Properties of Quantum Spin Systems and their Classical Limit

joint work with prof. Valter Moretti, prof. Klaas Landsman, Dr. Robin Reuvers & prof. Gerrit Groenenboom

Christiaan van de Ven

University of Trento

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Overview

• Quantum Curie-Weiss Hamiltonian as a discretization of a Schroedinger operator with a symmetric double well potential.

- Scientific paper yet available on the ArXiv. 'Quantum spin systems versus Schroedinger operators: A case study in spontaneous symmetry breaking'.

• Deformation quantization & application to quantum spin systems with their classical limit, special emphasis to spontaneous symmetry breaking (SSB).

- Publication in preparation.

Quantum Curie-Weiss Hamiltonian as a 1d discretization of a Schroedinger operator with a symmetric double well potential.

Properties of the quantum Curie-Weiss model

• Quantum Curie-Weiss Hamiltonian h_N^{CW} defined on $\mathcal{H}_N = \bigotimes_{n=1}^N \mathbb{C}^2$ by:

$$h_N^{CW} = -\frac{J}{2N}\sum_{i,j=1}^N \sigma_3(i)\sigma_3(j) - B\sum_{i=1}^N \sigma_1(i). \tag{1}$$

• Existence of an invariant subspace for h_N^{CW} and a basis such that the restriction to this subspace represented in this basis is a tridiagonal matrix. One can show that the ground state is in the subspace.

• This subspace is the symmetric subspace $\text{Sym}^N(\mathbb{C}^2)$, namely the range of the symmetrizer $S_N = \frac{1}{N!}\sum_{\sigma\in \mathbf{S}_N} L_\sigma$. The corresponding basis is the canoncial (Dicke) basis $\{|k, N-k\rangle\}$, where the vectors $|k, N-k\rangle$ are given by permutations of qubits:

$$|k, N-k\rangle = \frac{1}{\sqrt{\binom{N}{k}}}\sum_{j,l} P_{j,l}\,|\underbrace{\uparrow\uparrow\cdots\uparrow}_{\text{k times}}\underbrace{\downarrow\downarrow\cdots\downarrow}_{\text{N-k times}}\rangle, \quad (k = 0, ..., N). \tag{2}$$

Discretization: uniform case

• Principle: a process to approximate derivatives by linear combinations of function values at grid points.

• We focus on the central difference approximation method and apply this to the second order differential operator d^2/dx^2, which we would like to discretize with uniform grid spacing of $\Delta = 1/N$ on the domain $\Omega = [0, 1]$.

• The second order derivative for a single-variable smooth function f is then approximated by

$$f_i'' \approx \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta^2} \quad (i = 1, ..., N), \tag{3}$$

where $f_i = f(x_i) = f(i\Delta)$.

Discretization: uniform case

• In matrix form we find

$$f'' \approx \frac{1}{\Delta^2} \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & \mathbf{0} & \\ & \ddots & \ddots & \ddots & \\ & \mathbf{0} & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix} f. \tag{4}$$

• This matrix is the result of a central finite difference discretization method of the second order derivative on a uniform grid consisting of N points of length $\Delta \cdot N$, with uniform grid spacing Δ. In this specific case, we have $\Delta = 1/N$. We denote this tridiagonal matrix by $\frac{1}{\Delta^2}[\cdots 1 \; -2 \; 1 \cdots]_N$.

Discretization: uniform case

• The other way around: suppose we are given a symmetric tridiagonal matrix A of dimension N with constant off- and diagonal elements,

$$A = \begin{pmatrix} b & a & & & \\ a & b & a & \mathbf{0} & \\ & \ddots & \ddots & \ddots & \\ & \mathbf{0} & a & b & a \\ & & & a & b \end{pmatrix} \tag{5}$$

• Goal: rewrite this matrix as a sum of kinetic and potential energy:

$$A = a[\cdots 1 \ \frac{b}{a} \ 1 \cdots]_N = a[\cdots 1 \ -2 \ 1 \cdots]_N + \mathrm{diag}(b + 2a). \tag{6}$$

Discretization: uniform case

• It follows that $A = T + V$, , for $T = a[\cdots 1 \;\; -2 \; 1 \cdots]_N$, and $V = \mathrm{diag}(b + 2a)$.

• In view of the above, the matrix T corresponds to a discretization of a second order differential operator (kinetic energy), with uniform grid spacing $1/\sqrt{a}$ on the grid of length $N/\sqrt{a}$. Since the matrix V is a diagonal matrix, it can be seen as a multiplication operator. Hence, we can identify A with a discretization of a Schrödinger operator.

• Apply this idea to the quantum Curie-Weiss tridiagonal matrix $\rightarrow$ extract a discretized Schroedinger operator.

Curie-Weiss versus Schroedinger operator

• The Curie-Weiss tridiagonal matrix will be interpreted as an approximation (N large) of a $1d$ discretized Schrödinger operator on $L^2[0, 1]$ with a symmetric double well potential $V_N(x)$:

$$-\frac{1}{L^2N^2}\frac{d^2}{dx^2} + V_N(x), \tag{7}$$

where $1/N$ plays the role of $\hbar$.

• Idea: split the tridiagonal matrix into two parts, one corresponding to the kinetic energy and the other to the potential energy.

• Main problem, our tridiagonal matrix does not have constant off-diagonal elements (entries even vary with the dimension), so we cannot apply the previous theory directly.

Curie-Weiss versus Schroedinger operator

• However, In the semi-classical limit, the potential energy dominates the kinetic energy. We extracted this potential and observed that is has the shape of a symmetric double well.

• Spectral properties for bound states of our tridiagonal matrix and the discretization of (7), i.e., $-\frac{1}{L^2}[\cdots 1 \ -2 \ 1 \cdots]_N + V_N(x)$ have been compared. They coincide up to a very good approximation and improve with increasing N.

• Ground state is localized in the minima of these wells, and is Gaussian shaped, exactly as expected for such a Schroedinger operator.

• To conclude, the compressed quantum Curie-Weiss model can be seen as a discretization of a Schrödinger operator with a symmetric double well potential.

Deformation quantization & application to quantum spin systems with their classical limit, special emphasis to spontaneous symmetry breaking (SSB).

Introduction

• Example. Consider $h_\hbar = -\hbar \frac{d^2}{dx^2} + V(x)$, and the corresponding ground state eigenfunction $\psi_\hbar^{(0)}$, assuming the spectrum is discrete. How can $\lim_{\hbar \to 0} \psi_\hbar^{(0)}$ be interpreted?

• Framework to deal with this question exists under the name deformation quantization. Mathematical concept establishing a link between classical and quantum mechanics, using the language of C^* -algebras and the theory of Poisson manifolds.

• Basic idea: A continuous bundle of C^*-algebras over base space I consists of a C^*-algebra A, a collection of C^*-algebras $(A_\hbar)_{\hbar \in I}$ with norms $|| \cdot ||_\hbar$, and surjective homomorphisms $\varphi_\hbar : A \to A_\hbar$ for each $\hbar \in I$, such that several (continuity) properties are satisfied.

Deformation quantization

• A (strict) deformation quantization of a Poisson manifold X consists of a continuous bundle of C^*-algebras $(A, \{\varphi : A \to A_\hbar\}_{\hbar \in I})$ over I, along with maps

$$Q_\hbar : \tilde{A}_0 \to A_\hbar \quad (\hbar \in I),$$

where $\tilde{A}_0$ is a dense subspace of $A_0 = C_0(X)$, such that:

1. Q_0 is the inclusion map $\tilde{A}_0 \hookrightarrow A_0$;

2. Each map $Q_\hbar$ is linear and satisfies $Q_\hbar(f^*) = Q_\hbar(f)^*$.

3. For each $f \in \tilde{A}_0$, the following map is a continuous section of the bundle:

$$\begin{aligned} &0 \to f; \\ &\hbar \to Q_\hbar(f). \quad (\hbar > 0) \end{aligned} \tag{8}$$

4. For all $f, g \in \tilde{A}_0$ one has the Dirac-Groenewold-Rieffel condition:

$$\lim_{\hbar \to 0} || \frac{i}{\hbar}[Q_\hbar(f), Q_\hbar(g)] - Q_\hbar(\{f, g\})||_\hbar = 0.$$

• This map 'transfers' classical information to quantum data, and can therefore be used to identify classical theories as limits of quantum theories.

• Example 1. We define for any $\hbar \in [0, 1]$:

$$Q_\hbar : C_0(\mathbb{R}^2) \to B_\infty(L^2(\mathbb{R}));$$
$$Q_\hbar(f) = \int_{\mathbb{R}^2} \frac{dpdq}{2\pi\hbar} f(p, q) |\phi_\hbar^{(p,q)}\rangle\langle\phi_\hbar^{(p,q)}|,$$

where the projections $|\phi_\hbar^{(p,q)}\rangle\langle\phi_\hbar^{(p,q)}|$ are coming from so-called Schroedinger coherent states $\phi_\hbar^{(p,q)}$ on $\mathbb{R}^2$.

Deformation quantization

• Example 2. We define for any $1/N \in 1/\mathbb{N} \cup \{0\}$:

$$Q_{1/N} : C(S^2) \to B(\mathcal{H}_N);$$
$$Q_{1/N}(f) = \frac{N+1}{4\pi} \int_{S^2} d\mu(\Omega) f(\Omega) |\Omega_N\rangle\langle\Omega_N|,$$

where μ is a measure on the sphere S^2. The projections $|\Omega_N\rangle\langle\Omega_N|$ are coming from so-called spin coherent states, induced by points $\Omega \in S^2 = SU(2)/U(1)$.

• The maps $Q_\hbar$ and $Q_{1/N}$ satisfy the properties of a deformation quantization in the above sense.

• In the these two examples, both coherent states are involved to define the quantization map.

'Classical' limit

• Concerning example 2, the limit $N \to \infty$ will be defined as follows: given unit vectors $\psi_N \in \mathcal{H}_N$, we say that that these vectors have a 'classical' limit if

$$\lim_{N\to\infty} \langle \psi_N, Q_{1/N}(f)\psi_N \rangle = \omega_0(f) \quad (f \in C(S^2)), \tag{9}$$

where ω_0 is some probability measure on S^2, seen as a state on $C(S^2)$. A similar statement can be made for Example 1 sending $\hbar \to 0$, or for other quantization maps.

• In the context of Schroedinger operators (Example 1) the limit $\hbar \to 0$ typically means $m \to \infty$ at fixed $\hbar$ in $\hbar^2/2m$, so that one may physically see $\hbar \to 0$ as a special case of $N \to \infty$.

Intermezzo: Algebraic ground states and SSB

Definition

Let A be a C^*-algebra with time evolution, i.e., a continuous homomorphism $\alpha : \mathbb{R} \to \mathrm{Aut}(A)$. A *ground state* of (A, α) is a state ω on A such that:

1. ω is time independent, i.e., $\omega(\alpha_t(a)) = \omega(a)\ \forall a \in A\ \forall t \in \mathbb{R}$.
2. The generator h_ω of the ensuing continuous unitary representation

$$t \mapsto u_t = e^{ith_\omega} \tag{10}$$

of $\mathbb{R}$ on $\mathcal{H}_\omega$ has positive spectrum, i.e., $\sigma(h_\omega) \subset \mathbb{R}_+$, or equivalently $\langle \psi, h_\omega \psi \rangle \geq 0$ $(\psi \in D(h_\omega))$.

• The set of ground states forms a compact convex subset of $S(A)$, and we denote this set by $S_0(A)$. We moreover assume that pure ground states are pure states as well as ground states.

Definition

Suppose we have a C^*-algebra A, a time evolution α, a group G, and a homomorphism $\gamma : G \to \mathrm{Aut}(A)$, which is a symmetry of the dynamics α in that

$$\alpha_t \circ \gamma_g = \gamma_g \circ \alpha_t \quad (g \in G, t \in \mathbb{R}). \tag{11}$$

The G-symmetry is said to be spontaneously broken (at temperature $T = 0$) if

$$(\partial_e S_0(A))^G = \emptyset, \tag{12}$$

• Here $\mathscr{S}^G = \{\omega \in \mathscr{S} | \ \omega \circ \gamma_g = \omega \ \forall g \in G\}$, defined for any subset $\mathscr{S} \in S(A)$, is the set of G- invariant states in $\mathscr{S}$. (12) means that there are no G-invariant pure ground states. (12) means that there are no G-invariant pure ground states. This means also that if spontaneous symmetry breaking occurs, then invariant ground states are not pure.

Application to quantum spin Hamiltonians and SSB

• Special case. Assume $\psi_N^{(0)}$ is the ground state of some spin Hamiltonian on some Hilbert space $\mathcal{H}_N$ (or e.g. the ground state eigenfunction of a Schroedinger operator). Given a quantization map, in view of equation (9) one can ask if the limit exists on some commutative algebra $C(X)$.

• This is probably (numerical evidence) the case for the one-dimensional quantum Curie-Weiss model (for $X = B^3$ and some $Q_{1/N}$):

$$h_N^{QW} = -\frac{1}{N}\Big(\sum_{x,y=1}^{N} \sigma_3(x)\sigma_3(y) + B\sigma_1(x) \Big)$$

• Note that this limit (i.e. equation (9) with $\psi_N = \psi_N^{(0)}$) is different than the thermodynamic limit, where a infinite quantum spin system is considered.

Application to quantum spin Hamiltonians and SSB

• There is numerical evidence that the ground state eigenvector converges (in the above sense) to a classical mixed state given by $\omega_0^{(0)} = \frac{1}{2}(\omega_+ + \omega_-)$, where $\omega_0^{\pm}$ are Dirac measures (i.e. pure states) corresponding to the minima of the classical Hamiltonian on $C(B^3)$ which is given by $h = -(\frac{z^2}{2} + Bx)$.

• One can show that these degenerate pure classical ground states $\omega_0^{\pm}$ are not $\mathbb{Z}_2$-invariant (for $0 < B < 1$), under the homomorphism induced by the map $(x, y, z) \mapsto (x, -y, -z)$, which basically means that the pure classical ground states are not invariant under parity symmetry. According to our definition, one can show that the $\mathbb{Z}_2$-symmetry is spontaneously broken. However, for finite N it can be shown that the ground state is unique and hence $\mathbb{Z}_2$-invariant.

• Therefore, this theory also gives a mathematical explanation of spontaneous symmetry breaking (SSB).

Further research

• Generalize these type of quantization maps to more arbitrary spaces, like the state space $S(B)$ of a unital C^*-algebra B

$$Q_{1/N} : C(S(B)) \to B^{\otimes N}.$$

• Work in progress (with Valter Moretti): give a proof of the existence of a deformation quantization in the case $B = M_k(\mathbb{C})$. No coherent states, different approach is needed!

• Apply to spin Hamiltonians (e.g. quantum Curie Weiss-model or qauntum Ising model), and prove the possibly existence of classical limits. Try to understand natural emergent phenomena like SSB from this point of view.

• Different quantum Hamiltonians seem to share similar properties in their classical limit.

• Thank you for your attention! I hope you all enjoyed it.

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SSB

• The non-degenerate states $(\psi_N^{(0)}, \psi_N^{(1)})$ converge (in algebraic sense) to mixed classical states, i.e.,

$$\lim_{N\to\infty} \psi_N^{(0)} = \lim_{N\to\infty} \psi_N^{(1)} = \omega_0^{(0)},$$

where $\omega_0^{(0)} = \frac{1}{2}(\omega_0^+ + \omega_0^-)$.

• In contrast, the localized pure ground states

$$\psi_N^{\pm} = \frac{1}{\sqrt{2}}(\psi_N^{(0)} + \psi_N^{(1)}),$$

converge (in algebraic sense) to pure classical states, i.e.,

$$\lim_{N\to\infty} \psi_N^{\pm} = \omega_0^{\pm}.$$

Continuous bundle of C^*-algebras

Definition

Let I be a locally compact Hausdorff space. A continuous bundle of C^*-algebras over I consists of a C^*-algebra A, a collection of C^*-algebras $(A_\hbar)_{\hbar \in I}$ with norms $||\cdot||_\hbar$, and surjective homomorphisms $\varphi_\hbar : A \to A_\hbar$ for each $\hbar \in I$, such that

1. The function $\hbar \mapsto ||\varphi_\hbar(a)||_\hbar$ is in $C_0(I)$ for all $a \in A$.

2.The norm for any $a \in A$ is given by

$$||a|| = \sup_{\hbar \in I} ||\varphi_\hbar(a)||_\hbar. \tag{13}$$

3. For any $f \in C_0(I)$ and $a \in A$, there is an element $fa \in A$ such that for each $\hbar \in I$,

$$\varphi_\hbar(fa) = f(\hbar)\varphi_\hbar(a). \tag{14}$$

• A continuous (cross-) section of the bundle in question is a map $\hbar \mapsto a(\hbar) \in A_{\hbar}$, $(\hbar \in I)$, for which there exists an $a \in A$ such that $a(\hbar) = \varphi_{\hbar}(a)$ for each $\hbar \in I$.