The Dynamic Hubbard Model: studies with DMFT and exact diagonalization

Frank Marsiglio
University of Alberta, Edmonton

20th Mardi Gras Conference
Petascale Many Body Methods for Complex Correlated Systems
Feb. 12-14 2015 Baton Rouge
**High temperature superconductors:**
- discovered 1986
- copper oxygen planes
- theory not understood!!!

**Conventional or Low-Tc superconductors:**
- discovered 1911
- almost all metals (Hg, Pb, Nb, etc.)
- theory well understood

---

http://spot.colorado.edu/~dessau/HighTc.shtml
**High temperature superconductors:**
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**Conventional or Low-Tc superconductors:**
- discovered 1911
- almost all metals (Hg, Pb, Nb, etc.)
- theory well understood  ????

**Elements and Compounds:**
- Hg/Ba/Ca/Cu/O
- Tl/Ba/Ca/Cu/O
- Bi₂Sr₂CaCu₂O₈
- YBa₂Cu₃O₇
- (La₂, Sr₂)Cu₄O₄
- Ba-K-Bi-O
- K₃C₆₀
- MgB₂
- LaFeAsOF
- SmFeAsOF
- Organics
- Heavy Fermions
- Zintl phases
- Chevrel phases
- Borocarbides
Physica C Special Issue on Superconducting Materials
Dedicated to Theodore H. Geballe on the year of his 95th birthday
Edited by J.E. Hirsch, M.B. Maple, and F. Marsiglio

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What this talk is about

1) A ‘lightening-quick’ overview of Eliashberg Theory, as I would teach in a graduate course, for example.

2) Is there more, at least for the cuprates, for example?

3) The Dynamic Hubbard model --- is there more to Coulomb repulsions than $\mu^*$?
   (i) conceptual look
   (ii) DMFT solution
   (iii) 2-site model
   (iv) relation to high-Tc experiments (optics)
The conventional scenario: BCS

Electrons in solids

Fermi sphere

kinetic energy

$E_{\text{kin}} = 2 \sum \epsilon_k n_k$

finite temperature

$|k|$

$k_F$

$k_z$

$k_y$

$k_x$

$\mathbf{n}_k$

$\psi_{\text{BCS}} = \prod_k \left( u_k + v_k c_k^{\uparrow} c_{-k \downarrow}^{\dagger} \right) |0\rangle$

all k’s !! --- occupation is controlled by $u_k$ and $v_k$.

order parameter ($\Delta_k$) becomes non-zero, so, e.g.

$v_{k^2} = \frac{1}{2} \left( 1 - \frac{\epsilon_k}{E_k} \right)$

where

$E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$

$\sim 1$ for $\epsilon_k < 0$

$\sim 0$ for $\epsilon_k > 0$
It’s all about pairs…

In Ogg’s theory it was his intent
That the current keep flowing, once sent;
So to save himself trouble,
He put them in double,
And instead of stopping, it went.

George Gamow

Bose–Einstein Condensation of Trapped Electron Pairs. Phase Separation and Superconductivity of Metal-Ammonia Solutions

Richard A. Ogg, Jr.
Department of Chemistry, Stanford University, California
March 2, 1946

…Cooper pairs
normal state

superconducting state

why sacrifice kinetic energy?

Ans: gain potential energy

remember, \[ v_k^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta_k^2}} \right) \]
BCS formalism vs. Pairing Mechanism

\[ \Delta = |V| \frac{1}{N} \sum_k \frac{\Delta}{2E_k} \]

Tc equation (useless)

\[ \frac{2\Delta}{k_B T_c} = 3.53 \quad \text{Universality} \]

\[ \frac{\Delta C}{\gamma T_c} = 1.43 \]

Universality is wonderful

Universality is a curse!
Eliashberg Theory

• Extension of BCS formalism to include

S-STATE INSTABILITIES FOR RETARDED INTERACTIONS†

C. S. OWEN‡ and D. J. SCALAPINO§

Physics Dept., University of Pennsylvania, Philadelphia, Pa., USA

• loc

Physica 55, 691 (1971)

\[
\Delta(i\omega_n) Z(i\omega_n) = \pi T \sum_m \left[ \lambda (i\omega_n - i\omega_m) - \mu^* \right] \frac{\Delta(i\omega_m)}{\sqrt{\omega_m^2 + \Delta^2(i\omega_m)}}
\]

G. M. Eliashberg
Started graduate school in 1959
Wrote Eliashberg Theory paper in 1960
Graduated in 1963!
Eliashberg Theory

$$\Delta(k, \omega) = \mathcal{F}[V_{k,k'}(\omega, \omega')]$$

A functional of the interaction

**Question:** Can we invert the theory to extract the potential uniquely from a knowledge of \( \Delta(k, \omega) \)?
Answer is Yes!

**IMAGE OF THE PHONON SPECTRUM IN THE TUNNELING CHARACTERISTIC BETWEEN SUPERCONDUCTORS**

Bell Telephone Laboratories, Murray Hill, New Jersey
(Received 14 March 1963)

**EFFECTIVE TUNNELING DENSITY OF STATES IN SUPERCONDUCTORS**

J. R. Schrieffer, D. J. Scalapino, and J. W. Wilkins
University of Pennsylvania, Philadelphia, Pennsylvania
(Received 15 March 1963)
\[ \frac{dI}{dV} \sim N(\varepsilon) \]

\[ N(\omega) = \text{Re} \left( \frac{\omega}{\sqrt{\omega^2 - \Delta^2(\omega)}} \right) \]

**Fig. 10.** The relative conductance of a Pb-MgO-Mg sandwich plotted against energy. At higher energies there are definite divergences from the BCS density of states as can be seen from the bumps in the experimental curve. Note that the crossover point corresponds in energy to the Debye temperature.
requires Eliashberg theory:

- phonon dynamics (retardation) taken into account

\[ \Delta(\omega) = \mathcal{F}[\alpha^2 F(\omega), \mu^*] \]

- gap is a function of frequency

- density of states is modified:

\[ \frac{dI}{dV} \propto N(\omega) = N(\epsilon_F) \text{Re} \left( \frac{\omega}{\sqrt{\omega^2 - \Delta^2(\omega)}} \right) \]
$\omega$ (meV)

$$\alpha^2(\omega) \equiv \frac{\alpha^2 F(\omega)}{F(\omega)} \sim \text{constant}$$

$F(\omega)$: density of phonon states from neutron scattering (Brockhouse at Chalk River)
4 Electron–Phonon Superconductivity

F. Marsiglio  University of Alberta, Dept. of Physics, Edmonton, Canada and
J.P. Carbotte  McMaster University, Physics Dept. Hamilton, Canada

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So what’s wrong?

1) How did $\mu = \text{UN}(E_F)$ get reduced to $\mu^*$?

"We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?"

*Is There Glue in Cuprate Superconductors?*

Philip W. Anderson

*Science 316*, 1705 (2007);
Eliashberg Theory

But…
Never seen in QMC simulations
Many other ways for $U$ to be Reduced

Poor man’s Scaling (Tolmachev et al., Morel and Anderson)
FAST TRACK COMMUNICATION

The theory of electron–phonon superconductivity: does retardation really lead to a small Coulomb pseudopotential?

Retardation effects and the Coulomb pseudopotential in the theory of superconductivity

Johannes Bauer, Jong E. Han, and Olle Gunnarsson

Thursday, May 13, 2004

Sportsline

BCS formula up for tweaking

Stoops wants votes made public

By Steve Wieberg
USA TODAY

Architects of the Bowl Championship Series are close to drawing up a new formula that will essentially give one-third weight to the电脑 rating, one-third to the USA TODAY/ESPN Coach's Poll and a final one-third to a computer rating.

If no longer would include a separate strength-of-schedule rating, an emphasis for losses and probably rules for mercy wins. A final determination is being analyzed by outside mathematicians.

The modifications, he says, should avert a repeat of last year's messy split-championship outcome.

Stoops wants

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Copper-Oxygen Planes

http://www.cnms.ornl.gov/images/gordon-bell-1.gif

Fig. 1: (a) The crystal structure of La2CuO4, a typical cuprate, where black, red, and blue sphere represent Cu, O, and La, respectively. (b) The CuO2 plane with outlines of the Cu dx2-y2 and O px and py orbitals. Also shown in full color is the Zhang-Rice singlet state that forms from hybridization of the Cu orbitals with the neighboring O orbitals. (c) Pictorial representation of the single band 2D Hubbard model with on-site Coulomb repulsion U and inter-site hopping t.

High $T_c$ Cuprates: a Case Study
The (single band) Hubbard model

\[ H = -t \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]
Does it have the ‘right stuff’ (Doug Scalapino)?

Nearest neighbour interactions

\[
(ij| 1/r |ij) \sim \frac{2\epsilon - \kappa |\mathbf{R}_i - \mathbf{R}_j|}{|\mathbf{R}_i - \mathbf{R}_j|} \text{Ry (6 eV)}
\]

Electron correlations in narrow energy bands

By J. Hubbard

Theoretical Physics Division, A.E.R.E., Harwell, Didcot, Berks

(Communicated by B. H. Flowers, F.R.S.—Received 23 April 1963)


\[
(ii| 1/r |ij) \sim q \text{Ry} \sim \frac{1}{2}\text{eV},
\]

\[
(ij| 1/r |ik) \sim \frac{1}{4}q \text{Ry} \sim \frac{1}{10}\text{eV},
\]

\[
(ii| 1/r |jj) \sim (ij| 1/r |ji) \sim q^2 \text{Ry} \sim \frac{1}{40}\text{eV},
\]

Modulated hopping \( \Delta t \)

3-site hopping (t-J model)

Exchange term J

phonons, oxygen (or other) orbitals, longer range hopping, polarons, lunar effects, etc.
Or have we missed a key ingredient all along?

Dynamic Hubbard Model

J. E. Hirsch

*Department of Physics, University of California—San Diego, La Jolla, California 92093-0319*

(Received 24 July 2001; published 26 October 2001)

...a parable involving the lowly Helium atom...
Neutrons and protons are held together in the nucleus by the “strong” force, which has to overcome the electrical repulsion of the two positively charged protons in helium (and in more complex atoms too). Electrons are held around the atom by the electrical attraction between their negative charge and the positive charge of the protons in the nucleus.
But the real 2-electron wave function is given by

\[ |\psi\rangle = a_1|1s\ 1s\rangle + a_2|1s\ 2s\rangle + a_3|1s\ 3s\rangle + a_4|2s\ 2s\rangle + a_5|2p\ 2p\rangle + \ldots \]
Further Computations of the He Atom Ground State

Charles Schwartz *

Department of Physics, University of California
Berkeley, California 94720

Abstract

Recently reported computations have been extended to give ten more decimals of accuracy in the ground state energy of the Schrodinger equation for the idealized Helium atom. With the F basis - Hylleraas coordinates with negative powers and a logarithm of s - carried to the fiftieth order (N = 24,099 terms) we find the eigenvalue

\[
E = -2.90372 43770 34119 59831 11592 45194 40444 66969 25309 \ldots
\]
The spectral decomposition of the helium atom two-electron configuration in terms of hydrogenic orbitals

Joel Hutchinson¹, Marc Baker¹ and Frank Marsiglio¹,²,³

1s² energy

Exact energy

Table 1. Results for some overlaps, $a_i$.

| $i$ | Basis state | $a_i$  | $|a_i|^2$ | Total Probability |
|-----|-------------|--------|----------|-------------------|
| 1   | 100 100     | 0.9624 | 0.9263   | 0.9263            |
| 2   | 100 200     | −0.2148| 0.0461   | 0.9725            |
| 3   | 100 300     | −0.0752| 0.0057   | 0.9781            |
| 4   | 100 400     | −0.0427| 0.0018   | 0.9799            |
| 5   | 100 500     | −0.0289| 0.0008   | 0.9807            |
| 6   | 100 600     | −0.0213| 0.0005   | 0.9812            |
| 7   | 100 700     | −0.0166| 0.0003   | 0.9815            |
| 8   | 100 800     | −0.0146| 0.0002   | 0.9827            |
| 9   | 100 900     | −0.0146| 0.0002   | 0.9827            |
| 10  | 100 1000    | 0      | 0        | 0.9828            |

Not 1.000!
Why is this important?

\[ U(Z) = \int d^3r \, d^3r' \, |\varphi_{1s}(r)|^2 \frac{e^2}{|r - r'|} |\varphi_{1s}(r')|^2 \]

\[ = \frac{5}{4} Z \times 13.606 \text{ eV}, \]

\[ \varphi_{1s}(r) = \left( \frac{Z^3}{\pi a_0^3} \right)^{1/2} e^{-Zr/a_0} \]

Experimental values:

\[ U_{\text{eff}}(1) = I - A = 12.86 \text{ eV} = U(1) - 4.15 \text{ eV} \quad (2a) \]

\[ U_{\text{eff}}(2) = I_{II} - I_I = 29.92 \text{ eV} = U(2) - 4.10 \text{ eV}. \quad (2b) \]

\[ 4 \text{ eV} \approx 46 \, 000 \text{ K!} \]

J.E. Hirsch, PRL 87, 206402 (2001)
In essentially all the lattice models used to understand electron correlations in solids, the “playing field” is static (phonons are a different matter).

In He, when one electron is present, it occupies the 1s orbital:

When two electrons are present, in Hubbard-like models they (doubly) occupy the 1s orbital:

- For Hubbard model:

- For real atom

\[
\psi(\vec{r}_1, \vec{r}_2) = \Phi_{1s}(\vec{r}_1)\Phi_{1s}(\vec{r}_2)
\]

\[
\psi(\vec{r}_1, \vec{r}_2) = \sum_{mn} c_{mn} \Phi_m(\vec{r}_1)\Phi_n(\vec{r}_2)
\]
This is like what happens in general relativity; the presence of mass alters the underlying space-time structure.
This is like what happens in general relativity; the presence of mass alters the underlying space-time structure.

Here, the presence of a second electron alters the nature of the orbitals that model the conduction band.
Exact Diagonalizations (very small clusters!) AND Dynamical Mean Field Theory (DMFT)

FIGURE 4. Mean-field theory replaces a lattice model by a single site coupled to a self-consistent bath.

Antoine Georges, arXiv:cond-mat/0403123
\[ U_{eff} = E_0(N_e) + E_0(N_e - 2) - 2E_0(N_e - 1) \]
This is like what happens in general relativity; the presence of mass alters the underlying space-time structure.

Here, the presence of a second electron alters the nature of the orbitals that model the conduction band.

A simple way to model this: hopping term

\[ H_{DH} = - \sum_{<i,j>} t_{ij} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) - \mu \sum_{i\sigma} n_{i\sigma} + \]

\[ \sigma_z = +1 \]
\[ \Omega = \omega_0 \sqrt{1 + g^2} \]

\[ \sigma_z = -1 \]

\[ t_e = t \quad \text{(electron in an empty lattice)} \]

\[ t_h = t S^2 \quad \text{(electron in an almost full lattice)} \]

where \( S = \text{Franck-Condon factor.} \)
Dynamic Hubbard Model

\[ H_{\text{DHM}} = \sum_{<i,j>\sigma} t_{ij} (c_i^{\dagger} c_j \sigma + c_j^{\dagger} c_i \sigma) - \mu \sum_{i,\sigma} n_{i\sigma} \]

\[ + \sum_i \left( \omega_0 \sigma_i^x + g \omega_0 \sigma_i^z \right) + \sum_i \left( U - 2 g \omega_0 \sigma_i^z \right) n_{i\uparrow} n_{i\downarrow} \]

Parameter

- \( t \): electron hopping
- \( U \): ‘bare’ electron-electron repulsion
- \( g \): electron-pseudospin coupling strength
- \( \omega_0 \): energy (time) scale associated with pseudospin

**How do we check this out?**

(i) effective model

(ii) exact diagonalizations

(iii) Dynamical Mean Field Theory
Electron-hole asymmetry

Mott physics vs. orbital relaxation

Pseudospin expectation values

\[ \sigma_z = -1 \]

\[ \Omega = \omega_0 \sqrt{1+g^2} \]

\[ \sigma_z = +1 \]

G.H. Bach et al., PRB 82, 155122 (2010)

M. Potthoff, Phys. Rev. B 64, 165114 2001: 2-site DMFT
FIG. 12. (Color online) The spectral function for various energies, as shown, for (a) \( n = 0.2 \) and (b) \( n = 1.8 \). Here, we have used \( U = 1 \), \( g = 1 \), and \( \omega_0 = 2 \) (see pink curve in Fig. 9). The second last frame in each instance shows the spectral function at an energy corresponding to the Fermi level, and the weight under the peak at \( \omega = 0 \) corresponds to the quasiparticle residue, \( z \).

\[ U = 1, \ g = 1, \ \omega_0 = 2 \]
Optical conductivity

G.H. Bach et al., PRB 82, 155122 (2010)

See also G.H. Bach and F.M. PRB 85, 155134 (2012)
\[ \sigma_1^{(3)}(\omega) = \frac{\pi e^2 t}{2\hbar^2} \left[ S^2 \delta\left(\omega - \frac{2tS^2}{\hbar}\right) + 4S^2 \bar{S}^2 \frac{t}{\Omega_0} \delta\left(\omega - \frac{\Omega_0}{\hbar}\right) + \bar{S}^4 \frac{t}{\Omega_0} \delta\left(\omega - \frac{2\Omega_0}{\hbar}\right) \right]. \] (29)

Dimer calculations

G.H. Bach and F.M. PRB 85, 155134 (2012)
How do we measure this?

Optical Sum Rule (Kubo)

\[ \int_0^\infty d\nu \sigma_1(\nu) = \frac{\pi e^2}{\hbar^2} \frac{1}{N} \sum_k \left( \frac{\partial^2 \epsilon_k}{\partial k^2} \right) n_k \]

for all bands (or quadratic dispersion):

\[ = \frac{\pi e^2 n}{2m} = \omega_P^2 / 8 \]

for tight-binding band (with nearest neighbour hopping):

\[ \frac{\partial^2 \epsilon_k}{\partial k^2} = -a^2 \epsilon_k \]

\[ \int_0^\infty d\nu \sigma_1(\nu) = \frac{\pi e^2 a^2}{2\hbar^2} < -E_k > \]
Finite-energy $f$-sum rules for valence electrons

D. Y. Smith
Argonne National Laboratory, Argonne, Illinois 60439

E. Shiles
Argonne National Laboratory, Argonne, Illinois 60439
and Virginia Commonwealth University, Richmond, Virginia 23284

\begin{equation}
\text{ALUMINUM}
\begin{align}
n_{\text{eff}}(\omega)_k &= \frac{m}{2\pi^2e^2} \int_0^\omega \omega' \varepsilon'_2(\omega') d\omega', \\
n_{\text{eff}}(\omega)_k &= \frac{m}{\pi^2e^2} \int_0^\omega \omega' \varepsilon''(\omega') d\omega', \\
\text{and}
\end{align}
\end{equation}

\begin{align}
n_{\text{eff}}(\omega)|_{\varepsilon^{-1}} &= \frac{m}{2\pi^2e^2} \int_0^\omega \omega' \text{Im}[\varepsilon^{-1}(\omega')]] d\omega'. \tag{6}
\end{align}

\begin{align}
\int_0^\infty \omega \varepsilon_2(\omega) d\omega &= \frac{\pi}{2} \omega_p^2, \\
\int_0^\infty \omega \kappa(\omega) d\omega &= \frac{\pi}{4} \omega_p^2, \\
\text{and}
\int_0^\infty \omega \text{Im}[\varepsilon^{-1}(\omega)] d\omega &= \frac{\pi}{2} \omega_p^2.
\end{align}

See also Shiles et al. PRB22, 1612 (1980)
why is there temperature dependence in the normal state?

Answer:
1) $n_k \rightarrow f_k$ (Fermi-Dirac)
2) interactions

$$E_{\text{kin}} = 2 \sum \varepsilon_k n_k$$

Note: Absolute value of kinetic energy decreases in the superconducting state. This is conventional behaviour.
Superconductivity-Induced Transfer of In-Plane Spectral Weight in Bi$_{2}$Sr$_{2}$CaCu$_{2}$O$_{8+\delta}$

H. J. A. Molegraaf, C. Presura, D. van der Marel, P. H. Kes, M. Li

Science 22 March 2002 295: 2239-2241

In-plane optical spectral weight transfer in optimally doped Bi$_{2}$Sr$_{2}$Ca$_{2}$Cu$_{3}$O$_{10}$

F. Carbone, A. B. Kuzmenko, H. J. A. Molegraaf, E. van Heumen, E. Giamini and D. van der Marel

DPNC, University of Geneva, 24,
Quai Ernest-Ansermet, Geneva 4, Switzerland

FIG. 6: BCS prediction of the spectral weight function.
M.V. Klein and G. Blumberg, Science 283, 42 (1999)
Anomalous sum rule change at Tc

Using a phenomenology of scattering rate collapse:

---

FM, Phys. Rev. B73, 064507
microwave

use $1/\tau = 1/\tau_0 (T/T_c)^4$ below $T_c$
Also in photoemission, M.R. Norman et al.


FIG. 1. Comparison of data at $\bar{M}$ in the normal state (105 K, dashed line) and the superconducting state (13 K, solid line) for a slightly overdoped ($T_c = 87$ K) Bi2212 sample with photon polarization $\Gamma - \bar{M}$. 
Summary

I’ve tried to make the case that the BCS pairing formalism gives an excellent description of the superconducting state but…

The actual **mechanism** is an active subject of current interest for all superconductors.
Key Points

What are the essential ingredients buried in the parameter $\mu^*$?

(i) Maybe the Hubbard and Hubbard-like models don’t really capture the essence of electron correlations in metals.

(ii) The Dynamic Hubbard model tries to incorporate orbital relaxation --- the fact that orbitals expand, etc. when doubly occupied. Do these processes play an important role for superconductivity?

Moreover…

• We find a fundamental electron-hole asymmetry. This asymmetry is apparent in tunneling, and more indirectly through other probes.

• Pairing (requiring further study) results in energy lowering through kinetic energy (not potential energy), as seen in several optical conductivity studies (Basov, van der Marel, Bontemps, Timusk, etc.)
Many thanks to my collaborators: Benfatto, Carbotte, Knigavko, Schachinger, Timusk, van der Marel, Forestell, Kuzmenko, Carbone, van Heumen, Polachic, Chandler, Bach, Hirsch, Baillie, Blois, and Zhou

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Many thanks to my collaborators: Benfatto, Carbotte, Knigavko, Schachinger, Timusk, van der Marel, Forestell, Kuzmenko, Carbone, van Heumen, Polachic, Chandler, Bach, Hirsch, Baillie, Blois, and Zhou

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