Life as a theorist without a small parameter

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Dirac (1902-1984)

- 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.

  - Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, Vol. 123, No. 792 (6 April 1929)
• 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.
The rule of the small parameter

R. Feynman: 1918-1988

Equation of State Calculations by Fast Computing Machines

Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, and Augusta H. Teller,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

Edward Teller, Department of Physics, University of Chicago, Chicago, Illinois
(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

I. INTRODUCTION

The purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed, only two-body forces are considered, and the potential

II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number $N$ may be as high as several hundred. Our system consists of a square containing $N$ particles. In order to minimize the surface effects we suppose the complete substance to be periodic.
Broken symmetry – mean-field

Pierre Weiss: 1865 - 1940

Lev Landau: 1908-1968
The theory of everything

\[ H = K + V_{e-e} + V_{e-i} + V_{i-i} + V_{s-o} \]

- 10-1000 eV vs 10 meV (3-5 orders of magnitude)
- Broken symmetry (lattice) (Bands: Bloch)
- Density Functional Theory (Hohenberg-Kohn-Sham)
  - Ground state
  - Basis for perturbation theory
- Fermi liquid theory (Landau)
- Effective Hamiltonians (e.g. spin models)
- Moore’s law
- Better algorithms: beating Moore’s law.
Superconductivity

Leon Cooper

John Bardeen*

Robert Schrieffer
High temperature superconductors

Failure of
BCS theory
Band structure
and more
New and old superconductors

H. Takahashi: JPSJ Online—News and Comments [June 10, 2008]
Band structure for high Tc

W. Pickett, Rev. Mod. Phys. 1989
A puzzeling phase diagram
Breakdown of band theory: Half-filled band is metallic
Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949
Outline

• The model
• Beyond perturbation theory
  – Weak to intermediate correlations TPSC
    • Electron-doped cuprates
  – Strong correlations DMFT
    • Hole-doped cuprates
2. The model
Hubbard model

\[ H = - \sum_{<ij>\sigma} t_{i,j} \left( c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Effective model, Heisenberg: \( J = 4t^2 / U \)

Attn: Charge transfer insulator
Theoretical considerations
Another way to look at the many-particle problem

\[ F[\phi] = -T \ln Z[\phi] = -T \ln \text{Tr} \left[ e^{-\beta (H - \mu N)} T \int \int \psi^\dagger(\bar{1}) \phi(\bar{1}, \bar{2}) \psi(2) \right] \]

\[ \frac{1}{T} \frac{\delta F[\phi]}{\delta \phi(1, 2)} = G(2, 1) \]

\[ \Omega[G] = F[\phi] - \text{Tr} [\phi G] \]

\[ \frac{1}{T} \frac{\delta \Omega[G]}{\delta G(1, 2)} = -\phi(2, 1) \]

\[ \Omega[G] = \Phi[G] - \text{Tr} [(G_0^{-1} - G^{-1}) G] + \text{Tr} \left[ \ln \left( \frac{-G}{-G_\infty} \right) \right] \]

\[ \frac{1}{T} \frac{\delta \Phi[G]}{\delta G(1, 2)} = \Sigma(2, 1) \]

\[ U_{sp} = \frac{\delta \Sigma_{\uparrow}}{\delta G_{\downarrow}} - \frac{\delta \Sigma_{\uparrow}}{\delta G_{\uparrow}} \]

J. Schwinger: 1918-1994
Focus on physically meaningful quantities

\[ \Phi[G] = \quad \xrightarrow{\text{loop}} \quad + \quad \xrightarrow{\text{loop}} \quad + \quad \xrightarrow{\text{bubble}} \quad + \quad \ldots. \]

\[ \frac{\delta \Phi[G]}{\delta G} = \sum \]

Luttinger and Ward 1960, Baym and Kadanoff (1961)
Two-Particle Self-Consistent Theory
(Vilk)

Yury Vilkin
Two-Particle Self-Consistent Theory
(how it works, \( U < 8t \))

- General philosophy
  - Impose constraints and sum rules to find vertex
    - Conservation laws
    - \( U_{sp} = U \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle} \)
    - Pauli principle \( \langle n^2_\sigma \rangle = \langle n_\sigma \rangle \)
    - Local moment and local density sum-rules

- Get for free:
  - Mermin-Wagner theorem
  - Kanamori-Brückner screening
  - Consistency between one- and two-particle \( \Sigma G = U \langle n_\sigma n_{-\sigma} \rangle \)

Vilk, AMT J. Phys. I France, 7, 1309 (1997);
A.M.T. Chapt. 13, in *Theoretical Methods for Strongly Correlated Systems* Ed F. Mancini A. Avella,
(Mahan, third edition)
Benchmarks for TPSC
Proofs...

\[ U = +4 \]
\[ \beta = 5 \]

Monte Carlo

Many-Body

Flex

\[ \frac{\pi}{4}, \frac{\pi}{2} \]

\[ \frac{\pi}{4}, \frac{\pi}{4} \]

\[ \frac{\pi}{2}, \frac{\pi}{2} \]

\[ (0, \pi) \]

\[ (0,0) \]

\[ \omega/t \]

3. Electron-doped cuprates: normal state
Our road map
Fermi surface plots

Hubbard repulsion $U$ has to be not too large

increase for smaller doping

Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004

B. Kyung et al., PRB 68, 174502 (2003)
Hot spots from AFM quasi-static scattering

Mermin-Wagner

d = 2

Vilk, A.-M.S.T (1997)
Kyung, Hankevych, A.-M.S.T., PRL, 2004


Armitage et al. PRL 2001
4. Electron-doped cuprates: superconductivity
\[ \Delta p = -\frac{1}{2V} \sum_{p'} U(p - p') \frac{\Delta p'}{E_{p'}} \left( 1 - 2n(E_{p'}) \right) \]

Exchange of spin waves?
Kohn-Luttinger
\( T_c \) with pressure

Béal–Monod, Bourbonnais, Emery
P.R. B. 34, 7716 (1986).
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B 34, 8190-8192 (1986).
Kohn, Luttinger, P.R.L. 15, 524 (1965).

Results from TPSC

Satisfies Mermin-Wagner
Tc from TPSC


T. Maier et al. PRL 95, 237001 (2005)
5. Strong correlations: Dynamical Mean-Field Theory

Gabriel Kotliar

Antoine Georges
C-DMFT

\[ \Phi[G] = \bigcirc \bigcirc + \bigcirc \bigcirc + \bigcirc \bigcirc + \ldots \]
Mean-field is not a trivial problem! Many impurity solvers.

Here: continuous time QMC

P. Werner, PRL 2006
P. Werner, PRB 2007
K. Haule, PRB 2007
6. Hole-doped cuprates: normal state
Our road map
h-doped are strongly correlated: evidence from the normal state
Density of states (STM)

Khosaka et al. *Science* **315**, 1380 (2007);
Pseudogap (theory)

h-doped
How does the pseudogap develops as a function of $T$?
Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of $U$

Smaller $D$ and $S$
Density of states

- Mott insulator
- Pseudogap
- Critical point
- Correlated Fermi liquid

Graphs showing the relationship between density of states and temperature, with various parameters such as $\delta$ and $\omega$.
Density of states

Khosaka et al. *Science* **315**, 1380 (2007);
Spin susceptibility
Spin susceptibility

Underdoped Hg1223
Julien et al. PRL 76, 4238 (1996)
Pseudogap $T^*$ along the Widom line
7. Hole-doped cuprates: superconductivity
CDMFT global phase diagram


Armitage, Fournier, Greene, RMP (2009)
Finite $T$ phase diagram
Superconductivity

Sordi et al. PRL 108, 216401 (2012)
Strongly correlated superconductors

- $T_c$ does not scale like order parameter
- Superfluid stiffness scales like doping
- Superconductivity can be largest close to the metal-insulator transition
- Resilience to near-neighbor repulsion
First-order transition leaves its mark
Open problems
Conclusion
The dream

12 EVENTS
THAT WILL CHANGE EVERYTHING
AND NOT IN THE WAY YOU THINK

http://www.physique.usherbrooke.ca/taillefer/Vulgarisation.html
DFT + Methods from strongly correlated

Anisimov et al. J. Phys. 9, 7354 (1997)
G. Kotliar et al. RMP, 78, 865 (2006)
P. Sémon et al. arXiv:1403.7214
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