Introduction to Quantum Spin Systems Lecture 1

Bruno Nachtergaele

Mathematics, UC Davis

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Outline

What are Quantum Spin Systems?

Three reasons to study Quantum Spin Systems

Physics Mathematics Computer Science

Seminar organization

Quantum Systems with Finite-Dim. State Space

A Quantum Spin System (QSS) is a quantum system consisting of a collection of subsystems, each with a finite-dimensional Hilbert space of states.

States, for now, are $\psi \in \mathcal{H}$, $\|\psi\| = 1$, where \mathcal{H} is a complex Hilbert space. At first, we will only consider finite collections of spins and therefore dim $\mathcal{H} < \infty$, $\mathcal{H} \cong \mathbb{C}^n$, $n \ge 2$ (n = 1 is possible but trivial).

We call ψ a state because it is the mathematical object that allows one to calculate (model, predict, ...) the statistics of the outcomes of any measurement (observation) that can be performed on the corresponding physical system.

In general, there may be more than one mathematical way to represent a physical state of a system (e.g., density matrices). In simple cases one can describe a procedure to recover ψ from a set of measurements (quantum state tomography). A measurable quantity is mathematically represented by an **observable**, in this case a Hermitian linear transformation of \mathcal{H} : $A = A^* \in \mathcal{B}(\mathcal{H}) \cong M_n(\mathbb{C}).$

The mean or expectation of A in the state ψ is given by

$$\omega_{\psi}(\mathbf{A}) = \langle \psi, \mathbf{A}\psi \rangle.$$

Here, $\langle \cdot, \cdot \rangle$ denotes the inner product of \mathcal{H} . Following the convention most common in mathematical physics (as in physics, but not mathematics), our inner products are antilinear in the first and linear in the second argument.

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Example: spin 1/2-system, aka two-level atom, aka qubit (quantum bit). $\mathcal{H} = \mathbb{C}^2$. The basic observables for this system are the three Pauli matrices $\sigma^1, \sigma^2, \sigma^3$, which together with the identity matrix form a basis of $M_2(\mathbb{C})$:

$$\sigma^{0} = \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma^{1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$\sigma^{2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma^{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

As observables, $\sigma^1, \sigma^2, \sigma^3$ represent the components of the spin thought of as a vector in \mathbb{R}^3 .

Let (e_1, e_2) be the canonical orthonormal basis of \mathbb{C}^2 . For $a, b \in \mathbb{C}, |a|^2 + |b|^2 = 1, \psi = ae_1 + be_2$ is normalized vector and

$$\omega_{\psi}(\sigma^1) = \overline{a}b + \overline{b}a, \quad \omega_{\psi}(\sigma^3) = |a|^2 - |b|^2, etc.$$

The spin matrices are $S^{\alpha} = \frac{1}{2}\sigma^{\alpha}$, i = 1, 2, 3, and

$$[S^{lpha},S^{eta}]=i\epsilon_{lpha,eta,\gamma}S^{\gamma}$$

I.e., they generate the Lie algebra su(2), closely related to the rotations in \mathbb{R}^3 .

To be able to determine the full statistics of an observable quantity, we should be able to determine its moments and perhaps the characteristic function. It is therefore natural that the mathematical objects representing observables form an algebra of observables. If we lift the restriction that *A* is Hermitian, we have $A \in M_2(\mathbb{C})$, which is indeed an algebra and it makes sense to calculate quantities such as the variance of *A*:

$$\omega_{\psi}((\mathbf{A} - \omega_{\psi}(\mathbf{A}))^2),$$

and the characterisitic function:

$$f_{\psi,A}(\mathbf{x}) = \omega_{\psi}(\mathbf{e}^{i\mathbf{x}A}).$$

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In general then, a finite quantum system is described by a Hilbert space \mathcal{H} and a subalgebra \mathcal{A} of $\mathcal{B}(\mathcal{H})$ describing the observables. We assume that \mathcal{A} is closed for the *-operation and the operator norm, making it a *C**-algebra. We will always assume $\mathbb{I} \in \mathcal{A}$.

A state, in general, is a linear functional $\omega : \mathcal{A} \to \mathbb{C}$ with the properties $\omega(A^*A) \ge 0$, for all $A \in \mathcal{A}$ (positivity), and $\omega(\mathbb{1}) = 1$ (normalization).

If A happens to be abelian, the Riesz theorem tells us that states are in one-to-one correspondence with Borel probability measures on a compact space. Quantum systems, however, have non-abelian algebras of observables. In this sense, states generalize the notion of probability measures. $\rho \in \mathcal{B}(\mathcal{H})$ is called a density matrix if ρ is non-negative definite, trace class, and such that $\text{Tr}\rho = 1$. We will be primarily concerned with the finite-dimensional case. In that case, $\mathcal{H} = \mathbb{C}^n$, $\mathcal{A} = M_n$, the complex $n \times n$ matrices and all matrices are trace class.

Exercise: If ρ is a density matrix on M_n , then ω defined by

$$\omega(\mathbf{A}) = \mathrm{Tr}\rho\mathbf{A},\tag{1}$$

is state on M_n .

Exercise: The states ω on $\mathcal{A} = M_n(\mathbb{C})$ are in one-to-one correspondence with the $n \times n$ density matrices, i.e., for each state ω , there exists a unique density matrix $\rho \in M_n$ such that (1) holds.

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Interpretation: if $A = A^* \in M_n$, we have a spectral decomposition of the form $A = \sum_i \lambda_i P_i$, where the P_i are mutually orthogonal orthogonal projection and $\lambda_i \in \mathbb{R}$. We can assume $\sum_i P_i = \mathbb{1}$. Then, $p_i = \omega(P_i) \ge 0$ and $\sum_i p_i = 1$ and can be interpreted as the probabilities that A is found to take the value λ_i in a physical measurement of the quantity represented by A.

The problem in the physics and mathematics of quantum spin systems is to define and analyze the specific states that describe real experiments.

Physics

The theory of quantum spin systems was started by Heisenberg in 1926, shortly after the discovery that particles (electron, nuclei, atoms,...) have an intrinsic angular momentum called spin (Stern-Gerlach (1922, atoms), Goudsmit and Uhlenbeck (1925)). Heisenberg (and independently Dirac) proposed the exchange interaction. He introduced the model Hamiltonian named after him which remains till today the primary quantum spin model studied in mathematics and physics. It is essential to describe magnetic properties of matter and is an essential component in our understanding of many phenomena in condensed matter.

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Mathematics

In 1931 Hans Bethe introduced his famous *Ansatz*, which allowed him to 'solve' the one-dimensional Heisenberg model. The Bethe Ansatz is now not just a tool, but almost a field of research all by itself. Its development and application to a variety of other models repeatedly gave rise to the introduction of new structures and techniques studied in many areas of mathematics (algebra, algebraic geometry, representation theory, combinatorics,....)

The notion of quantum group is an example of an important mathematical structure that arose directly out of work on the Bethe Ansatz.

Its general impact on the development of representation theory of infinite-dimensional Lie and affine algebras is hard to overestimate.

CS: Quantum Information and Computation

Church-Turing thesis: *If we can compute a function f by a terminating procedure (algorithm), then we can construct a Turing machine for it.*

Turing machine:

- tape that can hold a string of binary data: $(\ldots, s_i, s_{i+1}, \ldots)$
- a head which holds one of a finite number of internal states q
- a function $(s, q) \mapsto (s', q', \pm 1)$.

The head reads state s_i at position *i*, depending on its state *q*, computes (s'_i, q') , and determines to move right or left (± 1) . Repeat until halt.

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The classical computer

The classical programmable computer is a universal Turing machine, meaning that it can simulate any Turing machine, much like a real computer but without the size limit. Universal or not, we can think of the Turing machine as executing a sequence of transformations on a string of bits (logic circuit): - memory to hold the internal states, the input bit string, and blank space

- an implementation of the algorithm as a sequence of logical gates acting on *k* bits at a time.

For all we know, the Church-Turing thesis holds.

Can be generalized to include the use of random bits: probabilistic algorithms.

Quantum computation (QC)

New ideas about the physical implementation of computation may change our ideas of what computable means, and perhaps the Church-Turing thesis does not hold in a more general context.

In QC bit strings are replaced by complex linear combinations of bit strings: $\psi \in \mathcal{H}_N$,

$$\psi = \sum_{s_1,\ldots,s_N=\pm 1} c_{s_1,\ldots,s_N} \ket{s_1,\ldots,s_N},$$

and logic gates are replaced by unitary transformations. Instead of reading of the answer at the end, perform a measurement following the prescriptions of quantum mechanics.

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Quantum circuits

Input + ancillas (internal states, spare memory) stored as a unit vector

$$\psi \in \mathcal{H}_{N} = \underbrace{\mathbb{C}^{2} \otimes \cdots \otimes \mathbb{C}^{2}}_{N}$$

Logic gates now become unitary operators on \mathcal{H} . They are assumed to *k*-local, meaning that they act as the identity on all but at most *k* of the tensor factors.

It is sometimes useful to replace *qbits* by *qdits* with a *d* dimensional state space \mathbb{C}^d .

The circuit is then of the form

$$C=\prod_{i=1}^{T}U(i)$$

Without loss of generality (properly interpreted) we can assume that each U(i) acts on 2 bits and is taken from a finite set of fundamental gates (Kitaev).

The circuit then takes the following form:

figure

In the simplest case the measurement is represented by an orthogonal projection *P*. The result of the computation is 'yes' (1), with probability $\|PC\psi\|^2$. If this probability is, say, 3/2 when the answer is in fact 'yes', we can verify this with any degree of certainty we want, by independently repeating the computation a number of times.

Quantum circuits generalize deterministic and probabilistic classical logic circuits.

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Quantum circuits include the classical case

The classical logic gates can be represented by permutations of the set of standard basis vectors in \mathcal{H}_N (provided we use ancillas).

The set of quantum circuits is vastly richer than the subset that represents the classical ones.

There is a lot of good evidence (but no proof yet) that quantum computers are qualitatively more powerful than classical computers.

The Hamiltonian class

Consider finite quantum systems of the following form:

- Finite collection of quantum systems (spins, qubits, qudits, atoms, quantum dots, ...) labeled by x ∈ Λ.
- ► Each system has a finite-dimensional Hilbert space \mathcal{H}_x . For simplicity, we assume dim $\mathcal{H}_x = r$, for all $x \in \Lambda$. The Hilbert space describing the total system is

$$\mathcal{H}_{\Lambda} = \bigotimes_{x \in \Lambda} \mathcal{H}_x.$$

The algebra of observables of the system is

$$\mathcal{A}_{\Lambda} = \bigotimes_{x \in \Lambda} \mathcal{B}(\mathcal{H}_x) = \mathcal{B}(\mathcal{H}_{\Lambda}).$$

If $X \subset \Lambda$, we have $\mathcal{A}_X \subset \mathcal{A}_\Lambda$, by identifying $A \in \mathcal{A}_X$ with $A \otimes \mathbb{I}_{\Lambda \setminus X} \in \mathcal{A}_\Lambda$.

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Interactions

The subsystems (qdits) interactions modeled by map Φ from the set of subsets of Λ to \mathcal{A}_{Λ} such that $\Phi(X) \in \mathcal{A}_X$, and $\Phi(X) = \Phi(X)^*$, for all $X \subset \Lambda$. The Hamiltonian is

$$H=\sum_{X\subset\Lambda}\Phi(X).$$

One says that *H* is *k*-local if for all *X* with |X| > k, $\Phi(X) = 0$. In the quantum computation it is common to assume that $\|\Phi(X)\| \le 1$, for all $X \subset \Lambda$.

The Schrödinger dynamcis is defined by the unitary group $U(t) = e^{-itH}$ on \mathcal{H}_{Λ} .

Ground states and the spectral gap

 H_{Λ} : finite system, includes boundary conditions described by additional terms in the Hamiltonian.

Ground state: eigenvector with eigenvalue $E_0 = \inf \operatorname{spec} H$. Spectral gap above the ground state: if dim $\mathcal{H}_{\Lambda} < \infty$, and H has eigenvalues $E_0 < E_1 < E_2 < \ldots$, we define $\gamma = E_1 - E_0 > 0$. In general

 $\gamma = \sup\{\delta \ge 0 \mid \operatorname{spec} H_{\Lambda} \cap (E_0, E_0 + \delta) = \emptyset\} \ge 0.$

If E_0 is simple, one says that the system has a unique (or non-degenerate) ground state.

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Organization

- Credit: 1 unit for attending, 3 units for giving a presentation on a topic mutually agreed upon with the instructor. If you signed up for 3 units, or plan to, please see me this week.
- Notes will be posted on ~bxn. Look for the link Introduction to Quantum Spin Systems under Seminars. http://www.math.ucdavis.edu/~bxn/ introduction_to_qss.html
- I will be away January 10, February 21, March 7.