High-temperature cluster expansion for classical and quantum spin lattice systems with multi-body interactions

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Canonical form

- Power expansion of the logarithm of the (grand-canonical) partition function.
- Expansion variables = "fugacities" (effective parameters)
- Interaction: gas of objects subject to pure hard-core exclusions.

Cluster-expansion technology: Rewrite your expansion so it takes the above form:

- High-temperature expansion
- Low-temperature (contour) expansion
- General perturbative methods (right choice of variables)

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Main issues

- Determine small-fugacity (poly)disk of convergence, hence analyticity.
- Through differentiation, full control of (reduced) correlation functions
- Through linear combinations, full control of expectations of more general observables.

Consequences:

- Lack of phase transition in the strongest sense.
- Full control of
  - Expectations
  - Finite volume corrections
  - Sensitivity to boundary conditions
  - etc.

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Mathematical aspects

The focus is on partition functions Ξ_Λ. Two steps:

(A1) ***Gas expansion*** = Ξ_Λ written as hard-core gas

- "Molecules" can be very general (e.g. subsets of lattice)
- Hard-core = incompatibility relation, also very general

(A2) ***Cluster expansion*** = formal series of $\log \Xi_\Lambda$ =

- Well known combinatoric expression
- Several approaches available to determine convergence

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Competing methods

Methods that avoid explicit consideration of the expansion:

Inductive (Dobrushin): No-cluster expansion approach.

- Easy to apply, hard to improve.
- A posteriori, convergence of the cluster expansion.
- Weaker than detailed cluster expansion analysis

Kirkwood-Salzburg: Coupled equations for the correlations.

- Correlation analyticity: Banach plus fix-point argument.
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Current situation

Classical stat mech

- Most only two-body interactions.
- Exceptions rely on a dominant two-body component.
- KS techniques OK for multi-body, but less precise.
- *Needed:* Multi-body HTE cluster expansion.

Quantum stat mech (lattice systems)

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Our results

Multi-body cluster expansions for both classical and quantum lattice spin systems.

- Interactions must be exponentially summable in the number of bodies.
- For quantum spin systems, this is needed for the dynamics to exist and for Gibbs = KMS.
- Our expansion is inspired in, and uses ideas of Park (1982)

Mathematical novelties:

- Gas expansion better done at the level of operators
- Canonical way to expand with or without commutativity

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The general setup

Countable family $\mathcal{P}$ of objects: *polymers*, animals, ..., characterized by

- An *incompatibility* constraint:

$$\begin{matrix} \gamma \nsim \gamma' \\ \gamma \sim \gamma' \end{matrix} \qquad \text{if } \gamma, \gamma' \in \mathcal{P} \qquad \begin{matrix} \text{incompatible} \\ \text{compatible} \end{matrix}$$

  For simplicity: each polymer incompatible with itself

- A family of *activities* $\boldsymbol{\rho} = \{\rho_\gamma\}_{\gamma \in \mathcal{P}} \in \mathbb{C}^{\mathcal{P}}$.

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Gas of polymers

For each *finite* family $\mathcal{P}_\Lambda \subset \mathcal{P}$,

Partition function

$$\Xi_\Lambda(\boldsymbol{z}) = 1 + \sum_{n\geq 1} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)\in\mathcal{P}_\Lambda^n} z_{\gamma_1} z_{\gamma_2} \ldots z_{\gamma_n} \prod_{j<k} \mathbb{1}_{\{\gamma_j \sim \gamma_k\}} \qquad (1)$$

and the **free energy** (modulo sign)

$$F_\Lambda(\boldsymbol{z}) \;=\; \log \Xi_\Lambda(\boldsymbol{z})$$

Probability weights

$$\mathrm{W}_\Lambda\big(\{\gamma_1,\gamma_2,\ldots,\gamma_n\}\big) \;=\; \frac{1}{\Xi_\Lambda(\boldsymbol{z})} z_{\gamma_1} z_{\gamma_2} \cdots z_{\gamma_n} \prod_{j<k} \mathbb{1}_{\{\gamma_j \sim \gamma_k\}}$$

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The questions:

In the limit $\mathcal{P}_\Lambda \to \mathcal{P}$ ("thermodynamic limit")

- Existence and analyticity of the free-energy density $F_\Lambda / |\Lambda|$
- Existence and properties of the measure defined by W_Λ.
- Asymptotic behavior of Ξ_Λ

The cluster expansion

Theorem [Canonical cluster expansion]

$$\log \Xi_\Lambda = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)\subset\Lambda^n} \omega_n^T(\gamma_1,\ldots,\gamma_n)\, z_{\gamma_1}\ldots z_{\gamma_n} \qquad (2)$$

(In the sense of formal power series) with

$$\omega_n^T(\gamma_1,\ldots,\gamma_n) = \begin{cases} 1 & n=1 \\ \displaystyle\sum_{\substack{G\subset\mathbb{G}(\gamma_1,\ldots,\gamma_n)\\ G\,\text{conn.spann.}}} (-1)^{|E(G)|} & n>1 \text{ and } \mathbb{G}(\gamma_1,\ldots,\gamma_n) \text{ conn.} \\ 0 & n>1 \text{ and } \mathbb{G}(\gamma_1,\ldots,\gamma_n) \text{ not conn} \end{cases}$$

$\mathbb{G}(\gamma_1,\ldots,\gamma_n)$ = graph of vertex set $\{1,\ldots,n\}$ and edge set

$$\{\{i,j\} : \gamma_i \nsim \gamma_j, 0 \le i < j \le n\},$$

The fundamental result

Theorem [Fundamental] Let $\boldsymbol{\varphi} : [0,+\infty)^{\mathcal{P}} \longrightarrow [0,+\infty]^{\mathcal{P}}$

$$\varphi_{Y_0}(\boldsymbol{\mu}) \;=\; 1+\sum_{n\geq 1}\sum_{\{Y_1,\dots,Y_n\}\subset\mathcal{P}}\prod_{i=1}^{n}\mathbf{1}_{\{Y_0\nsim Y_i\}}\prod_{1\leq k<\ell\leq n}\mathbf{1}_{\{Y_k\sim Y_\ell\}}\prod_{j=1}^{n}\mu_{Y_j} \tag{3}$$

If $\boldsymbol{\lambda} \in [0,+\infty)^{\mathcal{P}}$ satisfies

$$\lambda_Y \;\leq\; \frac{\mu_Y}{\varphi_Y(\boldsymbol{\mu})} \tag{4}$$

for each $Y \in \mathcal{P}$, for some $\boldsymbol{\mu} \in [0,+\infty)^{\mathcal{P}}$, then the following holds uniformly in Λ for $\boldsymbol{\rho} \in \mathcal{D}(\boldsymbol{\lambda})$.

(a) The cluster expansions (2) converge absolutely.

(b) The following bounds hold for each $Y \in \mathcal{P}(\Lambda)$:

$$\left|\frac{\Xi_{\Lambda\setminus Y}}{\Xi_\Lambda}\right| \;\le\; \frac{\mu_Y}{\lambda_Y} \tag{5}$$

$$\left|\log \frac{\Xi_\Lambda}{\Xi_{\Lambda\setminus Y}}\right| \;\le\; -\varphi_Y(\boldsymbol{\mu})\,\log(1-\lambda_Y) \tag{6}$$

Rules of the game:

- Write your partition function in the gas form (1)
- Use the fundamenta theorem to conclude

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Quantum lattice systems: Ingredients

Lattice: $\mathbb{L}$ = set of sites. E.g. $\mathbb{L} = \mathbb{Z}^d$

Spin spaces:

- $\mathcal{H}_x$ space at site x (often copies of a fixed space $\mathcal{H}$)
- Structure depends on whether classcal or quantum
- For each $\Lambda \subset\subset \mathbb{L}$, $\mathcal{H}_\Lambda = \otimes_{x\in\Lambda}\mathcal{H}_x$

Algebras of observables:

- Sequence of complex unital Banach algebras $\{\mathcal{A}_\Lambda : \Lambda \subset\subset \mathbb{L}\}$
- Increasing: $\Lambda_1 \subset \Lambda_2 \implies \mathcal{A}_{\Lambda_1} \subset \mathcal{A}_{\Lambda_2}$, with $\mathcal{A}_{\Lambda_1} \ni A_1 \longmapsto A_1 \otimes \mathbf{1}_{\Lambda_2\setminus\Lambda_1} \in \mathcal{A}_{\Lambda_2}$

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Traces: Maps $\mathrm{tr}_\Lambda : \mathcal{A}_\Lambda \longrightarrow \mathbb{C}$ satisfying

(T0) Lnearity and invariance under cyclic permutations of products

(T1) *Normalization:* $\mathrm{tr}_\Lambda(\mathbf{1}_\Lambda) = 1$

(T2) *Continuity:* If $A \in \mathcal{A}_\Lambda$, $|\mathrm{tr}_\Lambda(A)| \;\le\; \|A\|$

(T3) *Factorization:*

$$\mathrm{tr}_\Lambda \;=\; \bigotimes_{x\in\Lambda} \mathrm{tr}_{\{x\}}\;. \tag{7}$$

Main applications

Classical spin systems

- $\mathcal{H}_x$ = measure space with probability measure $d\mu_x$
- $\mathcal{A}_\Lambda$ = bounded measurable complex-valued functions on $\mathcal{H}_\Lambda$
- $\mathrm{tr}_\Lambda = \otimes_{x\in\Lambda} d\mu_x$

Quantum spin systems:

- $\mathcal{H}$ = finite-dimensional Hilbert space
- $\mathcal{A}_\Lambda$ = bounded operators on $\mathcal{H}_\Lambda$.
- Trace = normalization of the canonical trace $\mathrm{Tr}_{\mathcal{H}_\Lambda}$ of $\mathcal{H}_\Lambda$:

$$\mathrm{tr}_\Lambda = \frac{1}{\dim \mathcal{H}_\Lambda} \mathrm{Tr}_{\mathcal{H}_\Lambda} \tag{8}$$

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Finite-volume quantities

Interaction: Family $\Phi = \{\Phi(X) : X \subset\subset \mathbb{L}\}$ with $\Phi(X) \in \mathcal{A}_X$

Bonds: $\mathcal{B}_\Lambda = \big\{X \subset\subset \Lambda : \Phi(X) \neq 0\big\}$

Hamiltonian: $H_\Lambda \ = \ \sum_{X \subset \Lambda} \Phi(X) \ =: \ H_{\mathcal{B}_\Lambda}$

Finite-volume state: Defined by the expectations

$$\pi_\Lambda^\beta(A) \ = \ \frac{\mathrm{tr}_\Lambda\big(A\,\mathrm{e}^{-\beta H_\Lambda}\big)}{Z_\Lambda^\beta}$$

$A \in \mathcal{A}_\Lambda$, β = inverse temperature

Partition function: $Z_\Lambda^\beta \ = \ \mathrm{tr}_\Lambda\big(\mathrm{e}^{-\beta H_\Lambda}\big)$

Free energy: $-\beta F_\Lambda \ = \ \log Z_\Lambda^\beta$

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Classical gas expansion

Usual "±1 trick": $\mathrm{e}^{-\beta\Phi(X)} = 1 + \big(\mathrm{e}^{\Phi(X)} - 1\big)$:

$$\mathrm{e}^{-\beta H_\Lambda} = \prod_{X\in\mathcal{B}_\Lambda} \Big[1 + \big(\mathrm{e}^{\Phi(X)} - 1\big)\Big] = \sum_{\mathcal{B}\subset\mathcal{B}_\Lambda} \xi_{\mathcal{B}} \tag{9}$$

with

$$\xi_{\mathcal{B}} = \sum_{\widetilde{\mathcal{B}}\subset\mathcal{B}} (-1)^{|\mathcal{B}\setminus\widetilde{\mathcal{B}}|}\, \mathrm{e}^{-\beta H_{\widetilde{\mathcal{B}}}} = \xi_{\mathcal{B}_1}\cdots\xi_{\mathcal{B}_n} \tag{10}$$

$\{\mathcal{B}_1 \ldots, \mathcal{B}_n\}$ = maximally connected families of $\mathcal{B}$

Quantum: left identity in (9) is false, but last one is *true* (Möbius transform)

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Möbius transform

- $\mathcal{S}$ finite set,
- $\mathbb{V}$ vector space (product irrelevant, can be non-commutative),
- $F, G : \{\text{subsets of } \mathcal{S}\} \longrightarrow \mathbb{V}$

Then,

$$F(C) = \sum_{B \subset C} G(B) \; \forall C \quad \Longleftrightarrow \quad G(B) = \sum_{A \subset B} (-1)^{|B \setminus A|} F(A) \; \forall B$$

Möbius transform plus compatibility

In addition we assume a compatibility relation "$\sim$" such that

$$C_1 \sim C_2 \implies \left\{ \begin{array}{l} C_1 \cap C_2 = \emptyset \\ F(C_1 \cup C_2) = F(C_1)F(C_2) \end{array} \right\} \tag{11}$$

Then

$$C_1 \sim C_2 \implies G(C_1 \cup C_2) = G(C_1)\, G(C_2)$$

Say C is ***connected*** if

- C can not decomposed into two compatible subsets;
- $\equiv C$ is connected wrt the incompatibility relation

Then each $G(B)$ can be factored into contributions due to maximally connected components

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General gas expansion

Bottom line:

Theorem (General gas expansion)

Let $F : \{\textit{subsets of } \mathcal{S}\} \longrightarrow \mathbb{V}$ *satisfying* (11). *Then,*

$$F(C) \;=\; F(\emptyset) + \sum_{n=1}^{\infty} \sum_{\substack{\{B_1,\dots,B_n\} \\ \text{conn. } B_i \subset C}} \prod_{i=1}^{n} G(B_i) \prod_{1\le i<j\le n} \mathbf{1}_{\{B_i \sim B_j\}} \qquad (12)$$

with

$$G(B) \;=\; \sum_{A\subset B} (-1)^{|B\setminus A|} F(A)$$

Quantum gas expansion

For our basic application,

- $\mathcal{S} = \mathcal{B}_\Lambda$
- $\mathcal{B}_1 \sim \mathcal{B}_2$ if $X_1 \cap X_2 = \emptyset$ for all $X_1 \in \mathcal{B}_1$ and $X_2 \in \mathcal{B}_2$
- $F(\beta) = \mathrm{e}^{-\beta H_{\mathcal{B}}}$ ($H_{\mathcal{B}}$= *partially turned-on Hamiltonian*)

Then,

$$\mathrm{e}^{-\beta H_\Lambda} \;=\; 1 + \sum_{n=1}^{\infty} \sum_{\substack{\{\mathcal{B}_1,\ldots,\mathcal{B}_n\} \\ \text{conn.}\, \mathcal{B}_i \subset \mathcal{B}_\Lambda}} \prod_{i=1}^{n} \xi_{B_i} \prod_{1\le i<j\le n} \mathbf{1}_{\{\mathcal{B}_i \sim \mathcal{B}_j\}} \qquad (13)$$

with

$$\xi_{\mathcal{B}} \;=\; \sum_{\widetilde{\mathcal{B}} \subset \mathcal{B}} (-1)^{|\mathcal{B} \setminus \widetilde{\mathcal{B}}|}\, \mathrm{e}^{-\beta H_{\widetilde{\mathcal{B}}}}$$

Quantum partition functions as gas expansions

If we take the tr_Λ of the previous expansion (recall that the trace factorizes)

Theorem

The quantum partition function takes the form

$$Z_\Lambda \;=\; 1 + \sum_{n=1}^{\infty} \sum_{\substack{\{\mathcal{B}_1,\ldots,\mathcal{B}_n\} \\ \mathrm{conn.}\mathcal{B}_i \subset \mathcal{B}_\Lambda}} \prod_{i=1}^{n} \rho_{\mathcal{B}_i} \prod_{1\le i<j\le n} \mathbf{1}_{\{\mathcal{B}_i \sim \mathcal{B}_j\}} \;, \tag{14}$$

with

$$\rho_{\mathcal{B}} \;:=\; \sum_{\widetilde{\mathcal{B}} \subset \mathcal{B}} (-1)^{|\mathcal{B}\setminus\widetilde{\mathcal{B}}|}\, Z_{\widetilde{\mathcal{B}}} \quad , \; Z_{\mathcal{B}} \;:=\; \mathrm{tr}_\Lambda\Big(\mathrm{e}^{-\beta \sum_{X\in\mathcal{B}} \Phi(X)}\Big) \tag{15}$$

(Partially-turned-on partition functions)

Comments

- The form (15) of the fugacities is inspired in work by Park (1982), itself related to Greenberg (1969)
- These authors, however, mannouvered towards KS equations, and never wrote a full-fledged cluster expansion
- The expansion (13) can be subjected to other linear factorizable forms:
  - Can consider quantum boundary conditions
  - Can prove uniqueness of KMS=Gibbs state

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Convergence in terms of interactions

The cluster expansion takes of $\log Z_\Lambda$ the form (2)

We apply the fundamental convergence criterion (26) bounding $\rho_{\mathcal{B}}$ in terms of the interaction.

For the classical case,

$$\xi_{\mathcal{B}} = \sum_{\widetilde{\mathcal{B}} \subset \mathcal{B}} (-1)^{|\mathcal{B} \setminus \widetilde{\mathcal{B}}|} \, \mathrm{e}^{-\beta H_{\widetilde{\mathcal{B}}}} = \prod_{X \in \mathcal{B}} \left(\mathrm{e}^{-\beta \|\Phi(X)\|} - 1 \right)$$

For the quantum case this becomes an upper bound (Park)

$$\|\rho_{\mathcal{B}}\| \leq \prod_{X \in \mathcal{B}} \left| \mathrm{e}^{-\beta \|\Phi(X)\|} - 1 \right|$$

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Convergence criterion

This leads to convergence conditions

$$\sum_{\substack{\mathcal{B}\in\mathcal{P} \\ \mathcal{B}\,\text{connected} \\ \underline{\mathcal{B}}=Y}} \prod_{X\in\mathcal{B}} \left| e^{\beta\|\Phi(X)\|} - 1 \right| \;\le\; \lambda_Y$$

with

$$\lambda_Y \;\le\; \operatorname{argmax}_{\boldsymbol{\mu}} \left\{ \frac{\mu_Y}{\varphi_Y(\boldsymbol{\mu})} \right\}$$

Weaker explicit bounds

Change variables to $\mu_Y = \lambda_Y \, e^{a(Y)}$

The condition over $\boldsymbol{\lambda}$ becomes

$$\sup_{x \in X_0} \sum_{\substack{X \in \mathcal{P} \\ x \in X}} \lambda_X \, e^{a(X)} \leq e^{a(X_0)/|X_0|} - 1 \, ,$$

for each $X_0 \in \mathcal{P}$, for some $\boldsymbol{a} \in [0, +\infty)^{\mathcal{P}}$

[Improved Gruber-Kunz bound]

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- This dependence is usually not much off the mark.
- Optimization involves the single parameter a.

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Simplest bound

With this choice, the convergence condition is

$$T(a) \;\leq\; \mathrm{e}^{a} - 1 \tag{16}$$

with

$$T(a) \;:=\; \sup_{x} \sum_{n\geq 1} \sum_{\substack{\{X_1,\ldots,X_n\} \\ x\in X_1,\, G_n \text{ connected}}} \prod_{i=1}^{n} \left| \mathrm{e}^{\beta\|\Phi(X_i)\|} - 1 \right| \mathrm{e}^{a|X_i|}. \tag{17}$$

Notice that, for our criterion to apply,

$$\exists\, \alpha > 0 \quad : \quad \sup_{x\in\mathbb{Z}^d} \sum_{\substack{x\in X\subset\mathbb{Z}^d \\ X \text{ finite}}} \left| \mathrm{e}^{\|\Phi(X)\|} - 1 \right| \mathrm{e}^{\alpha|X|} < \infty\,.$$

Simplest bound

With this choice, the convergence condition is

$$T(a) \;\leq\; \mathrm{e}^{a} - 1 \tag{16}$$

with

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Sufficient condition for applicability

The above condition is equivalent to

$$\exists\, \alpha > 0 \quad : \quad \sup_{x \in \mathbb{Z}^d} \sum_{\substack{x \in X \subset \mathbb{Z}^d \\ X \text{ finite}}} \|\Phi(X)\|\, \mathrm{e}^{\alpha |X|} < \infty\,.$$

- Classical: Also necessary (Dobrushin-Martirosyan, 1988).
- Quantum: required for the existence of the dynamics.
- A posteriori, the above approximations are not that bad.

β-radius of analyticity

To disentangle the β-dependence: $|e^z - 1| \le z\, e^z$, $(z > 0)$
We obtain as sufficient condition

$$|\beta|\ \|\Phi\|_\infty \ \le\ \max_{a>0} W\left[\Gamma_\Phi(a)\right]$$

- W = Lambert function.
- $\Gamma_\Phi(a)$ includes a fixed-point condition.

Bounds for nearest-neighbor interactions

Our bound:

$$|\beta|\, \mathrm{e}^{|\beta|} \;\leq\; \frac{0.097619}{2d}\;.$$

Park (1982):

$$|\beta|\, \mathrm{e}^{|\beta|} \;\leq\; \frac{0.06}{2d}\Big(1+\frac{0.06}{2d}\Big)$$

[Ours = 62% improvement]

Simon (1993) (Example 2, page 462):

$$|\beta|\, \mathrm{e}^{|\beta|} \;\leq\; \frac{1}{48\, d^2}$$

[worse than Park's.]

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