Numerical Methods for the Many-Electron Problem

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Part of the Simons collaboration on the many-electron problem
Collaborators

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Ibn al-Haytham (‘al Basri’), 965-1040: systematic reliance on experimentation to check theories.


Scientific Method

Prediction

Experiment

Theory

Validation

Ibn al-Haytham (‘al Basri’), 965-1040: systematic reliance on experimentation to check theories.


Quantum Electrodynamics

Theory

Introduced by Sommerfeld, 1916

Proven to be exactly

\[
\alpha = \frac{e^2}{\hbar c} \\
\alpha \approx 1/137
\]

(A. Eddington, 1938)

Proper perturbation theory:

Experiment

Relationship between elementary charge, Planck constant, and speed of light.

Direct measurement from quantum Hall plateaus

\[
\alpha^{-1} = 137.0359979(32)
\]

Recoil speed measurements on Rubidium atoms

\[
\alpha^{-1} = 137.03599878(91)
\]

Combination of QED calculation and measurement of anomalous magnetic dipole moment

\[
\alpha = 1/137.035999084(51)
\]

Hanneke et al, PRL 100, 120801 (2008)

Tomonaga, Schwinger, Feynman
Few versus many particles

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

Paul Dirac, Proc. R. Soc. A 123 (1929), 714
Complicated equations? Different physics!

- Chemistry is based on the laws of physics, Molecular biology on the laws of Chemistry, …
- The language and tools of physics are inappropriate for describing, say, social science
- New phenomena where ‘many’ objects interact, fundamentally different from ‘few’: more is different

P.W. Anderson, Science 177, 393 (1972)
Collective quantum behavior

Levitating superconductor (YBCO)

Kondo resonance of Co adsorbed on Cu. From Nature 403, 512 (2000)


A QGP is formed at the collision point of two relativistically accelerated gold ions. RHIC, BNL

Collective quantum behavior

Oxide Electronics

High-Tc and High-Hc superconductors

Catalysis

Batteries

Solar cells

Electricity transport

Transistors

MRI
approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.
Breakdown of the scientific method

Theory

\[ H = \sum_{i=1}^{N} \frac{-\hbar^2}{2m} \nabla^2 + e^2 \sum_{i<j} v_{ee}(r_i, r_j) \]

Approximate solution

\[ v_{ee}(r, r') = \frac{1}{|r - r'|} \]

Low-energy effective theory

Approximation: restriction to ‘relevant’ low-energy degrees of freedom, construction of a model

Experiment

Approximate solution of a low-energy effective model
Approximation: restriction to ‘relevant’ low-energy degrees of freedom, construction of a model
Breakdown of the scientific method

Theory

Experiment

Approximate solution

Approximate solution of a low-energy effective model

H = \sum_{i=1}^{N} -\hbar^2 \frac{\nabla^2}{2m} + e^2 \sum_{i<j} v_{ee}(r_i, r_j)

v_{ee}(r, r') = \frac{1}{|r - r'|}

Approximation: restriction to ‘relevant’ low-energy degrees of freedom, construction of a model

Many particles
No small parameters
Perturbative methods fail

No controlled analytical approaches
Competing interactions and phenomena
Scenarios dependent on approximation, parameter regime,…
Numerical Methods for the Many-Electron Problem

Investigation of strongly correlated systems

Using modern computational methods

On large computers / supercomputers

...without too much computation...?
Numerical Methods

Theory

Experiment

Computation

Validation of simple model systems

'numerical experiment'

\[ H = \sum_{i=1}^{N} \frac{-\hbar^2}{2m} \nabla^2 + e^2 \sum_{i<j} v_{ee}(r_i, r_j) \]

\[ v_{ee}(r, r') = \frac{1}{|r - r'|} \]

added realism: materials specificity / chemistry. Numbers for calibration.
Numerical Methods

\[
H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m} \nabla^2 + e^2 \sum_{i<j} v_{ee}(r_i, r_j)
\]

\[
v_{ee}(r, r') = \frac{1}{|r - r'|}
\]
In this talk

Interplay with experiment, exact solution of many-body problem

Approximate solution of a many-body problem in a difficult regime

Theory

Validation of simple model systems. Numerical experiment

Computation

Experiment

added realism: materials specificity / chemistry. Numbers for calibration.
Lattice Model & Lattice Experiment

Fermionic model systems accessible with state of the art numerics & theory

some simple fermionic models now close to solution

Fermionic model systems accessible with optical precision experiments on ultracold atomic gases
One of the most simple interacting fermionic lattice models: Electrons on the sites of a lattice, no more than two (spin up and down) per site. Energetics is governed by Hamiltonian.

\[
H = - \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}.
\]

kinetic term describes electron hopping
potential energy term describes (screened) Coulomb repulsion

Model shows collective behavior (antiferromagnetism). Can we obtain the properties of this strongly interacting quantum many-body system?
Experimental realization: 3D Hubbard Model

Fermionic gases in atomic trap, held by counter-propagating laser beams.

Cooled to ultracold temperatures

Temperatures (in relevant units) in experiment are far above correlated AFM phase.

Systems are very clean and stable, no ‘dirt’, multi-band effects, or lattice vibrations as in real systems.

Numerical simulation

Map Hamiltonian onto a cluster quantum impurity model of size $N$, numerically solve it for a range of cluster sizes:

$N = 18, 36, 48, 56, 64, 84, 100$

Compute thermodynamics: energy, density, entropy, free energy, double occupancy, spin correlation functions, ...:

Observable estimates and errors for a finite size system.

Extrapolate observable estimate to the infinite system size limit using finite size scaling
Verification and validation

Small parameter 1/N for strongly correlated systems: precise control of error bars and convergence.
Comparison at a di-mogeneous system at µ approximated by the corresponding quantities in a homogeneous system with position-dependent chemical potential which is equal to the mean of the trapping frequencies taken from the experimental data the horizontal axis denotes the initial measured total particle number averaged over the trap to compare with the experimentally measured total particle number.

Without any free parameters and assuming no heating, we find excellent agreement for entropies of the DCA+LDA calculation for different anisotropies and interaction strengths. The entropies, the experimentally measured spin correlation per particle before loading into the lattice). In LDA, the local quantities at each position are calculated from the experimental data only. A similar situation arises from the experimental data with different anisotropy and interaction strengths. The upper axis of Fig.2(b) shows the temperature determined from the DCA+LDA calculation.

The comparison between the DCA+LDA calculations to the experimental results with different anisotropies and interaction strengths. The entropies are found. The theoretical prediction without heating is shown in blue, whereas the green data corresponds to an entropy increase of 0.6. This indicates that an anisotropic expansion parameter is needed to describe the data quite well. For increasing anisotropies, deviations from the HTSE breaks down quickly as the expansion parameter becomes large, see Fig.2(a) inset. The average normalized distance from the trap center and additionally the increasing effects in the Hubbard model Eq.(1). The local quantities at each position vary with the normalized distance from the trap center and at the same (trial)

\[ C(e_x) = \langle e_x^2 \rangle - \langle e_x \rangle^2 \]

is the geometric mean of the enhancement to the correlations. At a high temperature, the SU(2) invariance of the model can be accurately studied in this regime. For lower temperatures, the chemical potential in the calculation is extrapolated DCA results for a homogeneous system and mean fields, and additionally the increasing effects in the Hubbard model Eq.(1).

\[ \bar{C} = \frac{1}{N} \sum_{i=1}^{N} C(e_x) \]

The upper horizontal axis of Fig.2(b) shows the temperature. The chemical potential in the calculation is different anisotropy and interaction strengths.

\[ C(e_x) = \langle e_x^2 \rangle - \langle e_x \rangle^2 \]

The comparison between the experiment and numerics indicates heating. Numerics: Deviations from experiment visible for entropy S/N~ 1.0, indicate heating. Strong correlation physics at S/N~0.65.
Quantum Monte Carlo methods

Historical development in early 80s, lattice and impurity Monte Carlo methods

Hiatus until 2003-2005

Exponential growth of algorithms after 2006

Similar progress in other types of impurity algorithms, e.g. ED/FullCI/Ci

Blankenbecler, Sugar, Scalapino (1981)
Hirsch, Fye (1986)
Werner, Millis (2006)
Werner, Millis (2006)
Haule (2007)
Werner, Millis (2008)
Läuchli et al. (2009)
Werner, Millis (2008)
Otsuki et al. (2007)
Assad et al. (2008)
Mühlbacher et al. (2008)
Gull, Millis, et al. (2010)
Läuchli et al. (2009)
Koga et al. (2010)
Shiro (2010)
Gull, Millis, et al. (2011)
Lin, Gull, Millis (2012)
Gull et al. (2012)
Otsuki et al. (2013)
Hafermann et al., (2013)
Success of new algorithms

Solve impurity problems faster

- For the same problem: problem size reduced by ~30.
- Corresponds to time speedup of factor $30^3 = 27’000$ or ~25 years of Moore’s law

Avoid approximations

- Same problem can be tackled more accurately
- Elimination of bias and systematic errors
New physics accessible

- Real progress comes from access to physics that was previously inaccessible:

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<th>general interactions</th>
<th>very large systems</th>
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<td><img src="image8" alt="Phonons and screening" /></td>
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Diagrammatic Algorithms

Problem Setup

Partition function

\[ Z = \text{Tr} \left[ e^{-\beta H} \right] \]

Green’s function

\[ G(\tau) = \frac{1}{Z} \left[ e^{-(\beta-\tau)H} \right] \left[ e^{-\tau H} d^\dagger \right] \]

Feynman diagrammatic series expansion

\[ Z = \text{Tr} \left[ e^{-\beta H_1} T e^{-\int_0^\beta d\tau H_2(\tau)} \right] \]

\[ = \sum_{n=0}^\infty \int_0^\beta d\tau_1 \ldots \int_{\tau_{n-1}}^\beta d\tau_n \text{Tr} \left[ e^{-(\beta-\tau_n)H_1} (-H_2) \ldots e^{-(\tau_2-\tau_1)H_1} (-H_2) e^{-\tau_1 H_1} \right], \]

Taylor series

Trace expression illustrated as drawing of diagram

\[
\begin{align*}
\text{Diagrams} & \\
0 & \uparrow & \tau_1 & \uparrow & \tau_3 & \downarrow & \tau_2 & \beta
\end{align*}
\]

System described by Hamiltonian \( H = H_1 + H_2 \)
Use **Monte Carlo** methods to sample Feynman diagrams in diagram space.

Each diagram has a weight; Randomly insert and remove parts of diagrams according to that weight.

Typical diagram in this case has 50 vertices.

‘Large’ computational problem: 3000 interaction vertices.

Typical analytic methods: 2 to 4 interaction vertices.
Monte Carlo simulations of this type are **trivially parallel**: Scale to a very large (>10000) number of cores.

Ideally suited for modern supercomputers: little communications, lots of number crunching

Measurements are comparatively expensive; thermalization time small, Amdahl’s law relevant only at very large #cores.

Much of the time is spent doing non-equidistant fast Fourier transforms and matrix-matrix multiplications.

Numerical tricks: replace dger by dgemm:

\[ \text{Replace } d\text{ger} \quad \text{by } d\text{gemm} \]
What happens when T is lowered?

Interplay with experiment, exact solution of many-body problem

Approximate solution of a many-body problem in a difficult regime

**Theory**

Validation of simple model systems.
Numerical experiment

**Experiment**

added realism: materials specificity / chemistry.
Numbers for calibration.

**Computation**

Approximate solution of a many-body problem in a difficult regime
Experiments: The Cuprates
High Tc Superconductivity

Keller group, UniZH

The Nobel Prize in Physics 1987
J. Georg Bednorz, K. Alex Müller

for their important break-through in the discovery of superconductivity in ceramic materials
Experiments: Pseudogap

in high-Tc materials: Electronic spectral function is suppressed along the BZ face, but not along zone diagonal.

Key physics dependence on momentum around Fermi surface, Difference of spectral function around Fermi surface.

Doping dependence of region with quasiparticles

Experiments: Pseudogap

FIG. 1. Phase diagram of $n$- and $p$-type superconductors, showing superconductivity (SC), antiferromagnetic (AF), pseudogap, and normal-metal regions.

Pseudogap* appears only on the hole doped side.

Dopings smaller than optimal doping.

Temperatures up to $\sim 300$K.

Signatures also in NMR, Tunneling, c-axis conductivities, Raman…

*…of this type...
Experiments: d-wave superconductivity


He et al., Science 331, 1579 (2011)

FIG. 1. Phase diagram of n- and p-type superconductors, showing superconductivity (SC), antiferromagnetic (AF), pseudogap, and normal-metal regions.


Fig. 1. Temperature dependence of resistivity in Ba$_{1-x}$La$_x$CuO$_{4+y}, x$ for samples with $x$(Ba)$=1$ (upper curves, left scale) and $x$(Ba)$=0.75$ (lower curve, right scale). The first two cases also show the influence of current density.
Questions to theory

Theory claim: the important features of these materials are captured by a single-orbital Hubbard model in two dimensions, at large on-site Coulomb interaction $U$ and with 30-50% electron occupation.

Momentum space differentiation?

Pseudogap?

Superconductivity?

Simpler approximations?

Relation to experiment?

Analytic results are unreliable! Few limits (high $T$, infinitesimal interaction, infinite interaction, etc) but nothing in the regimes relevant for materials!
d-wave Superconductivity

It is now possible to reach low enough temperature to access the superconducting phase on large clusters that have a clear pseudogap state, different geometries!

- Interactions strong enough that half-filled system is Mott insulating
- Numerically exact algorithms (no bath fitting, no imaginary time discretization)
- Increase of CPU power makes surveys of phase space possible
- Precision good enough to do analytic continuation

d-wave superconductivity: anomalous antinodal self-energy


The issue may be cast in energetic terms. In the conventional BCS view, the driving force for superconductivity is an optimization of kinetic energy: by forming the superconducting state the electrons can take advantage of the low kinetic energy. In an alternative view, the superconductivity is an optimization of potential energy: by forming the superconducting state the electrons can take advantage of the low potential energy however costs kinetic energy, so that in the weak coupling limit the change from normal to superconductivity is an increase in the kinetic energy.

Changing the wave function to reduce the potential energy however costs kinetic energy, so that in the weak coupling limit the change from normal to superconductivity is an increase in the kinetic energy. In this paper we investigate the electronic energy to an applied pairing field, suggests that resonating valence bond physics is not the origin of the multiparticle physics of high-temperature superconductivity, as obtained in 8-site cluster dynamical mean field theory. Mott insulator at half filling for interaction strength $U/t > 0$) version of the model has been shown rigorously to have a d-wave superconducting ground state which the energy is computed are shown as arrows. Boundary of normal state pseudogap, defined as in Ref. 10, is indicated as dashed line (purple online). Trajectories along the superconducting state lowers the kinetic energy and increases the potential energy however costs kinetic energy, so that in the weak coupling limit the change from normal to superconductivity is an increase in the kinetic energy.

The repulsive- Hubbard model on the two dimensional square lattice Hubbard model in plane of density $\langle n \rangle$ at inverse temperature $T/t = 1/40$ is found to coincide with the boundary of the normal state pseudogap, providing further evidence of the unconventional nature of superconductivity. In at least some regions of the phase diagram.

The high transition temperature superconductivity expected for layered copper-oxide materials has been an important topic in condensed matter physics since its discovery in 1986. Broadly speaking, two views are currently held. One is that despite the various anomalous features of the materials the superconductivity may be captured by layered copper-oxide superconductivity is examined using the eight-site dynamical cluster approximation to the two-dimensional Hubbard model. Two regimes of superconductivity are found: a weak coupling/large interaction strength regime and a large coupling/weak interaction strength regime. In this paper we investigate the electronic energy to an applied pairing field, suggests that resonating valence bond physics is not the origin of the multiparticle physics of high-temperature superconductivity, as obtained in 8-site cluster dynamical mean field theory. Mott insulator at half filling for interaction strength $U/t > 0$) version of the model has been shown rigorously to have a d-wave superconducting ground state which the energy is computed are shown as arrows. Boundary of normal state pseudogap, defined as in Ref. 10, is indicated as dashed line (purple online). Trajectories along the superconducting state lowers the kinetic energy and increases the potential energy however costs kinetic energy, so that in the weak coupling limit the change from normal to superconductivity is an increase in the kinetic energy.

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FIG. 2. (Color online) Differences in total, kinetic, and potential energies (per site, in units of hopping $t$) between normal and superconducting states, obtained as described in the text at density $n = 1$ varying interaction strength (upper panel) and as function of density at fixed interaction strength $U = 6t$ (lower panel).
Analysis of superconducting state
overdoped / optimally doped region

- symmetric spectral function, quasiparticle peaks on both sides. Weight in peaks from vicinity of Fermi energy

- superconducting gap at the antinode

\[ \langle n \rangle = 0.92 \quad U/t = 6 \]
Pseudogap state at high T very different from SC state at low T: fundamental rearrangement of spectral weight on energy scales » Δ. Superconducting gap significantly smaller than pseudogap. (conclusion independent of continuation)
Solution of 2D Hubbard model?

Preliminary results from the Simons Collaboration on the Many-Electron Problem

Challenge: Obtain results for the Hubbard model in the thermodynamic limit

Many numerical methods, all of the have approximations, all have small parameter.

What happens when we take O(10) different many-body methods and compare results over a wide regime of the Hubbard model?

All controlled methods we tested are consistent: within error bars, no discrepancies found.

All of the ‘simple’, ‘weakly’ or ‘uncorrelated’ regimes work and are consistent.

Open questions exactly where superconductivity and the pseudogap occur…

Preliminary Data: Simons Collaboration on the Many-Electron Problem
from models to real compounds

Simple lattice structure

local interactions

nearest neighbor hopping

general lattice structure

ccomplicated non-local interactions

general orbital overlap

multi-orbital effects

Chemistry
Fermionic systems accessible with current numerics & theory

from models to real compounds

brute force numerics fails

hard exponential wall

GW+DMFT

Gradual improvements

…Here Be Dragons…

Correlated Condensed matter experiment

Dual Fermions

Diag. Vertex Approximation
Numerical Methods for the Many-Electron Problem

Part of the Simons collaboration on the many-electron problem