results are rigorous in the case of the *asymmetric* Hubbard model. Besides chessboard states, stabilizing effects of hopping yield other phases, such as planar and lamellar ones, depending on the relative strength of the hopping coefficients.

1. Introduction

The Hubbard model offers a simplified starting point for the study of electronic properties of condensed matter [Hub]. We can view it as describing electrons moving on a lattice and interacting via on-site repulsion. With $\Lambda \subset \mathbb{Z}^3$ a finite subset of the lattice, the phase space is the Fock space of antisymmetric wavefunctions on Λ for spin-$\frac{1}{2}$ particles, and the Hamiltonian is

$$H_\Lambda = -t \sum_{\substack{\langle x,y\rangle \subset \Lambda \\ \sigma \in \{\uparrow,\downarrow\}}} c^\dagger_{x\sigma} c_{y\sigma} + U \sum_{x\in\Lambda} n_{x\uparrow} n_{x\downarrow} - \mu \sum_{x\in\Lambda} (n_{x\uparrow} + n_{x\downarrow}) \tag{1.1}$$

where $c^\dagger_{x\sigma}$ and $c_{x\sigma}$ are creation and annihilation operators of a spin-σ electron at site $x \in \mathbb{Z}^3$, $n_{x\sigma}$ is the number operator of particles σ at site x and μ is the chemical potential. The first sum is over nearest neighbours and represents the kinetic energy, while the middle sum mimics the screened Coulomb repulsion between particles of different spins. Despite its simplicity, the Hubbard model remains very hard to study (see [Lieb2] for a review of rigorous results).

When the hopping coefficient t is small compared with the interaction U, the inverse temperature β is large, and at half-filling, one expects an antiferromagnetic behaviour, more precisely—a chessboard antiferromagnetism. Namely, an effective antiferromagnetic interaction of strength $-t^2/U$ stabilizes the chessboard pattern where the particles on one sublattice have the same orientation of spin, and the particles on the other sublattice have the opposite orientation. Broken symmetries include translation invariance (which is discrete) and rotation of spins (which is continuous).

The rigorous study of a breaking of continuous symmetry is extremely difficult; antiferromagnetism in the Hubbard model has been proven only for $\beta = \infty$ [Lieb1]. A

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method yielding many interesting results at low temperatures is the 'reflection positivity' [DLS], but it requires that the model has some special properties. Otherwise, we have either to sacrifice some mathematical rigour and use uncontrolled approximations, or to modify the model. We have chosen the latter approach and consider an *asymmetric Hubbard model* where the hopping depends on the spin of the particles. This artificially breaks the rotation symmetry of the spin because a special orientation is favoured; however, the Hamiltonian remains translation invariant, and we shall concentrate on the existence of periodic, non-translation-invariant Gibbs states. Note that allowing some asymmetry is not too misleading. Indeed, the antiferromagnetic phases that appear in our model find their origin in quantum fluctuations which yield a new 'classical' effective interaction, that is the same in both models. However, in our model some other effects of quantum fluctuations are diminished and we get good control of their full contribution; as a result, we have a proof that antiferromagnetism is present at low temperatures for any dimension greater than or equal to two. For symmetric Hubbard models, however, the control over the sum of additional terms is not sufficient. Indeed, we know from an extension of the Mermin–Wagner theorem that no long-range order appears in the two-dimensional model at non-zero temperature [WR, Gho], and antiferromagnetism is only expected for $D \geqslant 3$.

The derivation [Hub] of the model (1.1) neglects hoppings between sites that are not nearest neighbours. While this may be reasonable, in general, it is natural to expect that longer-range hoppings should be taken into account in certain materials, with certain lattice structures. To illustrate the differences that one can expect, we consider a Hubbard model with hopping that extends between first, second and third nearest neighbours on a cubic lattice $\mathbb{Z}^3$; we then show that for some choice of hopping coefficients, antiferromagnetic phases with periodicities other than that the chessboard one, are actually occurring. In order to formulate our results in the form of theorems, we consider asymmetric models, but we expect that they remain true for the symmetric case, for all dimensions greater than or equal to three.

The asymmetric Hubbard model with extended hopping describes a lattice system with two species of particles that we call spin-$\uparrow$ and spin-$\downarrow$ electrons; the Hamiltonian consists of a kinetic term and an on-site repulsion between different particles. Explicitly,

$$H_\Lambda = -\sum_{\substack{x,y\in\Lambda \\ \sigma\in\{\uparrow,\downarrow\}}} t_{xy,\sigma} c^\dagger_{x\sigma} c_{y\sigma} + U\sum_{x\in\Lambda} n_{x\uparrow} n_{x\downarrow} - \mu \sum_{x\in\Lambda} (n_{x\uparrow} + n_{x\downarrow}). \tag{1.2}$$

The hopping coefficients $t_{xy,\sigma}$ are supposed to be translation invariant, and to be non-zero only when x and y are at a distance of 1, $\sqrt{2}$ or $\sqrt{3}$:

$$t_{xy,\sigma} = \begin{cases} t^{(1)}_\sigma & \text{if} \quad \|x-y\| = 1 \\ t^{(2)}_\sigma & \text{if} \quad \|x-y\| = \sqrt{2} \\ t^{(3)}_\sigma & \text{if} \quad \|x-y\| = \sqrt{3} \\ 0 & \text{otherwise} \end{cases} \tag{1.3}$$

and $t^{(1)}_\sigma, t^{(2)}_\sigma, t^{(3)}_\sigma$ are real numbers, so that H is self-adjoint. The standard Hubbard model corresponds to the choice $t^{(k)}_\uparrow = t^{(k)}_\downarrow = \delta_{1,k}$, but we shall consider the parameters in the range $U \gg t^{(k)}_\uparrow \gg t^{(j)}_\downarrow$, corresponding to the assumption that $\uparrow$ species has a smaller mass and thus moves more easily. Quantum states will be defined in the grand-canonical ensemble, and the values of the chemical potential μ will be chosen to correspond to the half-filling situation, where the density of particles at zero temperature is one.

When $t^{(k)}_\downarrow = 0$, $k = 1, 2, 3$, and $t^{(2)}_\uparrow = t^{(3)}_\uparrow = 0$, we obtain the spinless Falicov–Kimball model (see [GM] for a review). For a chemical potential μ chosen so that the model is

symmetric with respect to the hole–particle transformation, Kennedy and Lieb proved that chessboard phases occur for any $t_\uparrow^{(1)} \neq 0$ [KL]†; when $t_\uparrow^{(1)}/U$ is small, this persists for values of μ close to the symmetry point [LM]. Other phases with higher periodicity also appear, as indicated by perturbative studies in powers of $t_\uparrow^{(1)}/U$ up to order four [GJL, Ken1, DFF], and to higher orders [Ken2, HK].

Clearly, there is no long-range order at high temperature (βU and $\beta|t_\sigma^{(j)}|$ small), and the free energy is real analytic in β and μ. This also holds under the sole assumption $\beta \max_{j,\sigma} |t_\sigma^{(j)}|$ is small, or $\beta \max_{j,\sigma} |t_\sigma^{(j)}|^2/U$ is small [KL] (see also [Uel] for a generalization that includes the standard Hubbard model).

When the hopping coefficients are small compared with the Coulomb repulsion U, it is natural to consider the model as a perturbation of a classical model that consists only of the interaction part plus the term with the chemical potential multiplied by the number of particles. These operators are diagonal in the basis of lattice site occupation numbers. Since this classical model involves only on-site terms, it is easy to check that the free energy is analytic for all β and all μ. What is the effect of the kinetic term treated as a quantum perturbation? The answer is that the kinetic operator yields an effective interaction between the particles that is classical in the sense that it is diagonal with respect to the basis in lattice site occupation numbers. This interaction, with a strength $t_{xy,\uparrow}^2 + t_{xy,\downarrow}^2$, favours pairs of opposite spins on sites x and y. Two general methods have been proposed to treat this effect in a rigorous fashion [DFFR, KU]. With their help one can obtain the properties of full quantum Gibbs states at sufficiently low temperatures and actually prove that they follow from the effective interaction. In fact, it is sufficient to take $\beta t^2/U$ large enough and to assume that other quantum effects are negligible (see the next section for a detailed formulation of a corresponding sufficient condition).

Consequently, the asymmetric extended Hubbard model, at sufficiently low temperatures, exhibits non-translation-invariant phases with various periodicities. For some values of the hopping coefficients, one obtains a chessboard order with a structure factor $S(k)$ that differs from zero only for $k = (\pi, \pi, \pi)$. For other values, the structure factor is non-vanishing only for $k = (\pi, 0, 0)$, $(0, \pi, 0)$ or $(0, 0, \pi)$—representing a situation where ferromagnetic planes with alternating spins are superimposed. Finally, we also observe cases where $S(k)$ is supported by $k \in \{(\pi, \pi, 0), (\pi, 0, \pi), (0, \pi, \pi)\}$, yielding a lamellar structure, where ferromagnetic lines are placed in antiferromagnetic order.

In section 2 we explain the ideas of [KU] for special case of models with on-site interactions and a small hopping operator. For these models, the general theory of [KU] is strongly simplified, making it worth presenting the crucial conditions and statements explicitly. This section can be skipped by the readers only interested in the application to the extended Hubbard model. In section 3, we discuss the asymmetric Hubbard model with extended hopping and show the existence of various antiferromagnetic phases.

2. Quantum perturbation of the model with on-site interactions

Here, we reformulate the theory of [KU] (see also [DFFR]) in the case of lattice models with an on-site interaction and small hopping term. We emphasize that both [DFFR] and [KU] apply to a much broader class of models than those considered in the present section. The interaction is assumed to be diagonal in the basis of classical configurations, so we start with

† Actually, their results also include the case where $t_\uparrow^{(3)} \neq 0$, since this represents hopping of electrons from one sublattice onto the other one.

the description of the corresponding classical system.

2.1. A general model with on-site interactions

Let Σ be a finite set describing the internal degrees of freedom of particles, and $\boldsymbol{N} = \{0, 1, \ldots, N\}$, where N is finite (it represents the maximum number of particles of a given species at a given site). The configuration on each site is an element of the finite set $\Omega = \boldsymbol{N}^{\Sigma}$; $|\Omega| = (N+1)^{|\Sigma|} =: S$. For fermion systems we actually have $N = 1$, but we can also consider boson systems with a hard-core condition that prevents more than N bosons of a given species from occupying the same site. The restriction to finite on-site configuration space is purely technical and can be removed. A *classical configuration* n_Λ is an element of Ω^Λ, where $\Lambda \subset \mathbb{Z}^\nu$ is the volume of the system, $\Omega^\Lambda \ni n = \{n_{x\sigma}; x \in \Lambda, \sigma \in \Sigma\}$ with $n_{x\sigma} \in \boldsymbol{N}$. We also write n_x for the vector $(n_{x\sigma}, \sigma \in \Sigma)$. The interaction is given by a collection of on-site potentials $(\Phi_x)_{x\in\mathbb{Z}^\nu}$, where $\Phi_x : \Omega \to \mathbb{R}$.

Here we consider a simple case involving only on-site interaction that is diagonal in the basis of lattice site occupation numbers and select a set of low-energy configurations. More precisely, we consider Hamiltonians of the form

$$H = V + T \tag{2.1}$$

with a potential part V and a hopping operator T. We introduce the following assumption on the potential part.

Assumption 1. *The potential part V of the Hamiltonian is given as $V = \sum V_x$ with*

$$V_x\,|n\rangle = \Phi(n_x)\,|n\rangle$$

in terms of an (translation invariant) on-site interaction Φ.

Moreover, we want to assume that there exists a set $G_0 \subset \Omega$, representing the low-energy states, such that Φ attains its minimum for a configuration in G_0 with other values on G_0 differing only slightly and has a large gap to the remaining values on $\Omega \setminus G_0$.

Assumption 2. *There exist a set $G_0 \subset \Omega$ and constants $\Delta_0 > 0$ and $\delta_0 < \infty$ such that*

$$\max_{g_x, g'_x \in G_0} \left|\Phi(g_x) - \Phi(g'_x)\right| \leqslant \delta_0 \tag{2.2}$$

and

$$\Phi(n_x) - \max_{g_x \in G_0} \Phi(g_x) \geqslant \Delta_0 \qquad \text{for all} \quad n_x \notin G_0. \tag{2.3}$$

Later on, we shall suppose that δ_0/Δ_0 is smaller than a small threshold that depends on the range of the effective interaction—see the assumptions of theorem 2.1.

We need an assumption ensuring that the quantum fluctuations increase the classical energy; this is achieved by the following.

Assumption 3.

(a) For any $g_x \in G_0$ and any $\sigma' \in \Sigma$, the configurations $(g_{x\sigma} \pm \delta_{\sigma\sigma'})$ do not belong to G_0.
(b) For any $g_x \in G_0$ and any $\sigma', \sigma'' \in \Sigma$, the configurations $(g_{x\sigma} + \delta_{\sigma\sigma'} + \delta_{\sigma\sigma''})$ and $(g_{x\sigma} - \delta_{\sigma\sigma'} - \delta_{\sigma\sigma''})$ do not belong to G_0. (This assumption will be necessary only when we consider the effective potential up to order four.)

Now, we introduce the set of low-energy configurations: for any $A \subset \mathbb{Z}^\nu$ we define

$$G_A = \{g \in \Omega^A : g_x \in G_0 \text{ for all } x \in A\} = G_0^A \tag{2.4}$$

(where G stands for 'ground states' even though these configurations are not necessarily absolutely minimizing the potential V). When $A = \mathbb{Z}^\nu$, we write $G \equiv G_0^{\mathbb{Z}^\nu}$.

The Hilbert space $\mathcal{H}_\Lambda$ is the Hilbert space spanned by classical configurations. The hopping operator T_Λ is

$$T_\Lambda = -\sum_{\substack{x,y\in\Lambda \\ \sigma\in\Sigma}} t_{xy,\sigma} c^\dagger_{x\sigma} c_{y\sigma} \tag{2.5}$$

where $c^\dagger_{x\sigma}$ and $c_{y\sigma}$ are the creation and annihilation operators whose definition is recalled below separately for bosons and fermions.

Assumption 4. *The hopping coefficients $t_{xy,\sigma} \in \mathbb{C}$ are such that $t^*_{yx,\sigma} = t_{xy,\sigma}$, they are invariant under translations, $t_{xy,\sigma} = 0$ if $\|x - y\| > r$ for some finite distance r, and $t_{xx,\sigma} = 0$ (i.e. T_Λ does not contain diagonal terms).*

To characterize the norm of the hopping operator, we introduce

$$\varepsilon = \max_{x,y,\sigma} |t_{xy,\sigma}|/\Delta_0. \tag{2.6}$$

At this stage the discussion becomes simpler if we treat fermions and bosons separately.

2.2. Bosons

Let us describe the action of creation and annihilation operators on states in occupation numbers of position operators.

$$c^\dagger_{x\sigma} |n_\Lambda\rangle = \begin{cases} \sqrt{n_{x\sigma}+1}\, |n'_\Lambda\rangle & \text{with} \quad n'_{y\sigma'} = n_{y\sigma'} + \delta_{xy}\delta_{\sigma\sigma'} \qquad \text{if} \quad n_{x\sigma} < N \\ 0 & \qquad\qquad\qquad\qquad\qquad\quad \text{if} \quad n_{x\sigma} = N \end{cases}$$

$$c_{x\sigma} |n_\Lambda\rangle = \sqrt{n_{x\sigma}}\, |n'_\Lambda\rangle \qquad \text{with} \quad n'_{y\sigma'} = n_{y\sigma'} - \delta_{xy}\delta_{\sigma\sigma'}.$$

The effect of moves of quantum particles can be combined with the diagonal term to yield an effective interaction, that can be expressed, when T_Λ is small, as a perturbation series in coefficients $\{t_{xy,\sigma}\}$.

Let us first note that, for any $g \in G$, a move of a particle σ from x to y increases the energy by

$$\phi_{xy,\sigma}(g) = \begin{cases} \Phi(\bar g_x) + \Phi_y(\bar g_y) - \Phi(g_x) - \Phi_y(g_y) & \text{if} \quad g_{x\sigma} > 0 \quad \text{and} \quad g_{y\sigma} < N \\ \infty & \text{otherwise} \end{cases} \tag{2.7}$$

where

$$\bar g_{x\sigma'} = g_{x\sigma'} - \delta_{\sigma\sigma'}$$

$$\bar g_{y\sigma'} = g_{y\sigma'} + \delta_{\sigma\sigma'}.$$

Note that $\phi_{xy,\sigma} \neq \phi_{yx,\sigma}$ in general. From assumption 3, this quantity is positive: $\phi_{xy,\sigma}(g) \geqslant 2\Delta_0$.

It turns out that, in the cases considered here, not all moves of quantum particles contribute significantly to the effective potential. It is useful to select a subset $\Sigma^* \subset \Sigma$ of those particles that we have taken into account. The smaller the set Σ^* we chose, the easier is the calculation

of the effective potential (fewer terms). On the other hand, the set Σ^* must be big enough, so that the overall contribution of hoppings that do not belong to Σ^* is small; see the definition (2.19), and the condition that ε^* should be small in theorem 2.1.

The effective interaction in lowest orders reads

$$\Psi = \Psi^{(2)} + \Psi^{(3)} + \Psi^{(4)} \tag{2.8}$$

$$\Psi^{(k)} = \sum_{A \subset \Lambda} \Psi_A^{(k)}. \tag{2.9}$$

Here $\Psi^{(k)}$ represents the contributions due to k transitions. For any $A \subset \mathbb{Z}^\nu$, and any $n_A \notin G_A$, we set

$$\Psi_A^{(k)}(n_A) = 0 \qquad k = 2, 3, 4. \tag{2.10}$$

For configurations $g \in G$, the first term contributing to the effective potential is

$$\Psi^{(2)}_{\{x,y\}}(g) = -\sum_{\sigma \in \Sigma^*} |t_{xy,\sigma}|^2 \left[\frac{g_{x\sigma}(g_{y\sigma}+1)}{\phi_{xy,\sigma}(g)} + x \leftrightarrow y \right]. \tag{2.11}$$

The term '$x \leftrightarrow y$' stands for the previous expression, but with x and y interchanged. This formula is a particular case of the term (2.8) from [KU]. It is obtained there by using a version of Feynman–Kac expansion and considering a particle $\sigma \in \Sigma^*$ hopping from x to y and returning back after time interval τ. This yields the contribution

$$-|t_{xy,\sigma}|^2 g_{x\sigma}(g_{y\sigma}+1) \int_0^\infty \mathrm{d}\tau \, \mathrm{e}^{-\tau \phi_{xy,\sigma}(g)}. \tag{2.12}$$

Considering also hopping first from y to x and then back, we get (2.11). The same can be obtained by other perturbative techniques—see, for example, the use of Lie–Schwinger expansion in [DFFR].

The next terms ($\Psi^{(3)}$ and $\Psi^{(4)}$) can be read directly from (2.9) and (2.10) in [KU]. Thus, for x, y, z distinct, we obtain

$$\Psi^{(3)}_{\{x,y,z\}}(g) = -\sum_{\sigma \in \Sigma^*} \left\{ t_{yx,\sigma} t_{zy,\sigma} t_{xz,\sigma} \left[\frac{g_{x\sigma}(g_{y\sigma}+1)(g_{z\sigma}+1)}{\phi_{xy,\sigma}(g)\phi_{xz,\sigma}(g)} + \frac{g_{x\sigma}(g_{y\sigma}+1)g_{z\sigma}}{\phi_{xy,\sigma}(g)\phi_{zy,\sigma}(g)} \right] \right.$$
$$\left. + \text{cyclic permutations of } (x, y, z) \right\}. \tag{2.13}$$

The first term corresponds to the three hoppings $x \to y$, $y \to z$ and $z \to x$; and the second term to $x \to y$, $z \to x$ and $y \to z$. If x, y, z are not distinct, the term $\Psi^{(3)}$ vanishes.

The fourth order is more intricate, and is not explicitly written down here. A preprint is available from the authors, or can be retrieved from the Internet (for example, at http://www.cts.cuni.cz/~kotecky/publications.html).

2.3. Fermions

To define the creation and annihilation operators, we need to specify an order on the configuration space. So we assume that an order is given on Λ, and also on Σ, and we define

$$(y, \sigma') < (x, \sigma) \quad \Longleftrightarrow \quad y < x \quad \text{or} \quad y = x \quad \text{and} \quad \sigma' < \sigma.$$

Then

$$c^{\dagger}_{x\sigma}\,|n_\Lambda\rangle = (1-n_{x\sigma})(-1)^{\sum_{(y,\sigma')<(x,\sigma)} n_{y\sigma'}}\,|n'_\Lambda\rangle \qquad \text{with} \quad n'_{y\sigma'} = n_{y\sigma'} + \delta_{xy}\delta_{\sigma\sigma'}$$

$$c_{x\sigma}\,|n_\Lambda\rangle = n_{x\sigma}(-1)^{\sum_{(y,\sigma')<(x,\sigma)} n_{y\sigma'}}\,|n'_\Lambda\rangle \qquad \text{with} \quad n'_{y\sigma'} = n_{y\sigma'} - \delta_{xy}\delta_{\sigma\sigma'}.$$

The increase of energy due to the move of a fermion from x to y takes the form (compare with (2.7) for bosons)

$$\phi_{xy,\sigma}(g) = \begin{cases} \Phi(\bar g_x) + \Phi_y(\bar g_y) - \Phi(g_x) - \Phi_y(g_y) & \text{if} \quad g_{x\sigma}=1 \quad \text{and} \quad g_{y\sigma}=0 \\ \infty & \text{otherwise} \end{cases} \tag{2.14}$$

where $\bar g_{x\sigma}=0$, $\bar g_{y\sigma}=1$ and $\bar g_{z\sigma'} = g_{z\sigma'}$ for $(z,\sigma') \neq (x,\sigma), (y,\sigma)$.

The effective interaction is similar to that of bosons, except for the multiplication by the number of particles and the signs due to anticommutation relations

$$\Psi^{(2)}_{\{x,y\}}(g) = -\sum_{\sigma\in\Sigma^*} |t_{xy,\sigma}|^2 \left[\frac{1}{\phi_{xy,\sigma}(g)} + \frac{1}{\phi_{yx,\sigma}(g)}\right]. \tag{2.15}$$

The next order is (still supposing x, y, z to be distinct, otherwise it is zero)

$$\Psi^{(3)}_{\{x,y,z\}}(g) = -\sum_{\sigma\in\Sigma^*} \left\{ t_{yx,\sigma}t_{zy,\sigma}t_{xz,\sigma}\left[\frac{1}{\phi_{xy,\sigma}(g)\phi_{xz,\sigma}(g)} - \frac{1}{\phi_{xy,\sigma}(g)\phi_{zy,\sigma}(g)}\right] \right.$$
$$\left. +\text{cyclic permutations of } (x,y,z) \right\}. \tag{2.16}$$

As before, the fourth order is very involved and has been hidden in a preprint.

It is interesting to compare the effective potential for bosons and fermions. For the Falicov–Kimball model, differences were put forward in [GMMU]. Here, one main difference comes from the fact that there can be more than one boson in the same quantum state (spin) at a given site. However, suppose we have hard-core bosons with $N=1$; then the formulae would be identical, except for signs. At order two, there is no difference. However, a minus sign shows up in (2.16), while its bosonic counterpart (2.13) is positive. In the path space formulation, this corresponds to a permutation of two fermions. The interpretation of the effective potential as 'to maximize quantum fluctuations' (see [KU]) does not make sense in the case of fermions, since the very possibility of making such fluctuations actually *decreases* the 'probability' of a configuration. It is somewhat amazing that it is still possible to carry out the method of [KU] in this situation.

2.4. Conditions for stability

Having defined the effective potential in both bosonic and fermionic situations, we now introduce sufficient conditions to ensure that the low-temperature phases are selected by the effective interaction, and that other quantum or thermal fluctuations are negligible.

Let us define the R-neighbourhood $U(x)$ of a site $x \in \mathbb{Z}^\nu$, with integer or half-integer radius R, by

$$U(x) = \begin{cases} \{y \in \mathbb{Z}^\nu : |y-x| \leqslant R\} & \text{if} \quad R \in \mathbb{N} \\ \{y \in \mathbb{Z}^\nu : |y-(x_1+\frac12,\dots,x_\nu+\frac12)| \leqslant R\} & \text{otherwise.} \end{cases} \tag{2.17}$$

To express our next assumption, we rewrite the effective interaction as an equivalent 'block interaction', i.e. we introduce $\Upsilon = (\Upsilon_x)_{x\in\mathbb{Z}^\nu}$, where $\Upsilon_x : \Omega^{U(x)} \to \mathbb{R}$, such that for any finite torus Λ (i.e. a rectangle with periodic boundary conditions), and any $n \in \Omega^\Lambda$, we have

$$\sum_{x\in\Lambda} \Phi(n_x) + \sum_{A\subset\Lambda} \Psi_A(n_A) = \sum_{x\in\Lambda} \Upsilon_x(n_{U(x)}) + C|\Lambda| \tag{2.18}$$

with C a constant. It means that $\Phi + \Psi$ and Υ yield the same Gibbs states. However, if suitably chosen, the potential Υ is easier to study. We state our conditions for the equivalent potential Υ.

Assumption 5. *There exists a suitable block interaction Υ, of range R such that $R^\nu \leqslant \Delta_0/\delta_0$, that is equivalent to $\Phi + \Psi$ and such that:*

(a) For any $x \in \Lambda$ and any n with $n_x \notin G_0$, we have

$$\Upsilon_x(n_{U(x)}) - \max_{g \in G} \Upsilon_x(g_{U(x)}) \geqslant \tfrac{1}{2}\Delta_0.$$

(b) There exists a finite subset $D \subset G$ of periodic configurations, and a strictly positive number Δ, such that:

- *any two elements of D are related by a translation, a reflection or a rotation;*
- *there is e_0 such that for all $x \in \mathbb{Z}^\nu$ and all $d_{U(x)} \in D_{U(x)}$, we have $\Upsilon_x(d_{U(x)}) = e_0$;*
- *for any $x \in \Lambda$ and any n with $n_{U(x)} \notin D_{U(x)}$, we have*

$$\Upsilon_x(n_{U(x)}) - e_0 \geqslant \Delta.$$

The set D contains classical configurations, that are 'stable' in the sense that at sufficiently low temperature, there exist Gibbs states that are close to projectors onto these configurations (see theorem 2.1 below). The condition that all elements of D are related by symmetries was not given in [DFFR, KU], but this simplifies the statement of the theorem.

The effective potential takes into account only the movement of particles with internal degrees of freedom in Σ^*, and we have to check that the effect of other 'quantum fluctuations' is negligible. To control what we have neglected, we introduce the parameter ε^*, that we shall require to be small in theorem 2.1,

$$\varepsilon^* = \max_{\substack{x,y \in \mathbb{Z}^\nu \\ \sigma \notin \Sigma^*}} \frac{|t_{xy,\sigma}|^2}{\Delta\Delta_0}. \tag{2.19}$$

Basically, all quantum lattice models show quantum fluctuations leading to effective interactions. The important question is whether other quantum effects may destabilize phases, i.e. whether there is 'quantum instability'. We introduce a parameter $\varepsilon^\perp$ that measures off-diagonal terms; this parameter will be supposed to be small in theorem 2.1. Let

$$\mathcal{T}(g_A, g'_A) = \left\{ (x_1, y_1, \sigma_1; \ldots; x_m, y_m, \sigma_m) : \langle g_A | \prod_{j=1}^m c^\dagger_{x_j\sigma_j} c_{y_j\sigma_j} | g'_A \rangle = \pm 1 \right\} \tag{2.20}$$

where $A = \cup_{j=1}^m \{x_j, y_j\}$. Then we define

$$\varepsilon^\perp = \frac{\Delta_0}{\Delta} \max_{\substack{g_A, g'_A \in G_A \\ g_A \neq g'_A}} \sup_{(x_1,y_1,\sigma_1;\ldots;x_m,y_m,\sigma_m) \in \mathcal{T}(g_A,g'_A)} \prod_{j=1}^m \frac{|t_{x_j y_j,\sigma_j}|}{\Delta_0}. \tag{2.21}$$

Here, we set $A = \cup_{j=1}^m \{x_j, y_j\}$.

Note that $\varepsilon^\perp$ cannot be made sufficiently small in the standard Hubbard model, and indeed the Mermin–Wagner theorem indicates that long-range order is destroyed by other quantum fluctuations at dimension two [WR, Gho].

2.5. Properties of low-temperature phases

Our results concern the existence of Gibbs states describing pure phases; let us start with a few mathematical definitions.

Let $\mathcal{K}$ be the set of operators that are given by finite polynomials in creation and annihilation operators. Each $K \in \mathcal{K}$ is a local operator. Gibbs states are functionals on $\mathcal{K}$; for each local operator we define the limit, whenever it exists,

$$\langle K \rangle = \lim_{\Lambda \nearrow \mathbb{Z}^\nu} \frac{\operatorname{Tr} K \, \mathrm{e}^{-\beta H_\Lambda}}{\operatorname{Tr} \mathrm{e}^{-\beta H_\Lambda}}. \tag{2.22}$$

Here, the limit is taken with any sequence of finite rectangles $(\Lambda_n)_{n \geqslant 0}$, whose sizes are multiples of the periods of configurations of D, and with periodic boundary conditions, such that $\Lambda_n \subsetneq \Lambda_{n+1}$. We say that the Gibbs state exists in the thermodynamic limit if the limit exists for all such sequences and all $K \in \mathcal{K}$.

We say that a Gibbs state is *thermodynamically stable* if it is insensitive to perturbations and that it is *pure* if it is a limit of thermodynamically stable phases (see [KU] for more explanations).

Theorem 2.1. *Suppose that assumptions 1–5 are satisfied. Then for all $\eta > 0$, there exist constants $\varepsilon_0 = \varepsilon_0(\nu, S, r, \eta) > 0$ and $\beta_0 = \beta_0(\nu, S, r, \eta) < \infty$ such that if $\varepsilon, \varepsilon^*, \varepsilon^\perp \leqslant \varepsilon_0$ and $\beta\Delta \geqslant \beta_0$, there exist $|D|$ infinite-volume, pure Gibbs states $\{\langle\cdot\rangle^d\}_{d \in D}$, with*

$$\big|\langle K \rangle^d - \langle d| \, K \, |d\rangle\big| \leqslant \eta |\operatorname{supp} K| \|K\|. \tag{2.23}$$

Each $\langle\cdot\rangle^d$ is exponential clustering,

$$\langle K K' \rangle^d - \langle K \rangle^d \langle K' \rangle^d \leqslant |\operatorname{supp} K| |\operatorname{supp} K'| \exp\big(-\operatorname{dist}(\operatorname{supp} K, \operatorname{supp} K')/\xi_d\big) \tag{2.24}$$

for a $\xi_d < \infty$ (independent of K, K').

The Gibbs state obtained with periodic boundary conditions is a linear combination of these pure Gibbs states,

$$\langle\cdot\rangle^{\mathrm{per}} = \frac{1}{|D|} \sum_{d \in D} \langle\cdot\rangle^d. \tag{2.25}$$

Proof. This theorem essentially follows from [KU]. Assumptions here are stronger than those of [KU]. There is a (minor) extension, however: we supposed in [KU] that the quantum perturbation only acts on connected sets, while here the sites x, y such that $t_{xy,\sigma} \neq 0$ are not necessarily nearest neighbours. Furthermore, an effort has been made here to get 'dimension-free' parameters, by dividing some quantities by Δ_0 when appropriate; this allows one to have constants ε_0 and β_0 independent of Φ, unlike in [KU]. A careful but straightforward check of the developments of [KU] proves theorem 2.1.

We supposed here that the configurations of D are related by symmetries. This implies that the function $f^\beta(d)$ in theorem 2.2 of [KU] is constant on D. Consequently, each element of D leads to a pure Gibbs state. □

3. Hubbard model with extended hoppings

Our abstract theory of section 2 finds an interesting application with fermion systems described by the Hubbard model (1.2). When the temperature is high, or if the interaction U is strong, there is a unique phase, which is translation invariant and shows exponential decay of

correlations. The results of [KL, Uel] can be summarized in the following manner: let $\Delta_0 = \min(\mu, U-\mu) > 0$ and $t = \max_{j,\sigma} |t_\sigma^{(j)}|$. Then for $\beta t < \varepsilon_1$, or $\beta t^2/\Delta_0 < \varepsilon_2(1 - Kt/\Delta_0)$ (for some $\varepsilon_1, \varepsilon_2 > 0$ and $K < \infty$), the Gibbs state is unique, exponentially clustering and stable against perturbations.

The structure factor $S(k)$ is the Fourier transform of the correlation functions. With $k \in [0, 2\pi)^3$, we set

$$S(k) = \lim_{\Lambda \nearrow \mathbb{Z}^\nu} \frac{1}{|\Lambda|^2} \sum_{x,y\in\Lambda} \mathrm{e}^{-\mathrm{i}k(x-y)} \langle (n_{x\uparrow} - n_{x\downarrow})(n_{y\uparrow} - n_{y\downarrow}) \rangle^{\mathrm{per}}. \tag{3.1}$$

Our aim in this paper is to show that phases displaying long-range order occur at low temperature; their existence can be proven in the case of *asymmetric* models.

The on-site term

$$U \sum n_{x\uparrow} n_{x\downarrow} - \mu \sum (n_{x\uparrow} + n_{x\downarrow})$$

has a gap: if $0 < \mu < U$, we define $G_0 = \{\uparrow, \downarrow\}$, and assumption 2 holds with $\Delta_0 = \min(\mu, U-\mu)$ and $\delta_0 = 0$. Assumptions 3 and 4 are also trivially satisfied.

3.1. Computation of the effective potential

We restrict our computations to the lowest order (in powers of t/U). Since we shall assume that hoppings of $\downarrow$-particles are much smaller than those for $\uparrow$-particles, we take $\Sigma^* = \{\uparrow\}$. It is useful to simplify the notation and to introduce $t_j := t_\uparrow^{(j)}$, $j = 1, 2, 3$. We also suppose t_j to be real numbers.

At second order, the effective interaction Ψ acts on pairs of sites at a distance less than or equal to $\sqrt{3}$, and is given by (2.15); explicitly,

$$\Psi_{\{x,y\}}(g) = \begin{cases} -t_j^2/U & \text{if} \quad \|x-y\| = \sqrt{j} \quad \text{and} \quad g_{\{x,y\}} \in \{(\uparrow,\downarrow),(\downarrow,\uparrow)\} \\ 0 & \text{otherwise.} \end{cases} \tag{3.2}$$

It is clear that antiferromagnetic pairs are favoured; however, we have to face a frustrated system. It is useful to inscribe this interaction in cubes of size 1 (i.e. with eight sites); therefore we define the equivalent interaction Υ to be

$$\begin{aligned} \Upsilon_x(n_{U(x)}) = {} & \frac{1}{8} \sum_{y\in U(x)} \big[\Phi_y(n_y) - \min_{g_y \in G_0} \Phi_y(g_y) \big] + \frac{1}{4} \sum_{\substack{\{y,z\}\subset U(x) \\ \|y-z\|=1}} \Psi_{\{y,z\}}(n_{\{y,z\}}) \\ & + \frac{1}{2} \sum_{\substack{\{y,z\}\subset U(x) \\ \|y-z\|=\sqrt{2}}} \Psi_{\{y,z\}}(n_{\{y,z\}}) + \sum_{\substack{\{y,z\}\subset U(x) \\ \|y-z\|=\sqrt{3}}} \Psi_{\{y,z\}}(n_{\{y,z\}}). \end{aligned} \tag{3.3}$$

Its range is $R = \frac{1}{2}$, see (2.17).

3.2. Analysis of the effective potential

To understand the low-temperature behaviour we have to look at configurations that minimize the effective potential. Only cubes where each site belongs to $\{\uparrow, \downarrow\}$ need to be considered, otherwise the energy increases by a large number μ or $U - \mu$.

The effective potential is symmetric under spin flip† and is rotation invariant. Up to spin flip and rotations, there are 14 configurations to be taken into account. In tables 1 and 2 we have written the effective energy for all of these configurations; in the pictures, '●' stands for '↑', and '•' stands for '↓'.

Table 1. Effective energy of cubes with one particle per site, and negative magnetization (i.e. more spins ↓ than spins ↑).

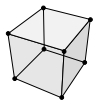
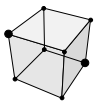
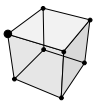
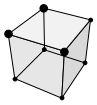
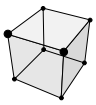
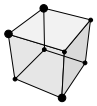
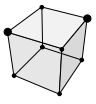
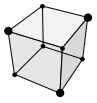
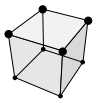
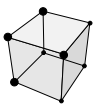
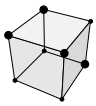
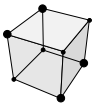
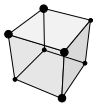
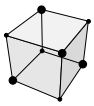
Config.	No	Effective energy	config.	No	Effective energy
	1	0		5	$-\frac{1}{U}[\frac{3}{2}t_1^2 + 3t_2^2]$
	2	$-\frac{1}{U}[\frac{3}{4}t_1^2 + \frac{3}{2}t_2^2 + t_3^2]$		6	$-\frac{1}{U}[\frac{5}{4}t_1^2 + \frac{7}{2}t_2^2 + 3t_3^2]$
	3	$-\frac{1}{U}[t_1^2 + 3t_2^2 + 2t_3^2]$		7	$-\frac{1}{U}[\frac{7}{4}t_1^2 + \frac{7}{2}t_2^2 + t_3^2]$
	4	$-\frac{1}{U}[\frac{3}{2}t_1^2 + 2t_2^2 + 2t_3^2]$		8	$-\frac{1}{U}[\frac{9}{4}t_1^2 + \frac{3}{2}t_2^2 + 3t_3^2]$

Table 2. Effective energy of cubes with one particle per site, and zero magnetization (i.e. equal number of spins ↓ and ↑).

Config.	No	Name	Effective energy	Config.	No	Name	Effective energy
	9	Planar	$-\frac{1}{U}[t_1^2 + 4t_2^2 + 4t_3^2]$		12	Enigmatic	$-\frac{1}{U}[\frac{3}{2}t_1^2 + 3t_2^2 + 4t_3^2]$
	10		$-\frac{1}{U}[2t_1^2 + 3t_2^2 + 2t_3^2]$		13	Lamellar	$-\frac{1}{U}[2t_1^2 + 4t_2^2]$
	11		$-\frac{1}{U}[\frac{3}{2}t_1^2 + 4t_2^2 + 2t_3^2]$		14	Chessboard	$-\frac{1}{U}[3t_1^2 + 4t_3^2]$

The 'zero-temperature' phase diagram is depicted in figure 1. There are three domains where one of the above configurations is minimum, namely the chessboard, planar and lamellar configurations. On the line that separates the chessboard and planar region, the enigmatic configuration is present. Between the chessboard and lamellar regions configuration no 10 appears, and configuration no 11, with an equal number of ↑ and ↓ spins, appears on the boundary between planar and lamellar regions. All other configurations have strictly greater effective energy than the minimum among those six above, whatever the hopping coefficients.

How many such configurations are there over the whole volume, for different values of t_1, t_2, t_3?

Inside the three domains with a unique minimizing cube (up to rotations), there are a finite number of ground configurations defining (separately for each domain) the set D: chessboard ($|D| = 2$), planar ($|D| = 6$), lamellar ($|D| = 6$). Assumption 5 is satisfied in these regions

† Although the asymmetric Hubbard model is not!

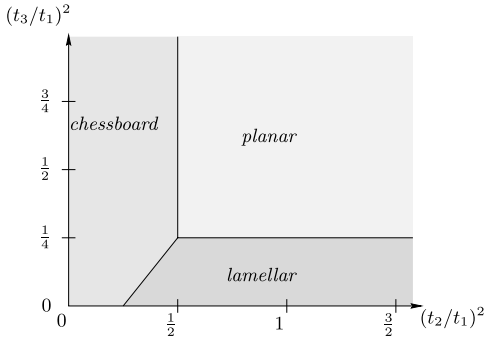


Figure 1. Zero-temperature 'phase diagram' of the asymmetric Hubbard model with extended hopping. The enigmatic configuration appears in between the chessboard and planar ones.

with a constant Δ that is vanishing when approaching the boundary of the region. While there is infinite degeneracy between chessboard and lamellar as well as between planar and lamellar regions, on the line separating the chessboard and planar region, there coexist only eight corresponding configurations with an additional eight enigmatic ones. Consequently, the transition from the planar to the chessboard region is first order and can be studied rigorously by the methods of [KU] and [DFFR]. However, one would have to make additional evaluations with the help of third- and fourth-order terms to determine whether the system passes from planar to chessboard regions directly or whether there is an additional enigmatic region sandwiched in between (and to clarify the number of corresponding transitions). In any case, using Pirogov–Sinai theory one can prove that there is a finite number of transitions on the way from planar to chessboard regions and all of them are first order.

As for transitions between other domains, we cannot say anything definite. It is reasonable to expect that the transitions is continuous, but it could also happen that higher-order terms in the effective potential select a finite number of configurations that would appear through first-order transitions between the domains.

We actually have inspected the effective potential at order three (see (2.16)); the equations for the coexistence lines are slightly modified, but the degeneracies remain the same. No conclusion can be drawn.

In order to state our theorem on the asymmetric Hubbard model with extended hopping, we define three subdomains in the phase diagram (see figure 2):

$$\mathcal{M}^{\gamma}_{\mathrm{cb}} = \left\{(a,b) \in \mathbb{R}^2 : a \leqslant \tfrac{1}{2} - \gamma \text{ and } b \geqslant a - \tfrac{1}{4} + \gamma\right\}$$

$$\mathcal{M}^{\gamma}_{\mathrm{pl}} = \left\{(a,b) \in \mathbb{R}^2 : a \geqslant \tfrac{1}{2} + \gamma \text{ and } b \geqslant \tfrac{1}{4} + \gamma\right\}$$

$$\mathcal{M}^{\gamma}_{\mathrm{lam}} = \left\{(a,b) \in \mathbb{R}^2 : b \leqslant \tfrac{1}{4} - \gamma \text{ and } b \leqslant a - \tfrac{1}{4} - \gamma\right\}.$$

In these domains assumption 5 is satisfied with a constant Δ that can be computed explicitly by comparing terms in tables 1 and 2. It turns out to be proportional to $\gamma \frac{t_1^2}{U}$. Recall that $t_j = t_{\uparrow}^{(j)}$.

Theorem 3.1. *Suppose $0 < \mu < U$, $t_1 \neq 0$, and $\eta > 0$. Then there exist constants $\varepsilon_0 > 0$ and $\beta_0 < \infty$ such that for all $\gamma > 0$: whenever the hopping parameters $\{t_{xy,\sigma}\}$ and inverse temperature β are such that*

$$(|t_1| + |t_2| + |t_3|)/U \leqslant \varepsilon_0 \min(\mu/U, 1 - \mu/U)$$

$$\frac{|t_j t_{\downarrow}^{(j)}| + |t_{\downarrow}^{(j)}|^2}{t_1^2} \leqslant \varepsilon_0 \gamma \min(\mu/U, 1 - \mu/U) \qquad j = 1, 2, 3$$

$$\beta \geqslant \beta_0 U/\gamma t_1^2$$

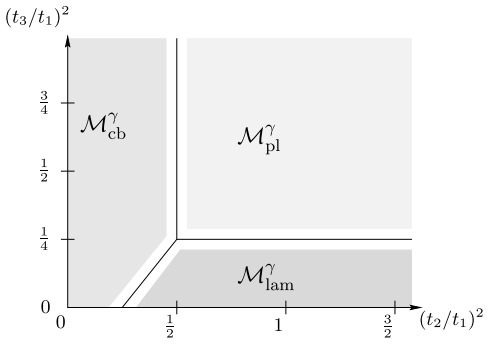


Figure 2. Domains of the phase diagram where low-temperature states can be rigorously described when hoppings are small. More can be said concerning the transition from $\mathcal{M}^{\gamma}_{\rm cb}$ to $\mathcal{M}^{\gamma}_{\rm pl}$: there are a finite number of first-order phase transitions, possibly by jumping to states close to the enigmatic configuration.

the following statements hold.

- *If* $\left((t_2/t_1)^2, (t_3/t_1)^2\right) \in \mathcal{M}^{\gamma}_{\rm cb}$*, there exist two pure Gibbs states with exponential decay of correlations, and the structure factor satisfies*

$$S(\pi,\pi,\pi) > 1-\eta \qquad |S(0,0,0)| < \eta$$

$$S(k) = 0 \qquad \text{if} \quad k \neq (\pi,\pi,\pi), (0,0,0).$$

- *If* $\left((t_2/t_1)^2, (t_3/t_1)^2\right) \in \mathcal{M}^{\gamma}_{\rm pl}$*, there exist six pure Gibbs states with exponential decay of correlations, and the structure factor satisfies*

$$S(\pi,0,0) = S(0,\pi,0) = S(0,0,\pi) > 1-\eta \qquad |S(0,0,0)| < \eta$$

$$S(k) = 0 \qquad \text{if} \quad k \neq (\pi,0,0), (0,\pi,0), (0,0,\pi), (0,0,0).$$

- *If* $\left((t_2/t_1)^2, (t_3/t_1)^2\right) \in \mathcal{M}^{\gamma}_{\rm lam}$*, there exist six pure Gibbs states with exponential decay of correlations, and the structure factor satisfies*

$$S(\pi,\pi,0) = S(\pi,0,\pi) = S(0,\pi,\pi) > 1-\eta \qquad |S(0,0,0)| < \eta$$

$$S(k) = 0 \qquad \text{if} \quad k \neq (\pi,\pi,0), (\pi,0,\pi), (0,\pi,\pi), (0,0,0).$$

Proof. The hypothesis of the theorem matches assumptions 1–5 of section 2. As mentioned above, we can take $\Delta = c\gamma\frac{t_1^2}{U}$ with $c > 0$; parameters ε, ε^*, $\varepsilon^{\perp}$ are

$$\varepsilon = \max_{j=1,2,3} \frac{|t_j|}{\min(\mu/U, 1-\mu/U)} \tag{3.4}$$

$$\varepsilon^* = \max_{j=1,2,3} \frac{|t_{\downarrow}^{(j)}|^2}{c\gamma t_1^2 \min(\mu/U, 1-\mu/U)} \tag{3.5}$$

$$\varepsilon^{\perp} = \max_{j=1,2,3} \frac{|t_j t_{\downarrow}^{(j)}|}{c\gamma t_1^2 \min(\mu/U, 1-\mu/U)}. \tag{3.6}$$

The assumptions of theorem 3.1 ensure that they will be small, so that theorem 2.1 applies.

Statements concerning Gibbs states are now clear. We present the proof for the structure factor only in the case of chessboard states (the generalization to other cases is immediate). We notice that from the decomposition (2.25) of Gibbs states with periodic boundary conditions,

and the exponential clustering of pure states, we have

$$S(k) = \tfrac{1}{2}\sum_{j=1}^{2} \lim_{\Lambda \nearrow \mathbb{Z}^v} \frac{1}{|\Lambda|^2} \sum_{x,y\in\Lambda} \mathrm{e}^{-\mathrm{i}k(x-y)} \langle (n_{x\uparrow} - n_{x\downarrow})(n_{y\uparrow} - n_{y\downarrow})\rangle^j$$

$$= \tfrac{1}{2}\sum_{j=1}^{2} \lim_{\Lambda \nearrow \mathbb{Z}^v} \left| \frac{1}{|\Lambda|} \sum_{x\in\Lambda} \mathrm{e}^{-\mathrm{i}kx} \langle (n_{x\uparrow} - n_{x\downarrow})\rangle^j \right|^2 . \tag{3.7}$$

Here, $\langle\cdot\rangle^j$ represents the Gibbs state associated with the chessboard j.

Now pure states can be defined as limits of states obtained with a perturbation, and periodic boundary conditions [KU]; here, we consider the Hamiltonian $H - h\sum_x (-1)^{|x|}(n_{x\uparrow} - n_{x\downarrow})$, and the corresponding infinite volume Gibbs state $\langle\cdot\rangle^{\mathrm{per},h}$. Then

$$\langle (n_{x\uparrow} - n_{x\downarrow})\rangle^1 = \lim_{h\to 0+} \langle (n_{x\uparrow} - n_{x\downarrow})\rangle^{\mathrm{per},h} \tag{3.8}$$

$$\langle (n_{x\uparrow} - n_{x\downarrow})\rangle^2 = \lim_{h\to 0-} \langle (n_{x\uparrow} - n_{x\downarrow})\rangle^{\mathrm{per},h}. \tag{3.9}$$

Clearly, these objects have periodicity 2 as a function of x; moreover,

$$\langle (n_{x\uparrow} - n_{x\downarrow})\rangle^1 = \begin{cases} a & \text{if} \quad (-1)^{|x|} = 1 \\ -b & \text{if} \quad (-1)^{|x|} = -1 \end{cases} \tag{3.10}$$

where a and b are close to 1, $|a-1| < \eta$, $|b-1| < \eta$. The structure factor is therefore close to 1 when $k = (\pi, \pi, \pi)$, close to 0 when $k = (0, 0, 0)$ and vanishes otherwise. □

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