STRONGLY CORRELATED SYSTEMS THROUGH COMPUTATION: FROM BAD METALS TO PERFECT INSULATORS

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EXECUTIVE SUMMARY:

Emergence is the principle where complicated phenomena arise from the interaction of simple rules. Two emergent phenomena in quantum mechanics include superconductivity, with its family of exotic neighboring phases, and many-body localization. It has often been said that the hardest part about understanding superconductivity is to make sense of the adjoining phases in which it is embedded; among these phases, the "bad metal," with gapless excitations but otherwise abnormal properties, stands apart [1].

Emergent phenomena in quantum mechanics can be particularly hard to understand as the computational complexity of simulating quantum mechanics scales exponentially. Using Blue Waters, we found and numerically simulated a model that supports a 2D bad metal phase. While superconductivity is the perfect conductor, the many-body localized (MBL) phase [2,3] is the exact opposite: a perfect insulator refusing to conduct even at infinite temperature. We numerically identified properties of the MBL phase, and found the algorithmic approach we developed transfers directly to a conceptual understanding of MBL. We pushed the limits of our simulations by developing improved algorithms.

INTRODUCTION

Bad Metals

In systems where you find superconductivity, you also often find the bad metal phase; understanding the bad metal phase is a likely way to make sense of superconductors. Unfortunately a simple mean field picture of the bad metal is absent and a tractable numerical model is needed. We find that fermions with a nearest-neighbor ring exchange term [4] fit the requirements.

Many-Body Localization

Quantum mechanics is usually seen at absolute zero (temperature). At high temperature, the strange nature of quantum mechanics is washed away leaving instead the classical physics we've understood for hundreds of years. One phase of matter, the many-body localized (MBL) phase, preserves the strangeness of quantum mechanics up to arbitrary temperatures. Many-body localization is formed in systems with simultaneous disorder and interactions. It is believed to form a perfect insulator and has emergent integrability. While much of the phenomenology of this phase is understood, what has been missing until now is a unifying framework in which to describe the wave-function of the MBL phase and a numerical approach for seeing the MBL phase on large systems.

New Algorithms

The limiting factor in solving much of materials and condensed matter physics is a combination of computational power and algorithmic techniques. There are two current de-facto simulation techniques for condensed matter problems: quantum Monte Carlo and tensor networks, but new ones are needed to move forward.

METHODS & RESULTS

Bad Metals

Using projector quantum Monte Carlo we computed the phase diagram of the ring exchange Hamiltonian. In addition to finding phase separation and a charge density wave, we discovered the first 2D system that convincingly demonstrates a bad metal phase—in this case an extremal d-wave Bose metal [5]. The smoking gun for this phase was the presence of two singular lines in the structure factor where it goes to zero and linear behavior in the structure factor at small momentum. Fig. 1 shows a canonical example from our simulation. Beyond finding the phase we also discovered a surprising feature—we could not identify any ordering in the spin sector, suggesting the possibility of a spin liquid riding on top of the bad-metal state.

Many-Body Localization

We devised a conceptual framework as well as a simulation approach for capturing the MBL phase through the matrix-product operator framework. A disordered non-interacting system is described by a simple product state. By turning on interactions, the product state turns into a matrix-product state where nearby states talk but distant ones have exponentially smaller effects. This defines local quasiparticles in terms of these matrices. In this language, the varied properties of the MBL phase are transparent. In addition, we have developed and used a variant of the density matrix renormalization group algorithm to capture the "finite temperature" eigenstates of the MBL phase from which we derived the properties.

New Algorithms

We found a way to combine the positive features of both quantum Monte Carlo and tensor network methods. Of particular interest is our ability to take an important algorithm that does not parallelize and use many of its features in a massively parallel way.

WHY BLUE WATERS?

Bad Metals

Unlike classical physics where single machines are able to simulate thousands of particles, simulating quantum physics is significantly more difficult. Even systems with hundreds of particles can be a computational tour de force. Blue Waters has been essential because any systems smaller than those we consider mask the physics of the bad metal phase. The quantum Monte Carlo algorithm required to simulate the bad metal phase requires 10^6 walkers and forward walking done to large imaginary time. With the next Track-1 system one could take the next step in understanding how this bad metal phase transitions into other nearby states, including the superconductor.

Many-Body Localization

Many-body localization is a phase where disorder is fundamental. Therefore, any simulations require an average over potentially thousands of disordered configurations to produce accurate statistics. Such averaging can be done only on large machines. In addition, to date there has been no reliable method of generating finite-temperature excited states. Finding the right approach required significant experimentation and each such experiment is computationally costly.

New Algorithms

Blue Waters was essential for developing these new algorithms. Not only was it necessary for testing the massive parallelization, but the benchmarking that was required to authenticate the methods required significant computational resources.

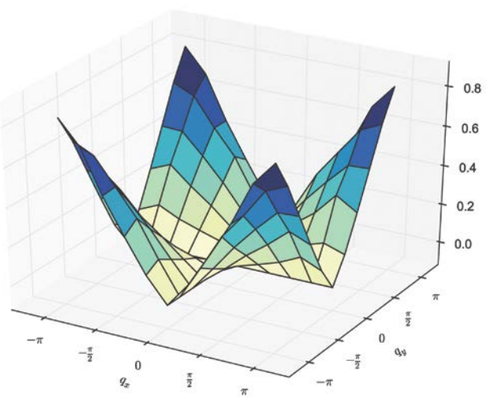

FIGURE 1: Charge structure factor of the ring-exchange Hamiltonian at density 4/10 on a 10 x 10 lattice with 10,000 walkers and tau=0.1. The singular lines show the characteristic gapless modes that are the smoking gun of the extremal DBL phase.