Introduction to Quantum Spin Systems

Lecture 5: SU(2)-invariant two-spin interactions

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SU(2)-invariant two-spin interactions

In almost all model Hamiltonians the most important, if not all, interaction terms are two-spin interactions, i.e., a self-adjoint $h_{x,y} \in \mathcal{A}_{\{x,y\}}$. For simplicity we will restrict ourselves here to the case where all spins are of equal magnitude S. Then, at each $x \in \Lambda$, we have a copy of the $2S+1$-dimensional irrep $D^{(S)}$ of $SU(2)$. h commuting with $D^{(S)} \otimes D^{(S)}$ are necessarily of the form

$$h = \sum_{j=0}^{2S} c_j P^{(j)}$$

with $c_j \in \mathbb{R}$ if $h = h^*$.

The Heisenberg interaction

The primary example of such h is the Heisenberg interaction

$$h = S^1 \otimes S^1 + S^2 \otimes S^2 + S^3 \otimes S^3$$

It will often be convenient to use indices to distinguish between tensor factors, e.g., $h = \mathbf{S}_0 \cdot \mathbf{S}_1$. The spectrum of h is easily found by considering its relation to the Casimir invariant $C = (\mathbf{S}_0 + \mathbf{S}_1) \cdot (\mathbf{S}_0 + \mathbf{S}_1) = \sum_{j=0}^{2S} j(j+1)P^{(j)}$:

$$\begin{aligned} h &= \frac{1}{2}\left[C - \mathbf{S}_0 \cdot \mathbf{S}_0 - \mathbf{S}_1 \cdot \mathbf{S}_1\right] = \frac{1}{2}\left[C - 2S(S+1)\mathbb{1}\right] \\ &= \sum_{j=0}^{2S} \left(\frac{1}{2}j(j+1) - S(S+1)\right)P^{(j)} . \end{aligned}$$

Polynomials of the Heisenberg interaction

Clearly, for any polynomial $Q(x) = a_0 + a_x + a_2 x^2 + \cdots a_n x^n$, with real coefficients $a_0, \ldots, a_n$, the operator $Q(h)$ also commutes with $SU(2)$ and is self-adjoint. Due to the finiteness of the spectrum of h, the number of linearly independent $Q(h)$ is finite (in fact, that number is $2S+1$ and the set of monomials of degree $\leq 2S$ is a basis). As a consequence, for any given half-integer value of S, there are unique polynomials $Q_j, j = 0, \ldots, 2S$, such that $P^{(j)} = Q_j(h)$.

Spin $1/2$

In the case $S = 1/2$, h itself is the only nontrivial interaction. Indeed,

$$h = -\frac{3}{4}P^{(0)} + \frac{1}{4}P^{(1)} = \frac{1}{4}\mathbb{1} - P^{(0)}$$

and, therefore,

$$(\frac{1}{4}\mathbb{1} - h)^k = (P^{(0)})^k = P^{(0)} = \frac{1}{4}\mathbb{1} - h$$

Another useful relation involves the transposition operator $T(u \otimes v = v \otimes u$:

$$T = P^{(1)} - P^{(0)},\ T^2 = \mathbb{1},$$

in terms of which we have

$$h = \frac{1}{2}(T - \frac{1}{2}\mathbb{1})$$

Spin 1

$$\begin{aligned} h^0 &= P^{(0)} + P^{(1)} + P^{(2)} \\ h^1 &= -2P^{(0)} - P^{(1)} + P^{(2)} \\ h^2 &= 4P^{(0)} + P^{(1)} + P^{(2)} \end{aligned}$$

From these expressions we can solve for the $P^{(j)}$:

$$\begin{aligned} P^{(0)} &= -\frac{1}{3}\mathbb{1} + \frac{1}{3}h^2 \\ P^{(1)} &= \mathbb{1} - \frac{1}{2}h - \frac{1}{2}h^2 \\ P^{(2)} &= \frac{1}{3}\mathbb{1} + \frac{1}{2}h + \frac{1}{6}h^2 \end{aligned}$$

Interactions with ferromagnetic ground states

We will call a two-spin interaction h, ferromagnetic if the eigenspace belonging to the smallest eigenvalue of h is the subspace of maximal total spin, i.e., with spectral projection $P^{(2S)}$. If all the interactions of a model with nearest-neighbor interactions on a graph are ferromagnetic, the model will have ferromagnetic ground states, i.e., on any finite subgraph the states with maximal total spin are ground states. E.g., this is always the case for the negative Heisenberg interaction itself:

$$H_\Lambda = -\sum_{(xy)\in\Lambda} J_{xy}\mathbf{S}_x \cdot \mathbf{S}_y$$

with $J_{xy} \geq 0$, is ferromagnetic.

Ferromagnetic Interactions for Spin 1 models

Let $h = \mathbf{S}_0 \cdot \mathbf{S}_1$ denote the Heisenberg interaction for $S = 1$ spins. Up to a trivial additive constant, the most general SU(2)-invariant two-spin interaction is then given by

$$J_1 h + J_2 h^2 = (-2J_1 + 4J_2)P^{(0)} + (-J_1 + J_2)P^{(1)} + (J_1 + J_2)P^{(2)}$$

The eigenvalue belonging to spin 2, $J_1 + J_2$, will be the smallest if

$$J_1 \leq 0, \text{ and } J_1 \leq J_2$$

Spin waves in the $S = 1/2-$ Heisenberg Model

The Hamiltonian is

$$H_\Lambda = -J \sum_{|x-y|=1, x,y\in\Lambda} \mathbf{S}_x \cdot \mathbf{S}_y = -\frac{J}{2} \sum_{|x-y|=1, x,y\in\Lambda} (t_{xy} - \frac{1}{2}\mathbb{1}),$$

with $J > 0$ and t_{xy} the unitary interchanging the tensor factors labeled by x and y.
Recall that the ground states are the symmetric states, which coincide with the SU(2) irrep of total spin $|\Lambda|/2$, the maximum possible value for the system. (under the assumption that Λ, considered as a graph with edges given by the distance 1 pairs, is connected.)

Clearly the ground states of the ferromagnetic model are the eigenvectors with smallest eigenvalue of the operator

$$\tilde{H}_\Lambda = - \sum_{|x-y|=1, x,y\in\Lambda} t_{xy}$$

Consider Λ as a graph with N vertices $x \in \Lambda$ and E edges (xy) given by the nearest neighbor pairs.

Theorem

Suppose Λ considered as a graph is connected. Then, the smallest eigenvalue of $\tilde{H}_\Lambda$ is $-E$ and its eigenspace has dimension $N + 1$ and consist of all vectors symmetric under permutations of the vertices.

Proof

Let $\{e_-, e_+\}$ be an o.n. basis of $\mathbb{C}^2$, and $\lambda_0(A)$ the smallest eigenvalue of a matrix A.

Observation 1)

For any Hermitian operators, $\lambda_0(A+B) \geq \lambda_0(A) + \lambda_0(B)$. (For any hermitian matrix the lowest eigenvalue satisfies the variational principle $\lambda_0(A) = \inf_{\psi \neq 0} \langle A \rangle_\phi$. Thus $\lambda_0(A+B) = \inf_{\psi \neq 0} \langle A+B \rangle_\psi$, while for any ψ, $\langle A+B \rangle_\psi = \langle A \rangle_\psi + \langle B \rangle_\psi \geq \lambda_0(A) + \lambda_0(B)$, which proves the observation.) Apply this to $\tilde{H}$ to obtain $\lambda_0(\tilde{H}) \geq -E$.

Observation 2)

$$\tilde{H}(\bigotimes_{x \in \Lambda} e_+) = -E \bigotimes_{x \in \Lambda} e_+$$

which implies that $\lambda_0(H)$ does equal $-E$.

Observation 3) If $\lambda_0(A+B) = \lambda_0(A) + \lambda_0(B)$ then $(A+B)\phi = \lambda_0(A+B)$ implies $A\phi = \lambda_0(A)\phi$ and $B\phi = \lambda_0(B)\phi$. (For a hermitian matrix A, ψ is an eigenvector for $\lambda_0(A)$ iff $\langle A \rangle_\psi = \lambda_0(A)$. Now suppose $\lambda_0(A+B) = \lambda_0(A) + \lambda_0(B)$ and ϕ is a ground state for $A+B$. Then

$$\langle A \rangle_\phi + \langle B \rangle_\phi = \langle A+B \rangle_\phi = \lambda_0(A+B) = \lambda_0(A) + \lambda_0(B)$$

Also, $\langle A \rangle_\phi \geq \lambda_0(A)$ and $\langle B \rangle_\phi \geq \lambda_0(B)$. So we have $\langle A \rangle_\phi = \lambda_0(A)$ and $\langle B \rangle_\phi = \lambda_0(B)$. And this implies $A\phi = \lambda_0(A)\phi$ and $B\phi = \lambda_0(B)\phi$.) Apply this to determine $H\phi = -E\phi$ only if $t_{xy}\phi = \phi$ for all $(xy) \in \Lambda$.

Observation 4) If Λ is a connected graph then any permutation of its vertices, π, can be written as a product of transpositions τ_{xy} where (xy) is an edge in the graph. Apply this to deduce that for any ground state ϕ, $U_\pi \phi = \phi$ for all permutations π, where U_π is the unitary determined by its action on simple tensors:

$$U_\pi(v_1 \otimes \cdots \otimes v_N) = v_{\pi_1} \otimes \cdots \otimes v_{\pi_N}$$

So, all ground states have to be permutation-invariant vectors, and vice-versa if $U_\pi \phi = \phi$ for all π then $t_{xy}\phi = \phi$ for all x, y (because $t_{xy} = U_{\tau_{xy}}$). An o.n. basis of permutation invariant vectors is given by

$$\psi_k = \frac{1}{N!} \sum_{\pi \in \mathrm{Perm}(\Lambda)} U_\pi(\underbrace{(e_- \otimes \cdots \otimes e_-)}_{k} \otimes \underbrace{(e_+ \otimes \cdots \otimes e_+)}_{N-k})$$

for $k = 0, 1, \cdots, N$.
This is also the maximum spin irreducible representation contained in $\otimes_{x \in \Lambda} \mathcal{D}^{(1/2)}$. More about that later.

(Let $\mathcal{G}$ be the group generated by $\{\tau_{xy} : (xy) \in \Lambda\}$. Prove by induction that $\tau_{xy} \in \mathcal{G}$ for all i and j, vertices in Λ. Induction is on

$$d(x, y) = \min\{n : (xx_2), (x_2x_3), \ldots, (x_{n-1}y) \in \Lambda\}$$

For $d(x, y) = 0$ it is trivial that $\tau_{xx} = id \in \mathcal{G}$. For the induction step assume that $\tau_{xy} \in \mathcal{G}$ whenever $d(x, y) \leq n$. If $d(x, y) = n + 1$ let $x_2, \cdots, x_n$ be a sequence s.t. $(xx_2), \ldots, (x_ny) \in \Lambda$. Then $\tau_{xx_n}, \tau_{x_ny} \in \mathcal{G}$ by the induction hypothesis. So $\tau_{xy} = \tau_{x_ny}\tau_{xx_n}\tau_{x_ny} \in \mathcal{G}$. Since the permutation group is generated by all transpositions, $\mathcal{G} = \mathrm{Perm}(\{x : x \in \Lambda\})$.)

Excited states; Spin waves

Note that the subspace $\mathcal{H}_\Lambda^{(S)}$ of the Hilbert space $\mathcal{H}_\Lambda$ belong to any given value S of the total spin is an invariant subspace. We just proved that the ground state space is $\mathcal{H}_\Lambda^{(S_{\max})}$, where $S_{\max} = |\Lambda|/2$.

It is reasonable to guess that the next-to-lowest eigenvalue would have an eigenvector in $\mathcal{H}_\Lambda^{(S_{\max}-1)}$. Next week, Stephen will some cases where we have a proof of this. For now, let us consider the Hamiltonian restricted to the invariant subspace with $S = S_{\max} - 1$, starting with the case where $\Lambda = \mathbb{Z}/\mathbb{Z}_L$, the one-dimensional lattice $[1, L]$ considered with periodic boundary conditions (a ring with L vertices).

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By the SU(2) symmetry, I will find all eigenvalues of the Hamiltonian restricted to $\mathcal{H}_\Lambda^{(S_{\max}-1)}$ if we diagonalize its restriction to the subspace of eigenvectors of $S_1^3+\cdots+S_L^3$ with eigenvalue $S_{\max}-1$. Consider the o.n. basis of this eigenspace given by the vectors $\psi_x, x\in[1,L]$, such that

$$S_y^3\psi_x=\frac{1}{2}((1-\delta_{xy})-\delta_{xy}).$$

It is now straightforward to calculate the matrix of $H_{[1,L]}$ restricted to $V_L=\operatorname{span}\{\psi_x \mid x\in[0,L]\}$ with this basis:

$$\langle\psi_y,H_{1,L]}\psi_x\rangle=(L-2)\delta_{xy}-(\delta_{y,x-1}+\delta_{y,x+1}),\quad 1\le x,y\le L,\quad \text{mod } L.$$

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The matrix is $(2-L)\mathbb{1}+T_L$, where

$$T_L=-\begin{bmatrix}0&1&0&0&\cdots&1\\1&0&1&0&\cdots&0\\\vdots&\cdots&\ddots&&\cdots&\vdots\\1&\cdots&&0&1&0\end{bmatrix}$$

The eigenvalue equation for T_L is easily written as follows:

$$T_L\phi=\lambda\phi;\quad \phi_0=\phi_{L+1};\quad \phi_{x-1}+\phi_{x+1}=-\lambda\phi_x,\quad 1\le x\le L$$

of which the solutions are given by $\lambda_n=-2\cos k_n, \phi_{n,x}=e^{ik_nx}$, with $k_n=2n\pi/L$, for $n=0,\dots,L-1$. The corresponding eigenvalues for the Hamiltonian are $-L+2(1-\cos k_n)$. Note that $n=0$ corresponds to a ground state. As L increases the eigenvalues fill up the interval $[-L,-L+4]$. In the limit $L\to\infty$, after resettting the ground state energy to 0, the system has a band of continuous spectrum above the ground state, $[0,4]$. One says that the spectrum of low-lying excitations is *gapless*.