On the spectral gap in mean field spin systems

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Work in progress with Simone Warzel

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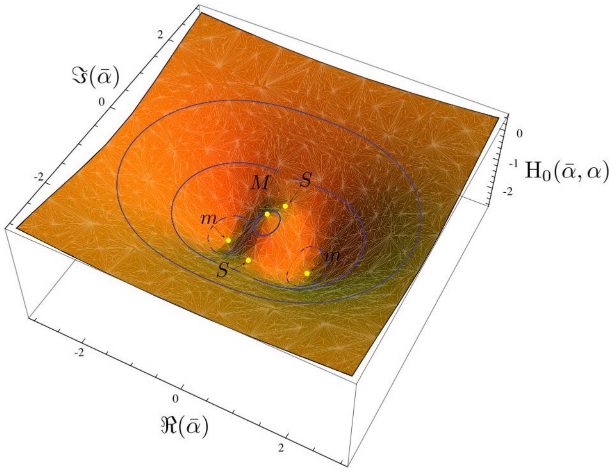


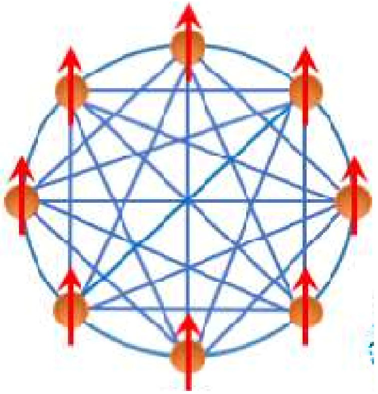
MCQST

DFG Deutsche Forschungsgemeinschaft

I. Thermodynamics of mean field models

Setup: N particles of spin s, Hilbert space $\mathcal{H}_N = (\mathbb{C}^{2s+1})^{\otimes N}$

fixed pair interaction $A = A^* \in \mathcal{B}((\mathbb{C}^{2s+1})^{\otimes 2})$



Mean field Hamiltonian: $H_N = \sum_{m \neq n} A(m, n)$

More general: p-interactions:

$$H = \sum_{n} A^{(1)}(n) + \sum_{m \neq n} A^{(2)}(m, n) + \sum_{k \neq m \neq n} A^{(3)}(k, m, n) + \cdots$$

with exchange symmetric p-spin interactions $A^{(p)}$

Pressure of mean-field models

pressure: $p_N(\beta) := \frac{1}{N} \ln Z_N(\beta) := \frac{1}{N} \ln \operatorname{Tr} e^{-\beta H}$

Approach based on quantum de Finetti theorem:

infinite volume thermal state $\omega_\beta = \int d\mu_\beta(\rho)\, \omega_\rho$ with $\omega_\rho = \rho^{\otimes\infty}$; ρ one particle density matrix

Fannes-Spohn-Verbeurre'80

$$p(\beta) = \lim_{N\to\infty} p_N(\beta) = \sup_{\varrho} \left[I(\varrho) - \beta \left(\operatorname{Tr} A^{(1)}\varrho + \operatorname{Tr} A^{(2)} \varrho \otimes \varrho + \dots \right) \right]$$

with entropy $I(\varrho) = -\operatorname{Tr} \varrho \ln \varrho$.

Maximizers satisfy self-consistent eqn.: $\varrho = e^{-\beta H_\varrho} / Z_\varrho(\beta)$ $\quad H_\varrho = A^{(1)} + \operatorname{Tr}_2 A^{(2)} \varrho + \dots$

Example: Exchange Hamiltonian $T(\psi \otimes \phi) := \phi \otimes \psi$ on $\mathbb{C}^d$

$$\operatorname{Tr} T \varrho \otimes \varrho = \sum_{i,j} \lambda_i \lambda_j \operatorname{Tr} T |u_i\rangle\langle u_i| \otimes |u_j\rangle\langle u_j| = \sum_i \lambda_i^2$$

$$\Rightarrow p(\beta) = \sup_{\lambda \in \Delta^d} \textstyle\sum_i -\beta\lambda_i^2 - \lambda_i \ln \lambda_i$$

Björnberg 15, ...

Mean-field spin systems

From now on $\mathbf{s} = \mathbf{1/2}$: model may be rewritten as

$$H = N\, P\left(\tfrac{2}{N}\, \mathbf{S}\right) \qquad \text{on} \quad \bigotimes_{n=1}^{N} \mathbb{C}^2$$

with a multivariate polynomial P

and $\mathbf{S} = \sum_{n=1}^{N} \mathbf{S}(n)$ the vector of **total spin**.

Prototype: $H = -\frac{2^p}{N^{p-1}} \left(\alpha S_z^p + \beta S_y^p \right) - 2\gamma S_x$ $\qquad \alpha = 1, \beta = 0$: Quantum p-Curie-Weiss

Why interesting? Mean-field models ('Kac potentials') in effective descriptions for:

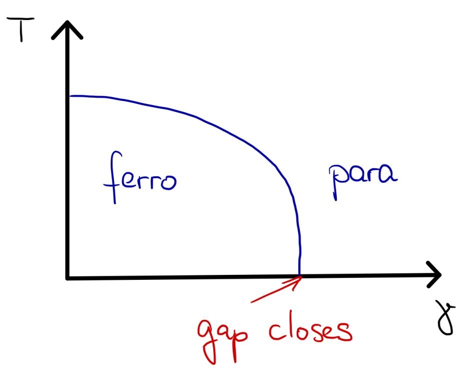
shape transitions of nuclei — Lipkin-Meshkov-Glick 65, ...

interacting Bosons in a double well — Turbiner '88, ... Cirac-Lewenstein-Mølmer-Zoller '98, ...

quantum annealing — Bapst-Semerjian '12, ...

- Equilibrium statistical mechanics and phase transitions
- **Spectral gap** away from quantum critical points

..., Fannes-Spohn-Verbeurre '80, ..., Ribeiro-Vidal-Mosseri '08, ...
Cayes-Crawford-Ioffe-Levit '08, ..., Björnberg-Fröhlich-Ueltschi '20, ...

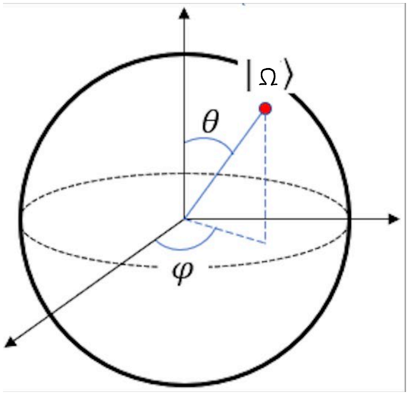


Bloch coherent states

Spin J operators: $[S_x, S_y] = iS_z$ (and cyclically) $S_\pm = S_x \pm iS_y$ on Hilbert space $\mathbb{C}^{2J+1}$

Bloch coherent state: $\Omega = (\theta, \varphi), \quad 0 \le \theta \le \pi, \ 0 \le \varphi \le 2\pi$

$$|\Omega\rangle := \exp\left(\frac{\theta}{2}\left(e^{i\varphi}S_- - e^{-i\varphi}S_+\right)\right)|J\rangle$$



Properties:

Concentration: $|\langle\Omega'|\Omega\rangle|^2 = [\cos(\Delta(\Omega', \Omega)/2)]^{4J}$ Overcompleteness: $\frac{2J+1}{4\pi}\int d\Omega\,|\Omega\rangle\langle\Omega| = \mathbb{1}$

Symbols of a linear operator G on $\mathbb{C}^{2J+1}$

Lower: $g(\Omega) := \langle\Omega|G|\Omega\rangle$ Upper: $G = \frac{2J+1}{4\pi}\int d\Omega\, G(\Omega)\,|\Omega\rangle\langle\Omega|$

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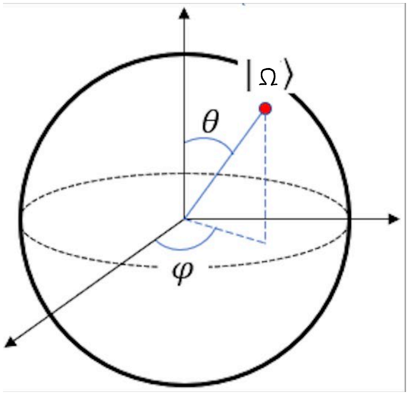

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Lower: $g(\Omega) := \langle \Omega | G | \Omega \rangle$

Upper: $G = \frac{2J+1}{4\pi} \int d\Omega\, G(\Omega)\, |\Omega\rangle\langle\Omega|$

Operator	$g(\Omega)$, (2.15)	$G(\Omega)$, (2.13)
S_z	$J\cos\theta$	$(J+1)\cos\theta$
S_x	$J\sin\theta\cos\varphi$	$(J+1)\sin\theta\cos\varphi$
S_y	$J\sin\theta\sin\varphi$	$(J+1)\sin\theta\sin\varphi$
${S_z}^2$	$J(J-\frac{1}{2})(\cos\theta)^2 + J/2$	$(J+1)(J+3/2)(\cos\theta)^2 - \frac{1}{2}(J+1)$
${S_x}^2$	$J(J-\frac{1}{2})(\sin\theta\cos\varphi)^2 + J/2$	$(J+1)(J+3/2)(\sin\theta\cos\varphi)^2 - \frac{1}{2}(J+1)$
${S_y}^2$	$J(J-\frac{1}{2})(\sin\theta\cos\varphi)^2 + J/2$	$(J+1)(J+3/2)(\sin\theta\cos\varphi)^2 - \frac{1}{2}(J+1)$

Lieb ’73

Mean-field models

H is block diagonal with respect to the decomposition of the Hilbert space according to total spin:

$$\bigotimes_{n=1}^{N} \mathbb{C}^2 \equiv \bigoplus_{J=\frac{N}{2}-\lceil\frac{N}{2}\rceil}^{N/2} \bigoplus_{\alpha=1}^{M_J} \mathbb{C}^{2J+1}$$

Basic observation / assumption: For some smooth $h : B_1(\mathbb{R}^3) \to \mathbb{R}$ and some $C \in [0,\infty)$:

$$\sup_N \sup_{J,\alpha} \left\| P_J^{(\alpha)} H P_J^{(\alpha)} - \frac{2J+1}{4\pi} \int d\Omega \, N \, h\big(\tfrac{2J}{N}\, \mathbf{e}(\Omega)\big) \, |\Omega, J\rangle\langle\Omega, J| \right\| \leq C$$

For polynomial Hamiltonian $H = N\, P\left(\frac{2}{N}\, \mathbf{S}\right)$: $\quad P = h$

Example: p-Curie-Weiss: $\quad h_p(r\mathbf{e}(\Omega)) = -r^p \cos^p\theta - \gamma r \sin\theta \cos\varphi, \quad r \in [0,1],\ \mathbf{e}(\Omega) = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}$

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Free energy becomes semiclassical in the limit $J \to \infty$

Semiclassical estimates on the quantum partition function of Hamiltonian G — Berezin, Lieb '73

$$\frac{2J+1}{4\pi} \int d\Omega \; e^{-\beta g(\Omega)} \leq \operatorname{Tr} e^{-\beta G} \leq \frac{2J+1}{4\pi} \int d\Omega \; e^{-\beta G(\Omega)}$$

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Consequence of Berezin-Lieb bounds for $N \to \infty$:

$$Z_N(\beta) = \operatorname{Tr} e^{-\beta H} = \sum_J M_J \operatorname{Tr} P_J^{(\alpha)} e^{-\beta P_J^{(\alpha)} H P_J^{(\alpha)}} \simeq \sum_J M_J (2J+1) \int \frac{d\Omega}{4\pi} \, e^{-\beta N h\left(\frac{2J}{N} \mathbf{e}(\Omega)\right)}$$

$$p(\beta) = \lim_{N\to\infty} N^{-1} \ln Z_N(\beta) = \max_{r\in[0,1]} \left[I(r) - \beta \min_{\Omega} h\big(r\mathbf{e}(\Omega)\big) \right]$$

with binary entropy $I(r) = -\frac{1+r}{2} \ln \frac{1+r}{2} - \frac{1-r}{2} \ln \frac{1-r}{2}$.

II. Ground-state and spectral gap

Motivating questions: Finite-size corrections to pressure?

Ground-state & **spectral gap** from semiclassical info $h \in C^2$ for models of form:

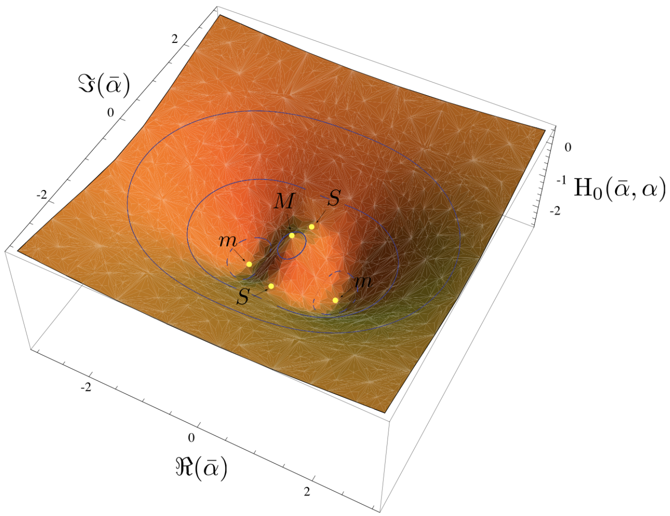
Basic assumption: For some smooth $h : B_1(\mathbb{R}^3) \to \mathbb{R}$ and some $C \in [0, \infty)$:

$$\sup_N \sup_{J,\alpha} \left\| P_J^{(\alpha)} H P_J^{(\alpha)} - \frac{2J+1}{4\pi} \int d\Omega\, N\, h\big(\tfrac{2J}{N}\, \mathbf{e}(\Omega)\big)\, |\Omega, J\rangle\langle\Omega, J| \right\| \leq C$$

Physicist's approach ???

$$\text{gap}\, H \approx \frac{1}{\text{Density of states at ground-state}}$$

Ribeiro-Vidal-Mosseri '08, . . . , Bapst-Semerjian '12, . . .



Lipkin-Meshkov-Glick model $p = 2$ with $\alpha = \frac{5}{2}$, $\beta = \frac{3}{2}$, $\gamma = -1$

semiclassical $h(\mathbf{m})$ at $|\mathbf{m}| = 1$ in stereographic coordinates

Set-up

Minimizers: $\mathcal{M} = \left\{ \operatorname{argmin} h(\mathbf{m}) \in B_1(\mathbb{R}^3) \right\}$

Assumption: $\mathcal{M} = \{\mathbf{m}_0\}$

- $\nabla h(\mathbf{m}_0) \parallel \mathbf{m}_0$ if $|\mathbf{m}_0| = 1$ or $\nabla h(\mathbf{m}_0) = 0$ else.
- **Subspace** at minimizing direction:

$$\mathcal{H}_J^K(\mathbf{m}_0) = \operatorname{span}\left\{ \psi \in \mathbb{C}^{2J+1} \mid \mathbf{m}_0 \cdot \mathbf{S}\, \psi = |\mathbf{m}_0|\,(J-k)\psi \text{ for some } k \in \{0,,1,\ldots,K\} \right\}$$

Quadratic approximation of h at $\mathbf{m}_0 \in B_1(\mathbb{R}^3)$ leads to:

$$Q_J(\mathbf{m}_0) := c + N\, h(\mathbf{m}_0) + 2\left(\mathbf{S} - \tfrac{N}{2}\mathbf{m}_0\right) \cdot \nabla h(\mathbf{m}_0) + \tfrac{2}{N}\mathbf{S} \cdot D_\perp(\mathbf{m}_0)\mathbf{S} \quad \text{on } \mathbb{C}^{2J+1}$$

with $D_\perp(\mathbf{m}_0)$ the Hessian of h projected on the directions perpendicular to $\mathbf{m}_0$.

Assumption on quadratic approximability at minimum $|\mathbf{m}_0| = 1$:

Let $P_{J,N}^{(\alpha)}$ be the projection onto $\mathcal{H}_J^{N^{1/6}}(\mathbf{m}_0) \subset \mathbb{C}^{2J+1}$. Then for all $J \geq \frac{N}{2} - N^{1/6}$:

$$\left\| (H - Q_J(\mathbf{m}_0)) P_{J,N}^{(\alpha)} \right\| = o(1)$$

- Trivially satisfied for $H = N \operatorname{Pol}_2\left(\frac{2}{N}\, \mathbf{S}\right)$.

Spectral gap in case $|\mathbf{m}_0| = 1$

Theorem (M.-Warzel '22)

Let $\omega_{1/2}$ are the eigenvalues of $D_\perp(\mathbf{m}_0)$ at $|\mathbf{m}_0| = 1$. Then

$$\operatorname{gap} H = 2\min\{\|\nabla h(\mathbf{m}_0)\|, \sqrt{(\|\nabla h(\mathbf{m}_0)\| + \omega_1)(\|\nabla h(\mathbf{m}_0)\| + \omega_2)}\} + o(1).$$

is the spectral gap above the unique ground state in case the rhs is strictly positive.

- Explicit asymptotic value also for ground-state energy and eigenvector as apparent from following

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Proof idea: w.l.o.g. $\mathbf{m}_0 = \mathbf{e}_z$ and $\nabla h(\mathbf{e}_z) = -\|\nabla h\|\, \mathbf{e}_z \neq 0$.

The 'outermost' irreducible subspaces corresponding to $\mathbf{S}^2 = J(J+1)$ with $J \geq \frac{N}{2} - N^{1/6}$ are decomposed into 'close to' and 'far from min': $\mathbb{C}^{2J+1} \equiv \mathcal{H}_J^{N^{1/6}}(\mathbf{m}_0) \oplus \mathcal{H}_J^{N^{1/6}}(\mathbf{m}_0)^\perp$.

On $\mathcal{H}_J^{N^{1/6}}(\mathbf{m}_0)$ the Hamiltonian is to $o(1)$ approximated by $Q_{N/2}(\mathbf{e}_z)$ which is of the form

$$\begin{aligned} Q_{N/2}(\mathbf{e}_z) - c_J + N\, h(\mathbf{m}_0) &= \|\nabla h\|\, (N - 2S_z) + \frac{2}{N}\left(\omega_1 S_x^2 + \omega_2 S_y^2\right) \\ &= \|\nabla h\| \, \frac{N^2 - 4S_z^2}{2N} + \frac{2}{N}\left(\omega_1 S_x^2 + \omega_2 S_y^2\right) + o(1) \\ &= \|\nabla h\| \left[\frac{N}{2} - \frac{2J(J+1)}{N}\right] + \frac{2}{N}\left[(\omega_1 + \|\nabla h\|)S_x^2 + (\omega_2 + \|\nabla h\|)S_y^2\right] + o(1) \end{aligned}$$

Note: $\left[\sqrt{\tfrac{2}{N}}S_x, \sqrt{\tfrac{2}{N}}S_y\right] = i\, 2S_z/N = i\,(1 + o(1))$.

Spectral gap in case $|\mathbf{m}_0| = 1$

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Since $h(\mathbf{m}) \geq h(\mathbf{e}_z) + c\,|\mathbf{m}_z - \mathbf{e}_z|$ for some $c > 0$, we have

$$H \geq c_J + Nh(\mathbf{e}_3) + c|2S_z - N|.$$

On $\mathcal{H}_J^{N^{1/6}}(\mathbf{m}_0)^\perp$, the last term causes a shift of $\mathcal{O}(N^{1/6})$. □

No gap in case $|\mathbf{m}_0| < 1$

Similar arguments as in the previous proof:

The quadratic approximation $Q_J(\mathbf{m}_0))$ near $J = N|\mathbf{m}_0|/2$ still yields the low-energy spectrum in those subspaces in the orthogonal decomposition:

$$\bigoplus_{J=\frac{N}{2}-\lceil\frac{N}{2}\rceil}^{N/2} \bigoplus_{\alpha=1}^{M_J} \mathbb{C}^{2J+1}$$

There are however $M_{N|\mathbf{m}_0|/2}$ copies corresponding to a fixed J.

Theorem (M.-Warzel '22)

If $|\mathbf{m}_0| < 1$ the ground state is exponentially degenerate above which the gap to the next eigenvalue vanishes with N.

Summary

Semiclassical criteria & expressions for spectral gaps in mean-field systems of N spin-$\frac{1}{2}$:

$$\text{If } |\mathbf{m}_0| = 1: \qquad \operatorname{gap} H = 2\min\{\|\nabla h(\mathbf{m}_0)\|, \sqrt{(\|\nabla h(\mathbf{m}_0)\| + \omega_1)(\|\nabla h(\mathbf{m}_0)\| + \omega_2)}\} + o(1).$$

Related results & questions:

- Limiting laws for spectral density, large deviation principles for observables ...
- Spectral gap in the Lebowitz-Penrose limit
- Generalization spin–$\frac{1}{2}$ to spin-s
- Semiclassical time evolutions
- ...

Hepp-Lieb '73, ..., Petz-Raggio-Verbeure '88, Raggio-Werner '88, ..., Fröhlich-Knowles-Lenzmann '07,
..., Cayes-Crawford-Ioffe-Levit '08, ...