Diffraction Spectrum of Lattice Gas Models above T_c

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Diffraction I

Objective: Atoms are distributed on a lattice $\mathbb{Z}^d$, we want to know the diffraction of this structure.

Model an atom at x by δ_x.
Then the structure is modeled by $\omega = \sum_{x \in S} \delta_x$, where $S \subset \mathbb{Z}^d$.

For diffraction, one needs the autocorrelation measure

$$\gamma_\omega = \sum_{z \in \Delta} \eta(z) \cdot \delta_z,$$

where $\Delta = S - S \subset \mathbb{Z}^d$ and

$$\eta(z) = \lim_{n \to \infty} \frac{1}{B_n} \sum_{\substack{x,y \in S \cap B_n \\ x - y = z}} 1.$$

Setting $\eta(z) = 0$ for $z \notin \Delta$ we obtain

$$\gamma_\omega = \sum_{z \in \mathbb{Z}^d} \eta(z) \cdot \delta_z.$$

Diffraction II

The diffraction measure is obtained from γ_ω by Fourier transform, $\hat{\gamma}_\omega$. It is a positive measure.

Decomposition (w.r.t. Lebesgue measure):

$$\hat{\gamma}_\omega = (\hat{\gamma}_\omega)_{\mathsf{pp}} + (\hat{\gamma}_\omega)_{\mathsf{sc}} + (\hat{\gamma}_\omega)_{\mathsf{ac}}$$

$(\hat{\gamma}_\omega)_{\mathsf{pp}}$: pure point measure (countable sum of point measures), Bragg part of the diffraction spectrum

$(\hat{\gamma}_\omega)_{\mathsf{sc}}$: singular continuous
$(\hat{\gamma}_\omega)_{\mathsf{ac}}$: absolutely continuous (Radon-Nikodym density)

How does the decomposition look like for lattice gases?

Lattice Gases I

Atoms with interaction: Spin-Models (Ising) (single spin space $\{\pm 1\}$) with pair potential $J(x) = J(-x)$.

Formal Hamiltonian: $H(\boldsymbol{\sigma}) = -\sum_{x,y\in\mathbb{Z}^d} J(x-y)\,\sigma_x\,\sigma_y$.

Probability space $\{\pm 1\}^{\mathbb{Z}^d}$ with product σ-algebra, associated measure(s): Gibbs measure(s)

prescribe conditional distributions of all finite collection of spins ($\tilde{\cdot}$ denotes restriction to finite collection):

$$\tilde{\mu}_\beta(\boldsymbol{\sigma}) = \frac{1}{\tilde{Z}_\beta}\exp(-\beta\tilde{H}(\boldsymbol{\sigma})),$$

where $\beta = \frac{1}{k_{\mathrm{B}}T}$ is the inverse temperature.

Infinite volume limit (thermodynamic limit) yields Gibbs measure(s) (under suitable conditions on J).

Lattice Gases II

The set of Gibbs measures is a non-empty simplex, extremal Gibbs measures are ergodic:

Quantities obtained as an average over the ensemble are valid almost surely for each member.

In the following, we will consider the case where the Gibbs measure is unique (therefore ergodic).

Interpretation:
$\sigma_x = +1$: atom at x
$\sigma_x = -1$: no atom at x
i.e., $n_x = \frac{1}{2}(\sigma_x + 1)$.

We get:

$$\eta(x) \overset{\text{erg.}}{=} \langle n_0 n_x \rangle_\beta \overset{\text{uniq.}}{=} \frac{1}{4}\langle \sigma_0 \sigma_x \rangle_\beta + \frac{1}{4}$$

Constant part yields $(\hat{\gamma}_\omega)_{\mathsf{pp}} = \frac{1}{4}\delta_{\mathbb{Z}^d}$ (as we will see) by Poisson's summation formula.

Bounds on Correlations

Suppose we have the following decay of the correlations:

1. $|\langle \sigma_0 \sigma_x \rangle_\beta| \leq C \cdot \mathrm{e}^{-\varepsilon \|x\|}$ $(C, \varepsilon > 0)$

   Note: $\sum\limits_{x \in \mathbb{Z}^d} \mathrm{e}^{-\varepsilon \|x\|} \leq (\coth(\frac{\varepsilon}{2\sqrt{d}}))^d < \infty$ (abs. conv.).

2. $|\langle \sigma_0 \sigma_x \rangle_\beta| \leq C \cdot \|x\|^{-p}$ $(C > 0, p > d)$

   Note: $\sum\limits_{x \in \mathbb{Z}^d \setminus \{0\}} \|x\|^{-p} \leq c_d \cdot \zeta(p + 1 - d) < \infty$ (abs. conv.).

Proposition 1. *The diffraction spectrum of lattice gas models on $\mathbb{Z}^d$, with correlation coefficients bounded as above, almost surely exists, is $\mathbb{Z}^d$-periodic and consists of the pure point part $\frac{1}{4}\delta_{\mathbb{Z}^d}$ and an absolutely continuous part with continuous density. No singular continuous part is present.*

Proof. Pure point part clear.
Have $f(x) := \langle \sigma_0 \sigma_x \rangle_\beta \in L^1(\mathbb{Z}^d)$ (by abs. conv.), then
$\hat{f} \in C(\mathbb{R}^d / \mathbb{Z}^d) \subset L^1(\mathbb{R}^d / \mathbb{Z}^d)$. $\square$

Decay of Correlations

Sufficient condition for uniqueness of Gibbs measure: Dobrushin's uniqueness theorem. Here:

$$\beta \sum_{x \in \mathbb{Z}^d} |J(x)| \le 1.$$

Observe that correlations decay at the same rate as the potential.

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

1. $\exists t > 0 : \quad \beta \sum_{x \in \mathbb{Z}^d} \mathrm{e}^{t\|x\|} \, |J(x)| < \infty$.

2. $\exists p > d : \quad \beta \sum_{x \in \mathbb{Z}^d} \|x\|^p \, |J(x)| < \infty$.

Then, for sufficiently high temperatures, the diffraction spectrum of such a model a.s. exists, is $\mathbb{Z}^d$*-periodic, ...*

Finite-Range Ferromagnets

Attractive lattice gas: $J(x) = J(-x) \geq 0$
Finite range: $\exists R > 0$ s.t. $J(x) = 0$ for $\|x\| > R$.

One knows:

- Phase transition at β_c, where $0 < \beta_c < \infty$ for $d \geq 2$.
- Autocorrelation coeff. non-negative (Griffiths ineq.).
- Autocorrelation coeff. decay exponentially for all(!) $\beta < \beta_c$.
  [Aizenman, Barsky Fernández 1987 & Simon-Lieb ineq. 1980]
  or [Campanino, Ioffe, Velenik 2003, `math.PR/0111274`]

Theorem 2. *For $\beta < \beta_c$, the diffraction spectrum of a lattice gas model on $\mathbb{Z}^d$ with finite-range ferromagnetic two-body interaction almost surely exists, is $\mathbb{Z}^d$ - ...*

Non-negative autocorr. coeff. $\Rightarrow$ Radon-Nikodym density of ac component assumes its maximal value at positions $k \in \mathbb{Z}^d$
(diffuse background concentrates around Bragg peaks)

Conclusions

- All results also hold for an arbitrary lattice.
- Singular continuous diffraction spectra should not be expected as the result of disorder of lattice gas type.
- Partial justification why sc spectra are usually not considered in classical crystallography.
- BUT: Evidence that for random tiling models with non-crystallographic symmetry in $d = 2$ the situation is different: here sc component is expected.

Poisson's summation formula

Poisson's summation formula for distributions:

$$\widehat{\delta_\Gamma} = \mathrm{dens}(\Gamma) \cdot \delta_{\Gamma^*},$$

where Γ is a lattice in $\mathbb{R}^d$,
$\Gamma^* = \{y \in \mathbb{R}^d \mid \langle x, y \rangle \in \mathbb{Z} \text{ for all } x \in \Gamma\}$ its dual lattice
and $\delta_\Gamma = \sum_{x \in \Gamma} \delta_x$.

For $\Gamma = \mathbb{Z}^d$ (self-dual) we have

$$\widehat{\delta_{\mathbb{Z}^d}} = \delta_{\mathbb{Z}^d}.$$