Dynamical Spectrum

vs

Diffraction Spectrum

in the

Description

of

Long-Range Order

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THE QUESTIONS:

What is Long-Range Order, and in particular Aperiodic Order?
Is it more like order or disorder? How could it originate as an equilibrium phase? What can we say mathematically?
Statistical Mechanics questions.

(Early speculation, long before quasicrystals, on " aperiodic crystal" by Schrödinger in "What is Life?"
as a model for chromosomes.)
Ruelle papers:
a) Do Turbulent Crystals Exist?-"
..fuzzy frequencies..." (1982)
b) Some Ill-formulated Problems on Regular and Messy Behavior...
(Earlier joint Ruelle-Sinai birthday meeting).

1) Spectral issues: Aperiodicity as order. Compare definition of (quasi-)crystals: point diffraction spectrum .

2)Existence of aperiodicity at zero and positive temperatures (where does aperiodicity come from?).

3) Aperiodicity as disorder, (spin-)glassy questions,

The questions in more detail

1) How can one describe general Long-Range Order, especially in terms of the (diffraction) spectrum?
2) Can one have a thermodynamically stable, non-periodically ordered phase for short-range translation-invariant interactions at zero or positive temperatures? In which dimension?
3) (Spin-)glass models. How disordered can tiling models be, without being so random as to be almost independent? Good as glass and spin glass models? Which kind of overlap distributions can one obtain for nonperiodic systems? What does it teach us about disordered systems?
Gibbs measure analysis, ($T > 0$) Ground state measure analysis ($T = 0$).

Spectral Issues, Configurations and Measures

In translation-invariant situations ergodic arguments imply that (almost) all configurations in the support of a translation-invariant Gibbs or ground state measure have the same global properties, in particular spectra.
Self-averaging (AvE+J.Miękisz, Dworkin).

Diffraction (atomic) Spectrum
versus
Dynamical (including molecular) Spectrum.

Probability Measures:

Lattice models, Gibbs -DLR- states.

These are probability measures on a spin configuration space which is a product of single-spin spaces: $\Omega = \Omega_0^{Z^d}$.

Their conditional probabilities of finding configurations σ_Λ in a finite Λ, given boundary condition (external configuration) ω^{Λ^c} (or probability densities) are of Gibbsian form for the local energy (Hamilton)$H^\omega_\Lambda(\sigma^\Lambda)$.

Here $H^\omega_\Lambda(\sigma^\Lambda) = \sum_{X \cap \Lambda \neq \emptyset} \Phi(X)$.

Thus $\mu^\alpha_\Lambda(\sigma^\Lambda | \omega^{\Lambda^c}) = \frac{exp(-\beta H^\omega_\Lambda(\sigma^\Lambda)}{Z^\omega_\Lambda}$,

for each choice of Λ, σ, and ω, and each Gibbs measure μ^α. Inverse temperature β.

Extremal translation-invariant (ergodic) Gibbs measures, finer decomposition into extremal Gibbs measures.

Statistical Mechanical notion of " order".
Disordered: Unique Gibbs measure.
Ordered: Multiple Gibbs measures.

Ground states, limits as β goes to infinity, of Gibbs states, live on ground state configurations, e.g. tiling configurations, substitution sequences (Dirac combs), often strictly ergodic measures.
Then statements for *all*, instead of *almost all*, ground state configurations.
Individual configurations are themselves measures, on R^d.

Spectral issues

Spectrum of Gibbs measures is expected to have absolutely continuous component due to thermal fluctuations.
Long-range order also other components (pure points and singular continuous).

Ground states can have (aperiodic) long-range order (violate tail triviality) with (dense) pure point spectrum -(quasi-)crystals-, (Regular)
or with (singular) continuous spectrum (Messy)
-weak or turbulent crystals.
(Non-canonical use of "crystal"
e.g. Ruelle, Ben-Abraham...)

Two notions of spectrum:
Full (Dynamical) Spectrum is the spectrum of the shift operator. The spectrum of the generator of the translations (as an operator on $L^2(\mu)$ for some translation invariant μ) is related to the observed Diffraction Spectrum, but it can be richer.

Diffraction Spectrum is the Fourier transform of covariance (autocorrelation function) of the measure, or of the Dirac combs in the support of this (translation-invariant) measure.

It is a (possibly proper) subset of the Dynamical Spectrum,
(In this context
A.v.E. + J.Miękisz, Dworkin).

The difference set can contain all the point spectrum.
Examples exist with
1) Diffraction Spectrum singular continuous, Dynamical Spectrum mixed, with p.p., (A.v.E.+ J.Miękisz).
or
2) Diffraction Spectrum absolutely continuous, Dynamical Spectrum mixed with p.p., (A.v.E. + M.Baake).

The other way around is impossible (Baake, Lee, Lenz, Moody, Solomyak):
Pure point Diffraction Spectrum implies pure point Dynamical Spectrum.

Old example (A.v.E + J.Miękisz):
((Prouhet)-Thue)-Morse sequences
.... $+--+-++--++-+--+$ ...
and orbits and orbit closure.
Strictly ergodic system with unique invariant measure, and singular Diffraction Spectrum.
Full Dynamical Spectrum is mixed (Keane), contains dyadic rationals.
Consider $Y_i = X_i X_{i+1}$, this provides period-doubling or Toeplitz sequences.
((Prouhet)-Thue)-Morse-sequence X_i
.... $+--+-++--++-+--+$ ...
goes into Y_i sequence
.... $-+---+-+-+---+--$ ...
(period-doubling, Toeplitz sequences).
These have pure point spectrum (dyadic rationals).
Recipe (Toeplitz):
Occupy odd or even sites with minus
(with probability $\frac{1}{2}$).
Occupy one half of the empty sites plus.
Occupy one half of the empty sites minus.
etc.....

Ergodic Theory Language: Toeplitz system is "factor" of P-T-Morse system.
Possible interpretation: molecular long-range order can be present in the absence of atomic long-range order.
Typical ground state example, strictly ergodic, no absolutely continuous part in the spectrum.

Positive temperatures: more randomness. Gibbs states are expected, and in various cases known, to have an absolutely continuous part in their spectrum (Baake, + Höffe, Sing, Zint... , Külske).

Randomizing independently (e.g. varying independently the position of each particle in an ordered structure) can produce an additional absolutely continuous part in the Dynamical (and Diffraction) Spectrum (Baake-Birkner-Moody).

However, by randomizing one can also remove points from the Diffraction Spectrum.

Simple example (A.v.E + M.Baake):

Take infinitely many dimers (two-site sets), fill Z with them. This can be done in two ways (left site in each dimer odd or even).

$[\cdot\ \cdot][\cdot\ \cdot][\cdot\ \cdot][\cdot\ \cdot][\cdot\ \cdot][\cdot\ \cdot][\cdot\ \cdot]$

Now take randomly $[-,+]$ or $[+,-]$ in each dimer, this creates two periodic measures μ_{odd} and μ_{even}. Their convex sum,

$\mu = \mu_{dimer} = \frac{1}{2}(\mu_{odd} + \mu_{even})$

is translation-invariant.

I claim that it has only absolutely continuous diffraction spectrum, but a period 2 (of the dimers) shows up as a point (delta-peak) in the Dynamical Spectrum.

Proof:
The correlation function between nearest-neighbor spins
$f(1) = \mu(S_i S_{i+1}) = -\frac{1}{2}$
and any other pair correlation between spins beyond nearest neighbors is zero: $f(n) = \mu(S_i S_{i+n}) = 0$.

On the other hand, if $Z_i = S_i S_{i+1}$,
(thus $\mu(Z_i) = -\frac{1}{2}$),
then for the "molecular" correlation holds
$g(2k) = \mu(Z_i Z_{i+2k}) = \frac{1}{2}$,
and $g(2k+1) = \mu(Z_i Z_{i+2k+1}) = 0$.

Such a 2-periodic function has an point (atom, delta-function) in its spectrum at $k = \frac{1}{2}$.

Further Questions:
1) Can one do this for a wide class of structures with non-absolutely-continuous spectrum, in particular including continuum cases?
To some extent -e.g. FLC systems- yes.
(A.v.E with M. Baake and D. Lenz).
In general infinitely many factors may be required (Herning), even though the covariance of a single, possibly nonlocal, continuous function, f, could produce the full Dynamical Spectrum (Fraczek).
Lattice also gives points in the spectrum, this should not be relevant.
2) If the Diffraction Spectrum does not possess an absolutely continuous component but has a singular component, can one prove that this also holds for the Dynamical Spectrum?
If one thinks of pure point, singular continuous and absolutely continuous spectrum as decreasing in order, this would extend the statement that molecules can be more but not less ordered than their constituent atoms.

QUESTION 2:

How to make models for quasicrystals?
By hand (cheating)...

Base on aperiodic sequences (Fibonacci, Thue-Morse, Rudin-Shapiro) and tilings (Penrose, Wang,...).
Construct translation-invariant interactions for which these are ground states.
Translation-invariant models with aperiodically ordered states.
Known results:
1 dimension: infinite-range interactions, fast decaying for ground states, slowly decaying for Gibbs states.
2 dimensions: Nearest-neighbor interactions via matching rules for tilings, give aperiodic ground states. Positive temperatures ?????
3 dimensions: Fast decaying in one direction, stabilizing ferromagnetic in the other two directions. Best result up to now (15 years old, with Miękisz and Zahradník.

QUESTION 3:

Aperiodicity as a form of disorder?

Tiling models either for quasicrystals or for glasses (Leuzzi-Parisi (2000), Levine-Kurchan-Wolff (2011–2013), Sasa(2012)).

Overlap distributions of aperiodic sequences.

Fibonacci, Toeplitz, period-doubling, Thue-Morse, paperfolding.... Unknown: Tilings?

Of interest in the theory of disordered systems, in particular spin glasses.

J.Kurchan (2010): "Is it possible that there will be new developments (in glass and spin glass theory) starting from the theory of low-dimensional amorphous order, as in nonperiodic tilings? It is amazing how little attention the glass community has paid to lessons that could be learned from quasicrystals and in general non-periodic systems."

Together with:

M. Baake, D. Lenz

(earlier J. Miękisz, C.Radin)

Acta Physica Pol. 126, p621 (2014)

J.Stat.Phys. 143, p88 (2011)(with M.Baake)

Erg.Th.Dyn.Sys 35, p2017 (2015)

(with M. Baake and D. Lenz)

To David Ruelle and Yasha Sinai

HAPPY BIRTHDAYS

and for many years of inspiration

THANK YOU !