DIFFRACTION SPECTRUM OF LATTICE GAS MODELS ABOVE $T_c$

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ABSTRACT. The diffraction spectra of lattice gas models on $\mathbb{Z}^d$ with finite-range ferromagnetic two-body interactions above $T_c$ or with certain rates of decay of the potential are considered. We show that these diffraction spectra almost surely exist, are $\mathbb{Z}^d$-periodic and consist of a pure point part and an absolutely continuous part with continuous density.

1. INTRODUCTION

In the following, we analyze the diffraction spectrum of translation invariant Ising type models on $\mathbb{Z}^d$, interpreted as a lattice gas. More specifically, we consider models with single spin space $\{-1,1\}$ and pair potentials which can be described by a real symmetric function $J(x) = J(-x)$ for $x \in \mathbb{Z}^d$ (so the Hamiltonian can formally be written as $H = -\sum_{x,y \in \mathbb{Z}^d} J(x-y) \sigma_x \sigma_y$, where $\sigma_x \in \{-1, +1\}$ denotes the spin at $x \in \mathbb{Z}^d$).

For a finite subsystem, $T \subset \mathbb{Z}^d$ (with periodic boundary conditions, say), the partition function in the spin-formulation is

$$Z_\beta = \sum_{\sigma} \exp(\beta \cdot \sum_{x,y \in T} J(x-y) \sigma_x \sigma_y)$$

where the sum runs over all configurations $\sigma = \{\sigma_x | x \in T\}$ on $T$. Via

$$\mu_\beta(\sigma) = \frac{1}{Z_\beta} \exp(\beta \cdot \sum_{x,y \in T} J(x-y) \sigma_x \sigma_y),$$

one defines a probability measure on the (finite) configuration space. In the infinite volume (or thermodynamic) limit, this leads to the corresponding Gibbs measure, compare [10, 21] for details.

The set of Gibbs measures is a non-empty simplex (see [10] Theorem 7.26), but it need not be a singleton set. If its nature changes as a function of $\beta$ (e.g., from a singleton to a 1-simplex), the system undergoes a phase transition. The point where this happens is characterized by $\beta_c = 1/k_B T_c$, the so-called inverse critical temperature. In the following, we will only consider cases where the Gibbs measure is unique, i.e., where we have a singleton set. Since extremal Gibbs measures are ergodic.
(see [10, Theorem 14.15]), the unique Gibbs measure is ergodic, and quantities obtained as an average over the ensemble (like the correlation functions which we consider next) are valid almost surely for each member of the ensemble (with respect to the Gibbs measure).

Assuming uniqueness of the Gibbs measure, the density-density correlation function \(\langle n_0 n_x \rangle_\beta\) in the lattice gas interpretation of the models considered can be deduced from \(n_x = \frac{1}{\beta} (\sigma_x + 1)\), where the site \(x\) is occupied by a particle iff \(n_x = 1\). This leads to the following relationship among the correlation functions (note that we assume uniqueness of the Gibbs measure, so \(\langle \sigma_x \rangle_\beta = 0\):

\[
\langle n_0 n_x \rangle_\beta = \frac{1}{4} \left( \langle \sigma_0 \sigma_x \rangle_\beta + 1 \right).
\]

This interpretation yields the following positive definite autocorrelation measure (almost surely, in the sense explained above):

\[
\gamma = \sum_{x \in \mathbb{Z}^d} \langle n_0 n_x \rangle_\beta \delta_x,
\]

where \(\delta_x\) denotes the Dirac or point measure at \(x\), compare [6, Chapter 7] and [2] for details on the autocorrelation of lattice systems. The diffraction spectrum of the lattice gas model is then the Fourier transform \(\hat{\gamma}\) of its autocorrelation measure \(\gamma\). The positive measure \(\hat{\gamma}\) can be uniquely decomposed as \(\hat{\gamma} = (\hat{\gamma})_{pp} + (\hat{\gamma})_{sc} + (\hat{\gamma})_{ac}\) by the Lebesgue decomposition theorem, see [17]. Here, \((\hat{\gamma})_{pp}\) is a pure point measure, which corresponds to the Bragg part of the diffraction spectrum, \((\hat{\gamma})_{ac}\) is absolutely continuous and \((\hat{\gamma})_{sc}\) singular continuous with respect to Lebesgue measure.

The constant part of (2) results in the pure point measure

\[
(\hat{\gamma})_{pp} = \frac{1}{4} \sum_{k \in \mathbb{Z}^d} \delta_k = \frac{1}{4} \delta_{\mathbb{Z}^d}
\]

in the diffraction spectrum (note that \(\mathbb{Z}^d\) is self-dual), as a consequence of Poisson’s summation formula for distributions, see [19, p. 254] and [5]. Strictly speaking, the validity of (3) is not clear at this stage, we have only shown that \((\hat{\gamma})_{pp}\) “contains” \(\frac{1}{4} \delta_{\mathbb{Z}^d}\). However, it is valid if \(\frac{1}{4} \sum_{x \in \mathbb{Z}^d} \langle \sigma_0 \sigma_x \rangle_\beta \delta_x\) is a null weakly almost periodic measure, see [2] Chapter 11. All examples we will consider here are of this type.

We will now show that, in addition to this pure point part, almost surely only an absolutely continuous part is present in the diffraction spectrum of models on \(\mathbb{Z}^d\) with finite-range “ferromagnetic” (i.e., attractive) two-body interactions for all temperatures above \(T_c\). We will also show that the same holds for models (deep) in the Dobrushin uniqueness regime that satisfy an additional condition on the rate of decay of their potential. Similar observations have also been made in [8, 3]. In view of the widespread application of such lattice gas models to disordered phenomena in solids, this gives a partial justification why singular continuous spectra are usually not considered in classical crystallography.
2. Fourier Series of Decaying Correlations

Let us assume that the correlation coefficients of a model considered is either exponentially or algebraically decaying. We first look at exponentially decaying correlations, i.e.,

\[(4) \quad |\langle \sigma_0 \sigma_x \rangle_{\beta}| \leq C \cdot e^{-\varepsilon \|x\|},\]

where \(C, \varepsilon\) are positive constants depending only on \(\beta\) and the model considered, and \(\| \cdot \|\) denotes the Euclidean distance.

We will now deduce from the absolute convergence of \(\sum_{x \in \mathbb{Z}^d} e^{-\varepsilon \|x\|}\) that the exponentially decaying part of the correlation yields an absolutely continuous part in the diffraction spectrum. From the inequality

\[\frac{1}{\sqrt{d}} (|x_1| + \ldots + |x_d|) \leq \|x\|,\]

we get

\[\sum_{x \in \mathbb{Z}^d} e^{-\varepsilon \|x\|} \leq \sum_{x \in \mathbb{Z}^d} e^{-\varepsilon \sqrt{\sum_{i=1}^{d} |x_i|}} = \left( \sum_{n \in \mathbb{Z}} e^{-\varepsilon \sqrt{d} |n|} \right)^d = \left( e^{\varepsilon/\sqrt{d} + 1} \right)^d = \left( e^{\varepsilon/\sqrt{d} - 1} \right)^d = \left( \coth \left( \frac{\varepsilon/\sqrt{d}}{2} \right) \right)^d.\]

So far, we have

**Lemma 1.** Let the correlation coefficients be bounded as in \(4\). Then the sum \(\sum_{x \in \mathbb{Z}^d} \langle \sigma_0 \sigma_x \rangle_{\beta}\) is absolutely convergent. \(\square\)

We now consider correlations with algebraic decay of power \(p > d\), i.e.,

\[(5) \quad |\langle \sigma_0 \sigma_x \rangle_{\beta}| \leq C \cdot \|x\|^{-p}\]

where \(C\) is positive constant.

We observe that \( |\langle \sigma_0 \sigma_x \rangle_{\beta}| \leq 1 \) for all \(x \in \mathbb{Z}^d\) and that \(\|x\|_\infty \leq \|x\|\) (where \(\|x\|_\infty = \max_i |x_i|\) denotes the maximum norm). Therefore, we get

\[\sum_{x \in \mathbb{Z}^d} |\langle \sigma_0 \sigma_x \rangle_{\beta}| \leq 1 + C \sum_{x \in \mathbb{Z}^d \setminus \{0\}} \|x\|^{-p} \leq 1 + C \sum_{x \in \mathbb{Z}^d \setminus \{0\}} \|x\|^{-p}.\]

Furthermore, we observe that there are \((2 \cdot n + 1)^d - (2 \cdot n - 1)^d = O(n^{d-1})\) lattice points \(x \in \mathbb{Z}^d\) with norm \(\|x\|_\infty = n\) (\(n \in \mathbb{N}\)); so there is a positive constant \(c_d\) such that

\[\sum_{x \in \mathbb{Z}^d \setminus \{0\}} \|x\|^{-p} \leq c_d \sum_{n \in \mathbb{N}} n^{-p+d-1} = c_d \cdot \zeta(p+1-d).\]

Here, \(\zeta\) denotes Riemann’s zeta function.

We have established the following variant of Lemma 1.

**Lemma 2.** Let the correlation coefficients be bounded as in \(5\) with \(p > d\). Then the sum \(\sum_{x \in \mathbb{Z}^d} \langle \sigma_0 \sigma_x \rangle_{\beta}\) is absolutely convergent. \(\square\)
With the same reasoning as in \cite{3} Proposition 5\slash and \cite{14} Satz 3.7, we now obtain

**Proposition 1.** The diffraction spectrum of a lattice gas model on $\mathbb{Z}^d$, with correlation coefficients bounded as in (4), or as in (5) with a power $p > d$, almost surely exists, is $\mathbb{Z}^d$-periodic and consists of the pure point part of (3) and an absolutely continuous part with continuous density. No singular continuous part is present.

**Proof.** Lattice gas models can also be treated as weighted lattice Dirac combs (with weight 1 if a site is occupied by a particle and weight 0 otherwise). So, the diffraction measure $\hat{\gamma}$ can be represented as

$$\hat{\gamma} = \rho \ast \delta_{\mathbb{Z}^d}$$

with a finite positive measure $\rho$ that is supported on a fundamental domain of $\mathbb{Z}^d$, by an application of \cite{2} Theorem 1. This yields the $\mathbb{Z}^d$-periodicity, which is also implied by the following more explicit arguments.

We have already treated the pure point part in (3).

Since the sum $\sum_{x \in \mathbb{Z}^d} \langle \sigma_0, \sigma_x \rangle_\beta$ is absolutely convergent, we can view the correlation coefficients $\langle \sigma_0, \sigma_x \rangle_\beta$ as functions in $L^1(\mathbb{Z}^d)$. Their Fourier transforms are uniformly converging Fourier series (by the Weierstraß M-test) and are therefore continuous functions on $\mathbb{R}^d/\mathbb{Z}^d$, see \cite{18} Theorem 1.2.4(a), which are then also in $L^1(\mathbb{R}^d/\mathbb{Z}^d)$. Applying the Radon-Nikodym theorem finishes the proof. □

**Remark:** The Riemann-Lebesgue lemma \cite{22} Corollary VII.1.11 states that if $f \in L^1(\mathbb{R}^d/\mathbb{Z}^d)$ and if $f$ admits a Fourier series ($\langle \cdot, \cdot \rangle$ denotes the scalar product)

$$\sum_{x \in \mathbb{Z}^d} a_x e^{2\pi i \langle k, x \rangle}$$

then $a_x \to 0$ as $\|x\| \to \infty$. Therefore, an algebraic decay of power $p \leq d$ might still give an analogous result, but (possibly) without the continuity of the Radon-Nikodym density. An example is the diffraction of the classical Ising lattice gas on $\mathbb{Z}^2$ at the critical point, $\beta = \beta_c$, see \cite{3} for details. In general, faster decay of correlations implies that higher derivatives of the density exist, see \cite{15} Chapter 3, §1.1. In particular, exponential decay implies that the Radon-Nikodym density is $C^\infty$.

3. **Uniqueness of the Gibbs Measure and Decay of Correlations**

A sufficient condition for the uniqueness of the Gibbs measure is stated in Dobrushin’s uniqueness theorem \cite{10} Theorem 8.7\slash. In the situation considered here, Dobrushin’s condition reads as follows (see \cite{10} Example 8.9(2)):

$$\beta \sum_{x \in \mathbb{Z}^d} \tanh |J(x)| < 1.$$  \hspace{1cm} (6)

Note that a sufficient condition for (6) to hold is $\beta \sum_{x \in \mathbb{Z}^d} |J(x)| \leq 1$.

This observation lines up with the following well-known result for finite range ferromagnets: For such models, we associate to each site $x \in \mathbb{Z}^d$ a nonnegative number $J(x) = J(-x) \geq 0$ (ferromagnetic interaction, i.e., we have an attractive lattice
gas) and we suppose that there exists an $R > 0$ such that $J(x) = 0$ if $||x|| > R$ (finite range). Obviously, we have $\sum_{x \in \mathbb{Z}^d} J(x) < \infty$, so for small $\beta$ (high temperature) we are in the Dobrushin uniqueness regime. More precisely, one knows [7, Section V.5] that $0 < \beta_c < \infty$ when $d \geq 2$, and $\beta_c = \infty$ for $d = 1$.

In the next step, we are interested in the decay of correlations. The result in [11] can be described succinctly by saying that the correlations decay (at high temperatures) at the same rate as the potential. Under Dobrushin’s condition, we will now consider two cases, exponential and algebraic decay, see [10, Sections 8.28 – 8.33].

**Lemma 3.** (Exponential decay) Suppose that, in addition to Dobrushin’s condition, we have, for some $t > 0$,

$$\beta \sum_{x \in \mathbb{Z}^d} e^{t||x||} |J(x)| < \infty.$$ 

Then, the correlation coefficients are exponentially decaying, i.e., there are constants $0 < \varepsilon, C < \infty$ such that

$$|\langle \sigma_0 \sigma_x \rangle^\beta| \leq C \cdot e^{-\varepsilon ||x||}.$$ 

(Algebraic decay) Alternatively, suppose that for some $p > 0$, in addition to Dobrushin’s condition, we have:

$$\beta \sum_{x \in \mathbb{Z}^d} ||x||^p |J(x)| < \infty.$$ 

Then, the correlation coefficients have an algebraic decay, i.e., there is a constant $0 < C < \infty$ such that

$$|\langle \sigma_0 \sigma_x \rangle^\beta| \leq C \cdot ||x||^{-p}.$$ 

\[\square\]

Note that for sufficiently high temperatures, the additional condition of either case implies Dobrushin’s condition. Combining this with Proposition 1 we get the following central result.

**Theorem 1.** Suppose that, for a lattice gas model on $\mathbb{Z}^d$ with two-body interaction, one of the following two conditions holds:

- There is a $t > 0$ such that

  $$\beta \sum_{x \in \mathbb{Z}^d} e^{t||x||} |J(x)| < \infty.$$ 

- There is a $p > d$ such that

  $$\beta \sum_{x \in \mathbb{Z}^d} ||x||^p |J(x)| < \infty.$$ 

Then, for sufficiently high temperatures, the diffraction spectrum of such a model almost surely exists, is $\mathbb{Z}^d$-periodic, and consists of a pure point part as in (3) and an absolutely continuous part with continuous density. It cannot have any singular continuous component. \[\square\]
Remark: Algebraic decay (of power \( p > d = 2 \)) of the correlations occurs in certain dimer models \( [3, 13] \) that can be interpreted as (crystallographic) random tiling models.

4. Models with Finite-Range Ferromagnetic Two-Body Interactions

For models with finite-range ferromagnetic two-body interaction, one even gets exponential decay for all supercritical temperatures \( \beta < \beta_c \) (and not only in the Dobrushin uniqueness regime \( \beta \ll \beta_c \)). Before stating the result, we note that \( \langle \sigma_0, \sigma_x \rangle_\beta \geq 0 \) by the first Griffiths inequality \( [7, \text{Section V.3}] \).

Theorem 2. [4, Theorem A] For a ferromagnetic model on \( \mathbb{Z}^d \) with finite-range two-body interaction, the following holds for \( \beta < \beta_c \) and uniformly in \( \|x\| \rightarrow \infty \):

\[
\langle \sigma_0, \sigma_x \rangle_\beta = \frac{\Phi_\beta(n(x))}{\|x\|^{(d-1)/2}} e^{-\|x\| \xi_\beta(n(x))} (1 + o(1))
\]

where \( n(x) \) is the unit vector in the direction of \( x \), \( n(x) = x/\|x\| \), \( \Phi_\beta \) is a strictly positive locally analytic function on \( S^{d-1} \), and \( \xi_\beta \) denotes the inverse correlation length.

The inverse correlation length \( \xi_\beta \) is a positive function by \([1, \text{Theorem 1}]\) in connection with \([20, \text{Theorems 1.3 & 2.1}]\).

Lemma 4. [4, Theorem 1.1] Under the assumption of Theorem 2, one has \( \xi_\beta > 0 \) on \( \mathbb{R}^d \setminus \{0\} \) iff \( \beta < \beta_c \).

Note that \( \xi_\beta \) is homogeneous of degree one, i.e., \( \xi_\beta(\alpha \cdot x) = \alpha \cdot \xi_\beta(x) \) for \( \alpha > 0 \). It also follows from the proof of [4, Theorem A] that \( \xi_\beta \) is an analytic and therefore continuous function on \( S^{d-1} \), see [4, p. 309].

One can now modify the bound (7) to meet our requirements.

Lemma 5. Under the assumption of Theorem 2 there are positive constants \( C, \varepsilon \), such that (7) can be bounded as in (4).

Proof. Since \( \xi_\beta \) is a positive continuous function over a compact set \( S^{d-1} \), we have

\[
\inf_{x \in S^{d-1}} \xi_\beta(x) \geq \varepsilon > 0.
\]

Similarly, since \( \Phi_\beta \) is locally analytic, we can also find an appropriate \( M > 0 \) such that

\[
\frac{\Phi_\beta(n(x))}{\|x\|^{(d-1)/2}} e^{-\|x\| \xi_\beta(n(x))} (1 + o(1)) \leq \frac{M}{\|x\|^{(d-1)/2}} e^{-\varepsilon \|x\|}.
\]

So far, we have an upper bound for the asymptotic behaviour of \( \langle \sigma_0, \sigma_x \rangle_\beta \). But \( |\langle \sigma_0, \sigma_x \rangle_\beta| \) is bounded by \( 1 \), so we can find a positive constant \( C \geq M \) such that

\[
\langle \sigma_0, \sigma_x \rangle_\beta \leq \frac{C}{(1 + \|x\|)^{(d-1)/2}} e^{-\varepsilon \|x\|} \leq C \cdot e^{-\varepsilon \|x\|}.
\]
This proves the claim.

It is possible to obtain the exponential decay also directly from [11] together with the Simon-Lieb inequality [20, 16]. However, we invoked the stronger result of [4] here because it might help to analyze some finer details of the diffraction in the future.

Combining the last Lemma with Proposition [11] we get our main result.

**Theorem 3.** For $\beta < \beta_c (T > T_c)$, the diffraction spectrum of a lattice gas model on $\mathbb{Z}^d$ with finite-range ferromagnetic two-body interaction almost surely exists, is $\mathbb{Z}^d$-periodic and consists of the pure point part $\hat{\gamma}_{pp} = \frac{1}{4} \delta_{\mathbb{Z}^d}$ and an absolutely continuous part whose Radon-Nikodym density is $C^\infty$. No singular continuous part is present.

One further qualitative property of the absolutely continuous component can be extracted without making additional assumptions. In our setting, we know inequality [4] and also that

$$\eta(x) = \langle \sigma_0 \sigma_x \rangle_\beta = \langle \sigma_0 \sigma_{-x} \rangle_\beta = \eta(-x)$$

which follows from the positive definiteness of the autocorrelation. Consequently, one has

$$\left( \sum_{x \in \mathbb{Z}^d} \eta(x) \delta_x \right)(k) = \sum_{x \in \mathbb{Z}^d} \eta(x) \cos(2\pi kx)$$

where the right hand side is a uniformly converging Fourier series of a $\mathbb{Z}^d$-periodic continuous function, as consequence of Lemma [11]. In fact, in our setting of exponential decay of $\eta(x)$, this function is $C^\infty$. Since $\eta(x) \geq 0$ for all $x \in \mathbb{Z}^d$, this function has absolute maxima at $k \in \mathbb{Z}^d$ (viewed as the dual lattice of $\mathbb{Z}^d$).

**Proposition 2.** Under the assumptions of Theorem [3] the absolutely continuous component of the diffraction measure is represented by a continuous function that assumes its maximal value at positions $k \in \mathbb{Z}^d$.

This result reflects the well-known qualitative property that the diffuse background (i.e., the continuous components) concentrates around the Bragg peaks if the effective (stochastic) interaction is attractive. Otherwise, the two components “repel” each other, as in the dimer models, see [6, 24] for details.

**Remark:** All results also hold – mutatis mutandis – for an arbitrary lattice $\Lambda \subset \mathbb{R}^d$, since there exists a bijective linear map $\Lambda \to \mathbb{Z}^d$, $x \mapsto Ax$ where $A \in \text{GL}_d(\mathbb{R})$ (i.e., $A$ is an invertible $d \times d$-matrix with coefficients in $\mathbb{R}$). E.g., we can interpret a finite-range model on $\Lambda$ with range $R$ as finite-range model on $\mathbb{Z}^d$ with range (bounded by) $\|A\|_2 \cdot R$, where $\| \cdot \|_2$ denotes the spectral norm of the matrix $A$. The ferromagnetic two-body interaction $\tilde{J}(x) = J(-x) \geq 0$ on $\Lambda$ changes to $J(y) = \tilde{J}(A^{-1}y) = \tilde{J}(-A^{-1}y) = J(-y) \geq 0$ for $y \in \mathbb{Z}^d$. Also, Dobrushin’s uniqueness condition does not require any specific underlying structure such as $\mathbb{Z}^d$, one can choose any lattice, and even more general structures.
5. CONCLUDING REMARKS

The precise analysis of diffraction spectra of mixed type (e.g., with non-trivial continuous components) has recently gained importance. This is caused by the existence of non-periodically ordered solids [23] and the observation that structural disorder is much more widespread than previously anticipated [24].

Our simple observation above shows that singular continuous diffraction spectra should not be expected as the result of disorder of (ferromagnetic) lattice gas type. It is plausible that also other types of disorder will tend to destroy rather than create singular continuous components.

However, there is very good evidence (based on scaling arguments and extensive numerical investigations [12] [14]) that this is different for random tiling diffraction with non-crystallographic symmetry in two dimensions. A rigorous proof of the latter claim would help to better understand the role of singular continuous spectra.

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