

ALGORITHMIC PERSPECTIVE ON STRONGLY CORRELATED SYSTEMS

(i.e. computational condensed matter)

Lecture: Introduction and Exact Diagonalization

Today: Heavy on logistics and philosophy about computing.

Later today/Thursday: Exact Diagonalization

Why computation?

Microscopic Hamiltonian



Emergent Degrees of Freedom

Computation

The act of figuring out how to get a computer to calculate properties of physical systems often gives deep understanding

All that happened at MIT was I got incredibly frustrated. Because of the slowness, nothing ever came out of that project. That was probably part of what helped me to move from actual computation to a lot of this conceptual idea of supposing that I had a computer that was big enough, which in the end, proved much more fruitful. That's the important part of the work I did through the 1960s, working with this conceptual idea of distinguishing between something that was large with finite degrees of freedom and therefore is computable and something that has infinite degrees of freedom and therefore is not. - **Ken Wilson**



Consider that tensor networks are amongst the best ways of understanding and classifying interacting topological systems.

A practical answer

Computers are getting more powerful and one of the few games in town - more problems you can solve.

Pencil and paper theorists are starting to heavily use computational techniques for strong correlations.

Leon Balent's Website

About our research (briefly):

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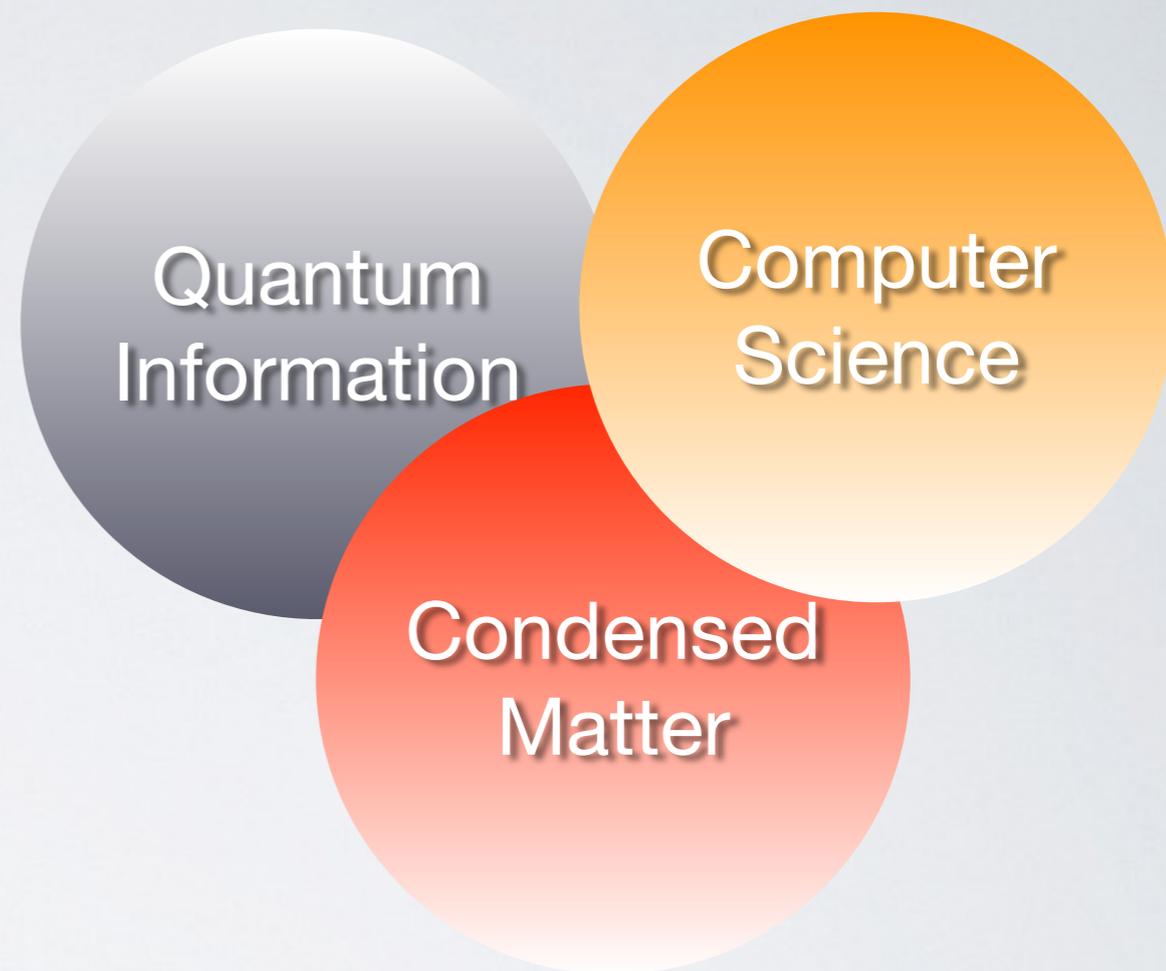
October 2011:

replica and other tricks for disorder averaging, applied mathematics and and some exact solutions. We can and do use some computational techniques as well (including rather sophisticated use of Mathematica), but stay away from really hard-core computational physics, like density functional calculations, quantum Monte Carlo, DMRG, or large-scale exact diagonalization. Luckily we have friends

October 2013:

How do we do this? We try not to rely too much on any one technique, and let the approach fit the problem. We're pretty comfortable with most analytical methods, including quantum/classical field theory, statistical mechanical methods, renormalization, symmetry analysis, replica and other tricks for disorder averaging, applied mathematics and and some exact solutions. We use computational techniques as well (including rather sophisticated use of Mathematica), and increasingly hard-core computational physics, like density functional calculations, quantum Monte Carlo, and DMRG.

We are at a tipping point in computational condensed matter; previously intractable problems are starting to be solved.

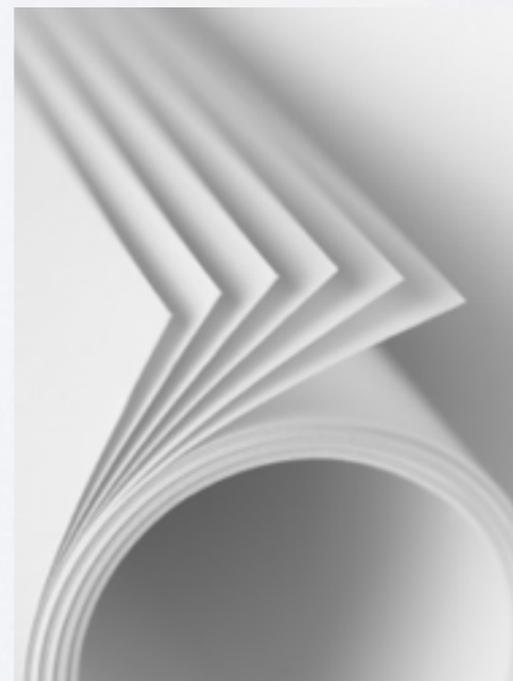


Do we need computers?

“A profound joke is that one can measure the progress of physics by the problems that can't be solved. In Newtonian gravity, the three-body problem is difficult, but the two-body problem can be done exactly; in general relativity, two bodies are difficult but one body can be done exactly; in quantum gravity, the vacuum is intractable.”

(Frank Wilczek, *Physics Today* 2003, pg. 11)

Fast forward theorem





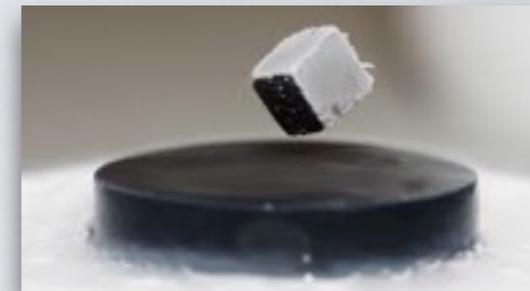
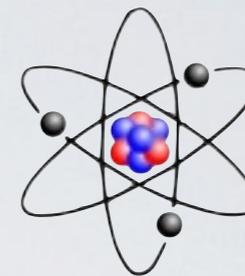
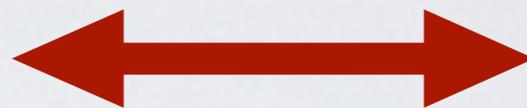
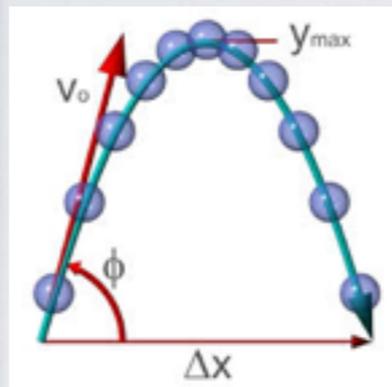
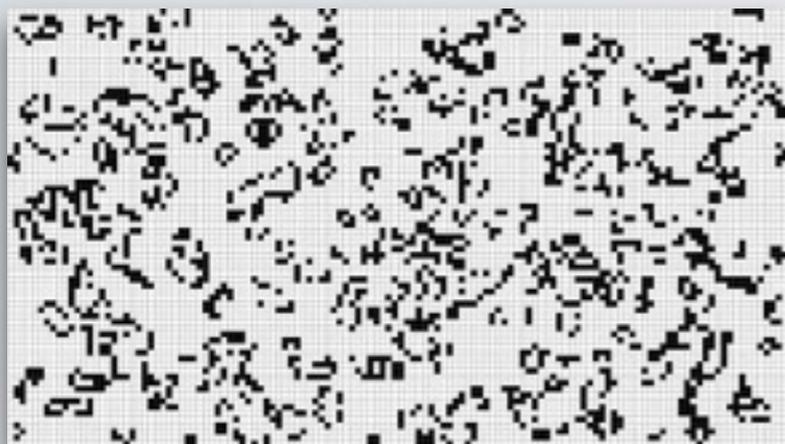
The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws lead to equations that are too complex to be solved.

- Paul Dirac

The Laws: $i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}, t) + V(\mathbf{r})\Psi(\mathbf{r}, t).$

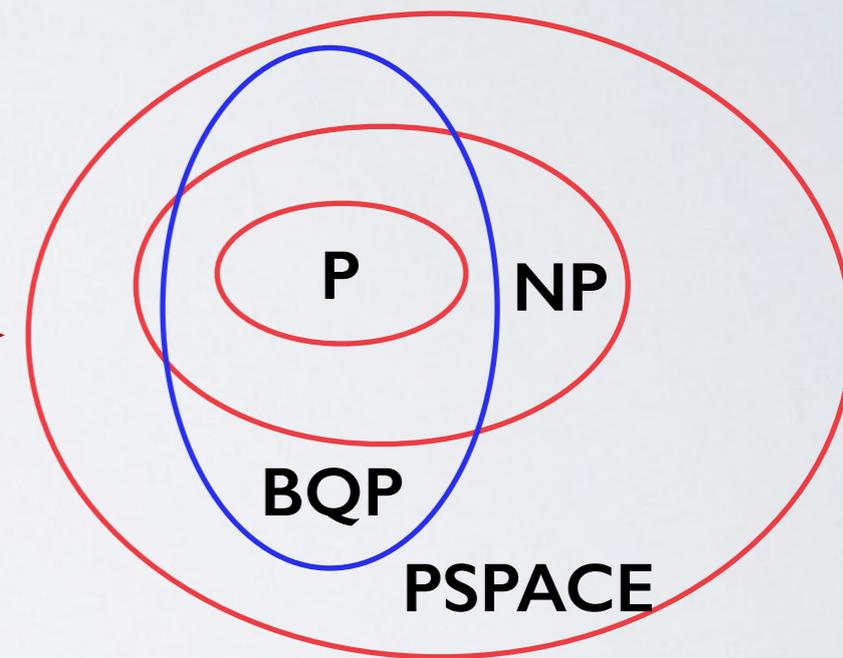
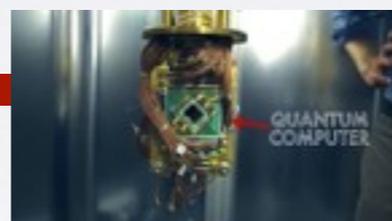
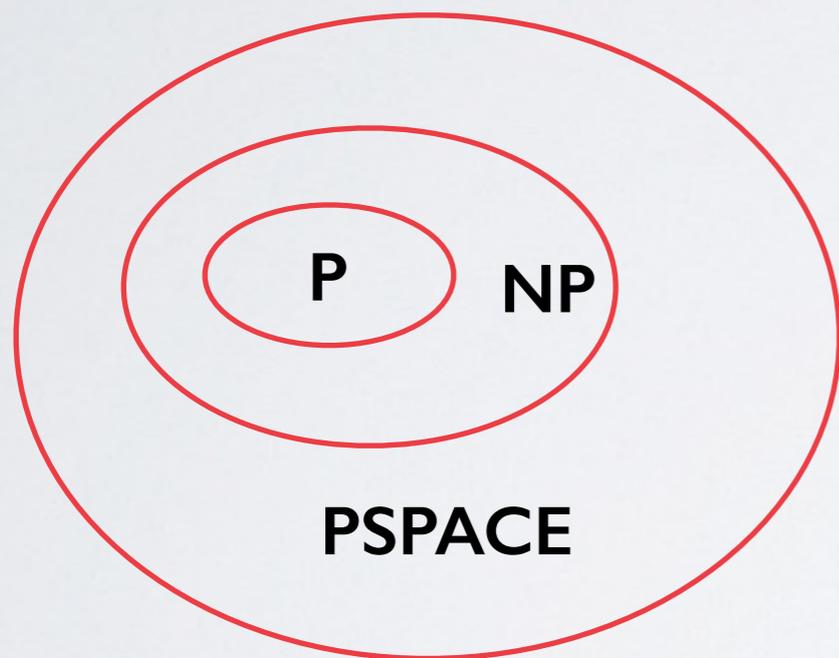
we will integrate out some unimportant degrees of freedom and end up with more minimal microscopic models in much of this class.

Classical vs. Quantum Simulation



Conway's game of life

Quantum Mechanics



(Modified) Church-Turing Thesis: All computers (physical systems) are essentially equivalent to your laptop.

Two Unifying Themes

Stochasticity and Signs

Quantum gates that are strictly real have no more power than classical computers.

Up to a question about MCMC mixing times, sign-free systems can be simulated efficiently.

Quantum Monte Carlo

Entanglement

A computation in which the entanglement stays low can be simulated. The essence of DMRG and matrix product states.

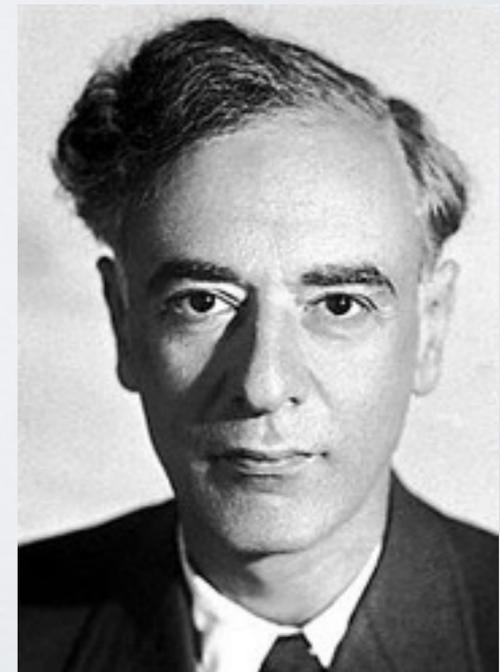
Schmidt Decomposition

Tensor Networks

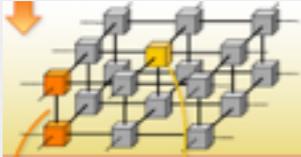
Without entanglement or signs, quantum computing stops working!

“A method is more important than a discovery, since the right method will lead to new and even more important discoveries.”

-Lev Landau



Ten algorithms that have changed the face of condensed matter.

1. Exact Diagonalization
2. Variational Monte Carlo
3. Diffusion (Projector) Monte Carlo
4. Fixed-node
5. Path Integral (World-line) Monte Carlo
6. SSE 
7. BSS
8. DMRG
9. Tensor Networks 
10. DMFT

In this course, you will learn these algorithms ranging from

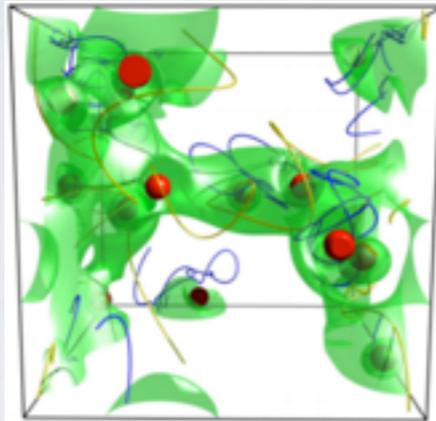
- nuts and bolts details;
- deep and beautiful algorithmic aspects;
- the way they reshape how we think about physical phenomena.

A deep question: We often say QMC fails because it propagates to the true ground state which is Bosonic. But if your matrix has a true state that is fermionic, why doesn't this solve the problem?

Fractional Quantum Hall Effect



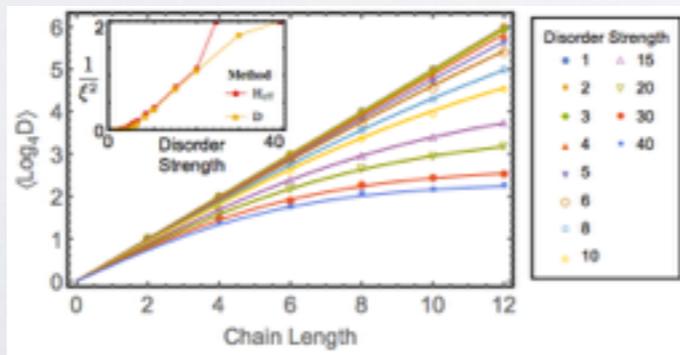
Supersolidity



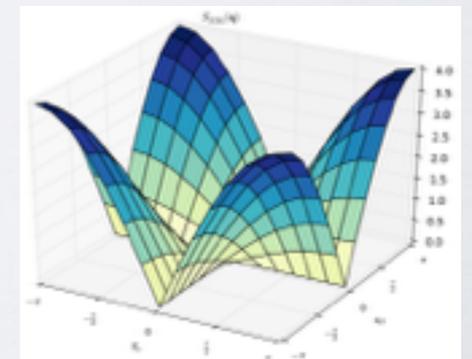
Spin liquids



Many-Body Localization



Non-fermi liquids



Course logistics

No good text (not even a bad text actually)

Not really any other course like this.

Going to learn to reason about algorithms

buzzword: Computational Thinking

understand what's going on under the hood

bring you to the research frontier

Not a:

programming course

numerical analysis course

computer science course (but a step in that direction on the physics-CS axis)

Programming language we will use for course: Julia

Why? good tradeoff of simple and fast

Office hours:

Homework

1. 4-6 problems sets
2. 'Present' one paper and discuss other papers on piazza site.
3. Final project
4. 'Module' for one lecture

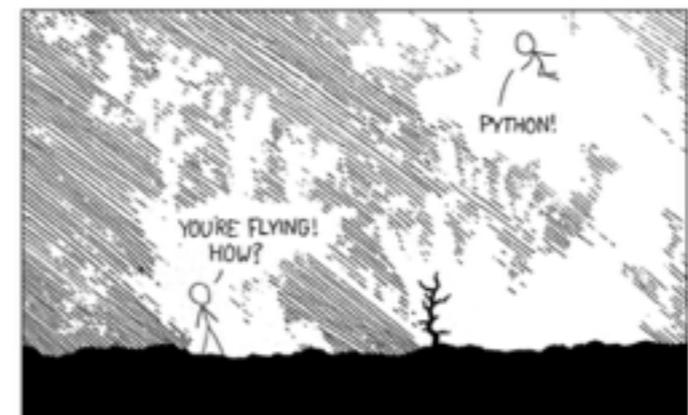
I hope you will learn a lot from the lectures but the heart of this course is the homework; this is where you will really wrestle with details and learn the materials.

This course is designed to be challenging but to bring you to the research frontier in this field.

Will try to post slides; solutions generated from your work; little partial credit for broken code;



Julia Examples



I LEARNED IT LAST NIGHT! EVERYTHING IS SO SIMPLE!
HELLO WORLD IS JUST
`print "Hello, world!"`

I DUNNO...
DYNAMIC TYPING?
WHITE SPACE?
COME JOIN US!
PROGRAMMING IS FUN AGAIN!
IT'S A WHOLE NEW WORLD UP HERE!
BUT HOW ARE YOU FLYING?

I JUST TYPED
`import ontigouty`
THAT'S IT?
... I ALSO SAMPLED EVERYTHING IN THE MEDICINE CABINET FOR COMPARISON.
BUT I THINK THIS IS THE PYTHON.

Course Outline

(currently under construction)

- Introduction (**1 day**)
 - Slides: [slides](#)
 - Additional Reading:
- Exact Diagonalization (**1 day**)
- Whirlwind introduction to Tensor Networks and QMC (**1 day**)
- Variational Ansatz (**2 weeks**)
 - Slides:
 - Additional Reading
 - [VMC Tutorial in Python](#) (you want to be running MathJax to see the equations)
- Projector Monte Carlo (**1 week**)
- World-line Monte Carlo (**1 week**)
- Determinant Monte Carlo/BSS/VBMC (**1 week**)
- DMRG (**1 week**)
- Tensor Networks (**1 week**)
- Fermion Sign Problem (**2 week**)
- Embedding Techniques: DMFT (**1 week**)
- Proof of 1D Area Law (**1 week**)
- Quantum Hamiltonian Simulations/Stabilizer Circuits/Matchgates (**1 week**)
- Perfect Tensors, QEC, and ADS/CFT (**1 week**)

Goal is to give a unified view of what appears to be many disparate algorithms.

Note: We may skip around a bit to make sure we cover the important stuff and to make the course isn't front loaded with all (or no) nuts-and-bolts details.