



A scalable and robust technique for identifying quantum phase transitions

ICFO researchers have reformulated the ground-state problem to solve it in a way that is both efficient and scalable. This relaxation method has theoretically identified quantum phase transitions in two-dimensional bilayer quantum spin systems, mapping out their entire phase diagram. The results, published in Physical Review Letters, establish relaxation methods as robust, scalable and accurate tools for exploring the phase diagrams of complex quantum systems, offering a significant advancement over previous computational techniques.

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In quantum physics, the ground state is the lowest energy state a system can be in, and it is typically reached at temperatures close to absolute zero. Under these conditions, changing certain external parameters, such as pressure or the magnetic field, can lead to quantum phase transitions, which are driven by quantum fluctuations rather than thermal ones. A system undergoing such a transition might, for instance, switch from being a conductor to an

insulator, or from an ordered ferromagnetic phase to a disordered one.

Studying quantum phase transitions can provide insights into the fundamental quantum effects governing material properties without the complicating influence of heat, helping us understand how quantum materials can exhibit vastly different behaviors. However, finding the ground state and determining its properties is increasingly challenging for increasingly complex systems.

ICFO researchers, **Dr. David Jansen**, **Dr. Luke Mortimer**, **Timothy Heightman**, **Dr. Andreas Leitherer**, and **Dr. Pere Mujal**, led by **ICREA Prof. Antonio Acin**, in collaboration with Universita degli Studi di Napoli Federico II, State Key Laboratory of Mathematical Sciences (China), and Quside, have recently reformulated the ground-state problem into a simplified, or *relaxed*, version that can be solved more **efficiently** and **scalably**. The **relaxation method**, published in Physical Review Letters, emerges as a **novel framework for mapping out phase diagrams**, something that was showcased with two-dimensional bilayer quantum spin systems.

These relaxations, expressed through semidefinite programming (SDP), **address the weaknesses of traditional exact and variational methods**. Exact methods are restricted to relatively small systems, which makes them impractical for larger and more complex models. Variational methods, while scalable, typically provide only upper bounds on the ground-state energy and can get stuck in local minima (that is, solutions that are not the system's true lowest-energy state), offering no guarantees about the results' accuracy.

In contrast, SDP relaxations scale much better than exact methods with the system size, they are not affected by local minima (ensuring more robust results), and provide lower bound on the ground-state energy. In the study, the researchers use SDPs not only to obtain the ground-state energy, but also to extract the so-called moment vectors of the system, which encapsulate other ground-state properties. Then, by analyzing how these moment vector change as certain parameters vary, the researchers identified phase transitions, **efficiently mapping out the complete phase diagram of a two-dimensional bilayer quantum spin system**.

Our method helps determine the accuracy of ground-state variational calculations for many-body systems, as well as provides a scalable, fast way to identify regions where the quantum phase transitions take place, says Dr. David Jansen, first author of the article. According to the researcher, the next step is to apply the framework to those two-dimensional quantum systems in which standard methods have been shown to struggle.

Reference:

David Jansen, Donato Farina, Luke Mortimer, Timothy Heightman, Andreas Leitherer, Pere Mujal, Jie Wang, and Antonio Acin, Mapping Phase Diagrams of Quantum Spin Systems through Semidefinite-Programming Relaxations, Phys. Rev. Lett. **136**, 050401 (2026).

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