Strongly correlated superconductivity

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Superconductivity
Attraction mechanism in the metallic state
Attraction mechanism in the metallic state
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Attraction mechanism in the metallic state
#1 Cooper pair, #2 Phase coherence

\[ E_P = \sum_{p,p'} U_{p-p'} \psi_{p^\uparrow,-p^\downarrow} \psi_{p'^\uparrow,-p'^\downarrow}^* \]

\[ E_P = \sum_{p,p'} U_{p-p'} \left( \langle \psi_{p^\uparrow,-p^\downarrow} | \psi_{p'^\uparrow,-p'^\downarrow}^* \rangle + \psi_{p^\uparrow,-p^\downarrow} \langle \psi_{p'^\uparrow,-p'^\downarrow}^* \rangle \right) \]

|BCS(\theta)\rangle = \ldots + e^{iN\theta} |N\rangle + e^{i(N+2)\theta} |N + 2\rangle + \ldots
Breakdown of band theory
Half-filled band is metallic?
Half-filled band: Not always a metal

NiO, Boer and Verway

Peierls, 1937

Mott, 1949
« Conventional » Mott transition

Figure: McWhan, PRB 1970; Limelette, Science 2003
2. The model

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

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

Attn: Charge transfer insulator
\[ U = 0 \]

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

\[ c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{i \mathbf{k} \cdot \mathbf{r}_i} c_{k\sigma} \]

\[ H = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} \]

\[ |\Psi\rangle = \prod_{k,\sigma} c_{k\sigma}^\dagger |0\rangle \]
\[ t_{ij} = 0 \]

\[ H = \]

\[ U \sum_i n_{i \uparrow} n_{i \downarrow} \]

\[ U \uparrow U \downarrow \]

\[ |\Psi\rangle = \prod_i c_{i \uparrow}^\dagger \prod_j c_{j \downarrow}^\dagger |0\rangle \]

\[ 2^N \]
Interesting in the general case

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

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

Meinders et al. PRB 48, 3916 (1993)
Outline

1. Introduction
2. The model
3. Weakly and strongly correlated antiferromagnets
   1. Qualitative
   2. Contrasting methods for weak and strong coupling
4. Weakly and strongly correlated superconductivity
   1. Qualitative
   2. Contrasting methods
5. High Tc and organics, the view from DMFT
   1. Quantum clusters
   2. Normal state and pseudogap
   3. SC state
6. Methods, 2 of them: C-DMFT and TPSC
7. Conclusion
3. Weakly and strongly correlated antiferromagnets

What is a phase?
Emergent properties
  - e.g. Fermi surface
    • Shiny
    • Quantum oscillations (in B field)

Many microscopic models will do the same
  - Electrons in box or atoms in solid, Fermi surface
  - Often hard to « derive » from first principles (fractionalization - gauge theories)
Antiferromagnetic phase: emergent properties

- Some broken symmetries
  - Time reversal symmetry
  - Translation by one lattice spacing
  - Unbroken Time-reversal times translation by lattice vector $\mathbf{a}$
    - Spin waves
    - Single-particle gap
Differences between weakly and strongly correlated

• Different in ordered phase (finite frequency)
  – Ordered moment
  – Landau damping
    • Spin waves all the way or not to J

• Different, even more, in the normal state:
  – metallic in $d = 3$ if weakly correlated
  – Insulating if strongly correlated
  – Pressure dependence of $T_N$
3. Strong vs weak coupling for an antiferromagnet

3.1 Qualitative
$n = 1$, unfrustrated $d = 3$ cubic lattice

$J = 4t^2 / U$

Slater $\leftrightarrow$ Heisenberg

AFM

Mott
Local moment and Mott transition

$n = 1$, $d = 2$ square lattice

Critical point visible in $V_2O_3$, $BEDT$ organics

Understanding finite temperature phase from a *mean-field theory* down to $T = 0$
4. Weakly and strongly correlated superconductivity

Analog to weakly and strongly correlated antiferromagnets
Superconducting phase: identical properties

• Emergent:
  – Same broken symmetry $U(1)$ for s-wave,
  – $U(1)$ and $C_{4v}$ for d-wave
  – Single-Particle gap, point or line node.
    • $T$ dependence of $C_p$ and $\kappa$ at low $T$
  – Goldstone modes (+Higgs)
Superconductivity not universal
even with phonons: weak or strong coupling

• In BCS universal ratios: e.g. $\Delta/k_BT_c$
  – Would never know the mechanism for sure if only BCS!
  – N.B. Strong coupling in a different sense
High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)

- Competing order
  - Current loops: Varma, PRB 81, 064515 (2010)
  - Stripes or nematic: Kivelson et al. RMP 75 1201(2003); J.C.Davis
  - d-density wave: Chakravarty, Nayak, Phys. Rev. B 63, 094503 (2001); Affleck et al. flux phase
  - SDW: Sachdev PRB 80, 155129 (2009) ...

What is under the dome?
Mott Physics away from $n = 1$

- Or Mott Physics?
Other class of strongly correlated SC

Phase diagram \((X=\text{Cu}[\text{N(CN)}_2]\text{Cl})\)

- \(S. \text{Lefebvre et al. PRL 85, 5420 (2000), P. Limelette, et al. PRL 91 (2003)}\)
- \(B_g \text{ for C}_{2h} \text{ and } B_{2g} \text{ for D}_{2h}\)

Powell, McKenzie cond-mat/0607078
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
h-doped are strongly correlated: evidence from the normal state
Mott-Ioffe-Regel limit

\[ \sigma = \frac{ne^2 \tau}{m} \]
\[ n = \frac{1}{2\pi d} k_F^2 \]
\[ \sigma = \left( \frac{1}{2\pi d} k_F^2 \right) \frac{e^2 \tau}{m} \]
\[ \ell = \left( \frac{\hbar k_F}{m} \right) \tau \]
\[ \sigma = \frac{1}{2\pi d} k_F e^2 \left( \frac{\ell}{\hbar} \right) \]
\[ k_F \ell = \frac{2\pi}{\lambda_F} \ell \sim 2\pi \]
\[ \sigma_{MIR} = \frac{e^2}{\hbar d} \]
Hole-doped cuprates and MIR limit

Gurvitch & Fiory
PRL 59, 1337 (1987)

MIR limit
Mean-free path
~ Fermi wavelength

LSCO 17%, YBCO optimal

Dominic Bergeron TPSC

Optical and dc conductivity of the two-dimensional Hubbard model in the pseudogap regime and across the antiferromagnetic quantum critical point including vertex corrections
Experiment: X-Ray absorption

Chen et al. PRL 66, 104 (1991)

Peets et al. PRL 103, (2009),

Number of low energy states above $\omega = 0$ scales as $2x +$
Not as $1+x$ as in Fermi liquid

Meinders et al. PRB 48, 3916 (1993)
Thermopower

Hall coefficient

Ando et al. PRL 92, 197001 (2004)
Density of states (STM)

Khosaka et al. Science 315, 1380 (2007);
e-doped cuprates

Less strongly coupled: evidence from the normal state
Electron-doped and MIR limit

NCCO

Dominic Bergeron et al. TPSC
PRB 84, 085128 (2011)

Onose et al. 2004
TPSC vs experiment for $\xi$

Kyung et al. PRL 93, 147004 (2004)

ξ(T) at the QCP

NCCO
Matsui et al. PRB 2007

z = 1
Motoyama, Nature 2007

U=6, t’=-0.175, t”=0.05, n=1.2007

Dominic Bergeron TPSC
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

Motoyama, E. M. et al..

Armitage et al. PRL 2001
$$T$$

I

$$E$$

$$\mathbf{k}_F$$

$$\omega$$

II

$$A(\omega)$$

$$\mathbf{k}_F$$

III

$$2\Delta$$

$$\mathbf{k}_F$$

$$\omega$$
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)
4. Weakly and strongly correlated superconductivity

Weakly correlated case
\[ \Delta_p = -\frac{1}{2V} \sum_{p'} U(p - p') \frac{\Delta_{p'}}{E_{p'}} \left( 1 - 2n\left( E_{p'} \right) \right) \]

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
QMC: symbols.
Solid lines analytical.

Kyung, Landry, A.-M.S.T.
Relation between symmetry and wave vector of AFM fluctuations

Hassan et al. PRB 2008
$T_c$ depends on $t'$

FIG. 5. (Color online) The $d_{x^2−y^2}$ superconducting critical temperature $T_c$ as a function of $t'$ at $U=2.5$, $3$, and $4$ for $n=1$. The inset shows the $d_{xy}$ superconducting critical temperature $T_c$ as a function of $t'$ for $U=3.6$ and 4.

Hassan et al. PRB 2008
Tc in RC regime or not

\[ \xi_{th} > \xi_{AFM} \]

\[ \xi_{AFM} \sim 10 \text{ at optimal } Tc \]

FIG. 6. (Color online) Logarithm base ten of the antiferromagnetic correlation length (in units of the lattice spacing) as a function of inverse temperature for three values of \( t' = 0.15, 0.21, 0.31 \) at \( U = 4 \) for \( n = 1 \). The value of \( T_c \) for the corresponding \( t' \) is shown on the plot.

Hassan et al. PRB 2008
Organics & Pnictides

Organic

Pnictide

Bourbonnais, Sedeki, 2012

Doiron-Leyraud et al., PRB 80, 214531 (2009)
Correlation resistivity vs \( T_c \)

Dominic Bergeron et al. TPSC
PRB 84, 085128 (2011)
4. Weakly and strongly correlated superconductivity

Strong coupling point of view
A cartoon strong coupling picture


\[ J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J \sum_{\langle i,j \rangle} \left( \frac{1}{2} c_i^\dagger \vec{\sigma} c_i \right) \cdot \left( \frac{1}{2} c_j^\dagger \vec{\sigma} c_j \right) \]

\[ d = \langle \hat{d} \rangle = 1/N \sum_{\vec{k}} (\cos k_x - \cos k_y) \langle c_{\vec{k},\uparrow} c_{-\vec{k},\downarrow} \rangle \]

\[ H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} - 4Jm\hat{m} - Jd(\hat{d} + \hat{d}^\dagger) + F_0 \]

Pitaevskii Brückner:
Pair state orthogonal to repulsive core of Coulomb interaction

Miyake, Schmitt–Rink, and Varma
P.R. B 34, 6554-6556 (1986)
5. High-temperature superconductors and organics: the view from dynamical mean-field theory

5.1: Quantum cluster approaches
Mott transition and Dynamical Mean-Field Theory.
The beginnings in $d = \infty$

- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy ($\omega$ dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.

W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

DMFT, ($d = 3$)
2d Hubbard: Quantum cluster method

Hettler ... Jarrell ... Krishnamurty PRB 58 (1998)
Kotliar et al. PRL 87 (2001)

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar et al. RMP (2006)
AMST et al. LTP (2006)
• Long range order:
  – Allow symmetry breaking in the bath (mean-field)
• Included:
  – Short-range dynamical and spatial correlations
• Missing:
  – Long wavelength p-h and p-p fluctuations
Two solvers for the cluster-in-a-bath problem
Competition AFM-dSC

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
At finite T, solving cluster in a bath problem

- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.


5.2 Normal state and pseudogap
High-temperature superconductors

Armitage, Fournier, Greene, RMP (2009)

[Graph showing phase transitions for La$_{2-x}$Sr$_x$CuO$_4$ and Re$_{2-x}$Ce$_x$CuO$_4$ superconductors with temperature ($T$) and doping levels as variables.]
Three broad classes of mechanisms for pseudogap

• Rounded first order transition
• $d = 2$ precursor to a lower temperature broken symmetry phase
• Mott physics

• Competing order
  – Current loops: Varma, PRB 81, 064515 (2010)
  – Stripes or nematic: Kivelson et al. RMP 75 1201(2003); J.C.Davis
  – d-density wave: Chakravarty, Nayak, Phys. Rev. B 63, 094503 (2001); Affleck et al. flux phase
  – SDW: Sachdev PRB 80, 155129 (2009) ...

• Or Mott Physics?
Doping driven Mott transition, $t' = 0$

<table>
<thead>
<tr>
<th>Method</th>
<th>$t'$</th>
<th>Orbital selective</th>
<th>U</th>
<th>Critical point</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>D+C+H 8</td>
<td></td>
<td></td>
<td>7</td>
<td></td>
<td>Werner et al. cond-mat (2009)</td>
</tr>
<tr>
<td>D+C+H 4</td>
<td></td>
<td></td>
<td>10,6</td>
<td></td>
<td>Gull et al. EPL (2008)</td>
</tr>
<tr>
<td></td>
<td>-0.3</td>
<td></td>
<td>10,6</td>
<td></td>
<td>Liebsch, Merino… (2008)</td>
</tr>
<tr>
<td>D+C+H 8</td>
<td></td>
<td></td>
<td>7</td>
<td></td>
<td>Ferrero et al. PRB (2009)</td>
</tr>
</tbody>
</table>

K. Haule, G. Kotliar, PRB (2007)  
Vildhyadhiraja, PRL (2009)
Doping driven Mott transition

\[ T = 0.25 \, t \]

Gull, Parcollet, Millis
arXiv:1207.2490v1

Gull, Werner, Millis, (2009)
Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of $U$
First order transition at finite doping.


\( n(\mu) \) for several temperatures: 
\( T/t = 1/10, 1/25, 1/50 \)
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
Khosaka et al. *Science* **315**, 1380 (2007);
Density of states
Density of states
Spin susceptibility
Spin susceptibility

Underdoped Hg1223
Julien et al. PRL 76, 4238 (1996)
Plaquette eigenstates
What is the minimal model?

H. Alloul arXiv:1302.3473

Fig 1 Spin contribution $K_s$ to the $^{89}$Y NMR Knight shift [11] for YBCO$_{5.6}$ permit to define the PG onset $T^*$. Here $K_s$ is reduced by a factor two at $T\sim T^{*}/2$. The sharp drop of the SC fluctuation conductivity (SCF) is illustrated (left scale) [23]. We report as well the range over which a Kerr signal is detected [28], and that for which a CDW is evidenced in high fields from NMR quadrupole effects [33] and ultrasound velocity data [30]. (See text.)
Pseudogap $T^*$ along the Widom line
The Widom line

G. Sordi, *et al.* Scientific Reports 2, 547 (2012)
What is the Widom line?

- it is the continuation of the coexistence line in the supercritical region
- line where the maxima of different response functions touch each other asymptotically as $T \to T_p$
- liquid-gas transition in water: max in isobaric heat capacity $C_p$, isothermal compressibility, isobaric heat expansion, etc

**DYNAMIC crossover arises from crossing the Widom line!**

Phase diagram
What is the minimal model?

H. Alloul arXiv:1302.3473

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Spin susceptibility
Two crossover lines

Sordi et al. PRL 108, 216401 (2012)
PRB 87, 041101(R) (2013)
C-axis resistivity

Summary: normal state

- Mott physics extends way beyond half-filling
- Pseudogap is a phase
- Pseudogap $T^*$ is a Widom line
- High compressibility (stripes?)
Finite $T$ phase diagram
Superconductivity

Sordi et al. PRL 108, 216401 (2012)
Unified phase diagram
Cuprates (doping driven transition)

Giovanni Sordi

Patrick Sémon
Cuprates (doping driven transition)

Pseudogap vs pair

F. Rullier-Albenque, H. Alloul, and G. Rikken,

Giovanni Sordi

Patrick Sémon
Meaning of $T_c^d$: Local pair formation


However, our measurements demonstrate that the nodal gap does not change with reduced doping. The pairing strength does not get weaker or stronger as the Mott insulator is approached; rather, it saturates.
Fluctuating region

Infrared response

Dubroka et al. PRL 106, 047006 (2011)
$T_{\text{pair}}$


ARPES

Bi2212
Magnetoresistance, LSCO
Fluctuating vortices

Actual $T_c$ in underdoped

• Quantum and classical phase fluctuations

• Magnitude fluctuations

• Competing order

• Disorder
Larger clusters

- Is there a minimal size cluster where $T_c$ vanishes before half-filling?
- Learn something from small clusters as well
- Local pairs in underdoped
Larger cluster 8 site DCA

Gull, Millis, arxiv.org:304.6406

FIG. 8. Superfluid stiffness $\rho_s$ determined in the superconducting state at $T = t/60$ from Eq. 15, as a function of doping.
Gaussian amplitude fluctuations in Eu-LSCO

Chang, Doiron-Leyraud et al.
Effect of disorder

First-order transition leaves its mark
Summary

- Below the dome finite $T$ critical point (not QCP) controls normal state
- First-order transition destroyed but traces in the dynamics
- $T^*$ different from $T_c^d$
- Actual $T_c$ in underdoped
  - Competing order
  - Long wavelength fluctuations (see O.P.)
  - Disorder
$T = 0$ phase diagram: superconductivity

Mechanism at strong coupling
Theory: $T_c$ down vs Mott

Dome vs Mott (CDMFT)

Kancharla, Kyung, Civelli, Sénéchal, Kotliar AMST
CDMFT global phase diagram

AND Capone, Kotliar PRL (2006)

Armitage, Fournier, Greene, RMP (2009)
The glue
Im $\Sigma_{an}$ and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)
The glue


Wakimoto … Birgeneau
PRL (2004)
The glue and neutrons

**FIG. 3** (color online). $Q$-integrated dynamic structure factor $S(\omega)$ which is derived from the wide-$H$ integrated profiles for LBCO 1/8 (squares), LSCO $x = 0.25$ (diamonds; filled for $E_i = 140$ meV, open for $E_i = 80$ meV), and $x = 0.30$ (filled circles) plotted over $S(\omega)$ for LBCO 1/8 (open circles) from [2]. The solid lines following data of LSCO $x = 0.25$ and 0.30 are guides to the eyes.

Frequencies important for pairing

\[ I_F(\omega) = - \int_0^\omega \frac{d\omega'}{\pi} \text{Im} F_{ij}^{R}(\omega'). \]

\[ \langle c_{i\uparrow} c_{i\downarrow} \rangle \]

for \( \omega \rightarrow \infty \)

Resilience to near-neighbor repulsion $V$

In mean-field, $J - V$

$J = 130 \text{ meV}$

$V = 400 \text{ meV}$

The $\ln(E_F/\omega_D)$ necessary to screen $V$, for $\mu^*$ not enough

Weak-coupling: $V < U (U/W)$ for survival of d-wave

Resilience to near-neighbor repulsion

\[ J = \frac{4t^2}{U-V} \]

Sénéchal, Day, Bouliane, ÁMST PRB 87, 075123 (2013)
$T = 0$ phase diagram

Normal state and large anisotropy
Underdoped metal very sensitive to anisotropy

FIG. 3: (Color online) Anisotropy in the CDMFT conductivity $\delta_\sigma = 2 [\sigma_x(0) - \sigma_y(0)] / [\sigma_x(0) + \sigma_y(0)]$ as a function of filling $N$ for various values of $U$ and $\eta = 0.1$, $\delta_0 = 0.04$.

Okamoto, Sénéchal, Civelli, AMST
Phys. Rev. B 82, 180511R 2010

D. Fournier et al. Nature Physics (Marcello Civelli)
Methods
Measurable quantities: Green’s functions

\[ \langle O \rangle \equiv \frac{\text{Tr}[e^{-\beta(H-\mu N)}O]}{\text{Tr}[e^{-\beta(H-\mu N)}]} \]

\[ G_{k\sigma}(\tau) = -\langle T_\tau [c_{k\sigma}(\tau)c_{k\sigma}^\dagger] \rangle \]

\[ = -\theta(\tau)\langle c_{k\sigma}(\tau)c_{k\sigma}^\dagger \rangle + \theta(-\tau)\langle c_{k\sigma}^\dagger c_{k\sigma}(\tau) \rangle. \]

\[ c_{k\sigma}(\tau) = e^{(H-\mu N)\tau}c_{k\sigma}e^{-(H-\mu N)\tau} \]

\[ G_{k\sigma}(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n\tau} G_{k\sigma}(\tau) \]

\[ \omega_n = (2n + 1)\pi T \]
Green’s function: free electrons, atomic limit

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

\[ \mathcal{G}_{k\sigma}(i\omega_n) = \frac{1}{i\omega_n - (\varepsilon_k - \mu)} \]

\[ H = U \sum_i n_{i\uparrow} n_{i\downarrow} \]

\[ \langle n \rangle = 1 \quad \mathcal{G}_{\sigma}(i\omega_n) = \frac{1/2}{i\omega_n + \frac{U}{2}} + \frac{1/2}{i\omega_n - \frac{U}{2}} \]
Self-energy and all that

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

\[ G_{k\sigma}(i\omega_n) = \frac{1}{i\omega_n - (\epsilon_k - \mu) - \Sigma_{k\sigma}(i\omega_n)} \]

\[ G_{k\sigma}^{-1}(i\omega_n) = G_{k\sigma}^{0-1}(i\omega_n) - \Sigma_{k\sigma}(i\omega_n) \]

Self-energy in the atomic limit for \( n = 1 \)

\[ G_\sigma(i\omega_n) = \frac{1/2}{i\omega_n + \frac{U}{2}} + \frac{1/2}{i\omega_n - \frac{U}{2}} \]

\[ G_\sigma(i\omega_n) = \frac{1}{i\omega_n + \frac{U}{2} - \Sigma(i\omega_n)} \]

\[ \Sigma(i\omega_n) = \frac{U}{2} + \frac{U^2}{i\omega_n} \]
Self-consistency

\[ G_{\sigma}^{\text{imp}}(i\omega_n)^{-1} = G_{\sigma}^{0-\text{imp}}(i\omega_n)^{-1} - \Sigma_{\sigma}(i\omega_n) \]

\[ N_c \int \frac{d^d \mathbf{k}}{(2\pi)^d} \frac{1}{G_{k\sigma}^{0}(i\omega_n)^{-1} - \Sigma_{\sigma}(i\omega_n)} = G_{\sigma}^{\text{imp}}(i\omega_n) \]
Methods of derivation

• Cavity method
• Local nature of perturbation theory in infinite dimensions
• Expansion around the atomic limit
• Effective medium theory
• Potthoff self-energy functional

DMFT as a stationary point
Another way to look at this (Potthoff)

\[ \Omega_t[G] = \Phi[G] - Tr[(G_{0t}^{-1} - G^{-1})G] + Tr \ln(-G) \]

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

\[ \Omega_t[\Sigma] = \Phi[G] - Tr[\Sigma G] - Tr \ln(-G_{0t}^{-1} + \Sigma) \]

Still stationary (chain rule)

\[ \Omega_t[\Sigma] = F[\Sigma] - Tr \ln(-G_{0t}^{-1} + \Sigma) \]

SFT : Self-energy Functional Theory

With $F[\Sigma]$  Legendre transform of Luttinger-Ward funct.

$$\Omega_t[\Sigma] = F[\Sigma] + \text{Tr} \ln(-(G_0^{-1} - \Sigma)^{-1})$$

is stationary with respect to $\Sigma$ and equal to grand potential there.

$$\Omega_t[\Sigma] = \Omega_{t'}[\Sigma] - \text{Tr} \ln(-(G_0'^{-1} - \Sigma)^{-1}) + \text{Tr} \ln(-(G_0^{-1} - \Sigma)^{-1}).$$

Vary with respect to parameters of the cluster (including Weiss fields)

Variation of the self-energy, through parameters in $H_0(t')$

CT-QMC impurity solver
Monte Carlo method

Gull, Millis, Lichtenstein, Rubtsov, Troyer, Werner,
Rev.Mod.Phys. 83, 349 (2011)

\[ Z = \int_{c} dx p(x). \]

\[ \langle A \rangle_p = \frac{1}{Z} \int_{c} dx \mathcal{A}(x) p(x). \]

\[ \langle A \rangle_p \approx \langle A \rangle_{MC} = \frac{1}{M} \sum_{i=1}^{M} \mathcal{A}(x_i). \]

\[ \langle A \rangle = \frac{1}{Z} \int_{c} dx \mathcal{A}(x) p(x) = \frac{\int_{c} dx \mathcal{A}(x)[p(x)/\rho(x)] \rho(x)}{\int_{c} dx [p(x)/\rho(x)] \rho(x)} \equiv \frac{\langle A(p/\rho) \rangle_p}{\langle p/\rho \rangle_p}. \]
Monte Carlo: Markov chain

- Ergodicity
- Detailed balance

\[
\frac{W_{xy}}{W_{yx}} = \frac{p(y)}{p(x)}
\]

\[
W_{xy} = W_{xy}^{\text{prop}} W_{xy}^{\text{acc}}
\]

\[
W_{xy}^{\text{acc}} = \min[1, R_{xy}]
\]

\[
R_{xy} = \frac{p(y) W_{yx}^{\text{prop}}}{p(x) W_{xy}^{\text{prop}}}
\]
Reminder on perturbation theory

\[ \exp(-\beta(H_a + H_b)) = \exp(-\beta H_a)U(\beta) \]

\[ \frac{\partial U(\beta)}{\partial \beta} = -H_b(\beta)U(\beta) \]

\[ U(\beta) = 1 - \int_0^\beta d\tau H_b(\tau) + \int_0^\beta d\tau \int_0^\tau d\tau' H_b(\tau)H_b(\tau') + \ldots \]
Partition function as sum over configurations

\[ Z = \text{Tr}[\exp(H_a + H_b)] \]

\[ = \sum_k (-1)^k \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \text{Tr}[e^{-\beta H_a} H_b(\tau_k) \times H_b(\tau_{k-1}) \cdots H_b(\tau_1)]. \]

\[ Z = \sum_{k=0}^{\infty} \sum_{\gamma \in \Gamma_k} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k w(k, \gamma, \tau_1, \ldots, \tau_k). \]

\[ x = (k, \gamma, (\tau_1, \ldots, \tau_k)), \quad p(x) = w(k, \gamma, \tau_1, \ldots, \tau_k) d\tau_1 \cdots d\tau_k, \]
$W_{(k, \tilde{\tau}), (k+1, \tilde{\tau}')}^{\text{prop}} = \frac{d\tau}{\beta}$

$W_{(k+1, \tilde{\tau}'), (k, \tilde{\tau})}^{\text{prop}} = \frac{1}{k + 1}.$

$R_{(k, \tilde{\tau}), (k+1, \tilde{\tau}')}(k, \tilde{\tau}) = \frac{p((k + 1, \tilde{\tau}'))}{p((k, \tilde{\tau}))} \frac{W_{(k+1, \tilde{\tau}'), (k, \tilde{\tau})}^{\text{prop}}}{W_{(k, \tilde{\tau}), (k+1, \tilde{\tau}')}}$

$= \frac{w(k + 1) d\tau'_1 \cdots d\tau'_{k+1}}{w(k) d\tau_1 \cdots d\tau_k} \frac{1/(k + 1)}{d\tau/\beta}$

$= \frac{w(k + 1)}{w(k)} \frac{\beta}{k + 1}.$


Solving cluster in a bath problem

- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.
Expansion in powers of the hybridization

\[ H_{\text{hyb}} = \sum_{p} (V_{p} c_{p}^{\dagger} d_{j} + V_{p}^{*} c_{p} d_{j}^{\dagger}) = \tilde{H}_{\text{hyb}} + \tilde{H}_{\text{hyb}}^{\dagger} \]

\[ Z = \sum_{k=0}^{\infty} \int_{0}^{\beta} d\tau_{1} \cdots \int_{\tau_{k-1}}^{\beta} d\tau_{k} \int_{0}^{\beta} d\tau'_{1} \cdots \int_{\tau'_{k-1}}^{\beta} d\tau'_{k} \]
\[ \times \sum_{j_{1}, \ldots, j_{k}} \sum_{p_{1}, \ldots, p_{k}} V_{j_{1}}^{p_{1}} V_{j_{1}}^{p_{1}}^{*} \cdots V_{j_{k}}^{p_{k}} V_{j_{k}}^{p_{k}}^{*} \]
\[ \times \text{Tr}_{d}[T e^{-\beta H_{\text{loc}}} d_{j_{k}}(\tau_{k}) d_{j_{k}}^{\dagger}(\tau'_{k}) \cdots d_{j_{1}}(\tau_{1}) d_{j_{1}}^{\dagger}(\tau'_{1})] \]
\[ \times \text{Tr}_{c}[T e^{-\beta H_{\text{bath}}} c_{p_{k}}^{\dagger}(\tau_{k}) c_{p_{k}}(\tau'_{k}) \cdots c_{p_{1}}^{\dagger}(\tau_{1}) c_{p_{1}}(\tau'_{1})]. \]

\[ P_{m} = \frac{\langle m | e^{-\beta H_{\text{loc}}} d_{j_{k}}(\tau_{k}) d_{j_{k}}^{\dagger}(\tau'_{k}) \cdots d_{j_{1}}(\tau_{1}) d_{j_{1}}^{\dagger}(\tau'_{1}) | m \rangle}{\sum_{n} \langle n | e^{-\beta H_{\text{loc}}} d_{j_{k}}(\tau_{k}) d_{j_{k}}^{\dagger}(\tau'_{k}) \cdots d_{j_{1}}(\tau_{1}) d_{j_{1}}^{\dagger}(\tau'_{1}) | n \rangle} \]
Sign problem

\[ S = S_{\text{cl}}(c^\dagger, c) + \int_0^\beta d\tau d\tau' c^\dagger(\tau') \Delta(\tau' - \tau) c(\tau) \]

P. Sémon, A.-M.S. Tremblay, (unpub.)
Two-Particle Self-Consistent Approach (U < 8t)
- How it works

• General philosophy
  – Drop diagrams
  – Impose constraints and sum rules
    • Conservation laws
    • Pauli principle ( \(<n_\sigma^2> = <n_\sigma>\) )
    • Local moment and local density sum-rules

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

Vilk, AMT J. Phys. I France, 7, 1309 (1997); Allen et al. in *Theoretical methods for strongly correlated electrons* also cond-mat/0110130
(Mahan, third edition)
TPSC approach: two steps

I: Two-particle self consistency

1. Functional derivative formalism (conservation laws)
   
   (a) spin vertex:
   
   \[ U_{sp} = \frac{\delta \Sigma_{\uparrow}}{\delta G_{\downarrow}} - \frac{\delta \Sigma_{\uparrow}}{\delta G_{\uparrow}} \]

   (b) analog of the Bethe-Salpeter equation:
   
   \[ \chi_{sp} = \frac{\delta G}{\delta \phi} = GG + GU_{sp}\chi_{sp}G \]

   (c) self-energy:
   
   \[ \Sigma_{\sigma} (1, \bar{1}; \{ \phi \}) G_{\sigma} (\bar{1}, 2; \{ \phi \}) = -U \langle c^\dagger_{-\sigma} (1^+) c_{-\sigma} (1) c_{\sigma} (1) c^\dagger_{\sigma} (2) \rangle_{\phi} \]
   
   \[ \approx A_{\phi} G_{-\sigma}^{(1)} (1, 1^+; \{ \phi \}) G_{\sigma}^{(1)} (1, 2; \{ \phi \}) \]

2. Factorization
3. The F.D. theorem and Pauli principle

\[
\langle (n_{\uparrow} - n_{\downarrow})^2 \rangle = \langle n_{\uparrow} \rangle + \langle n_{\downarrow} \rangle - 2\langle n_{\uparrow} n_{\downarrow} \rangle
\]

\[
\frac{T}{N} \sum_q \chi_{sp}^{(1)}(q) = n - 2\langle n_{\uparrow} n_{\downarrow} \rangle
\]

II: Improved self-energy

Insert the first step results into exact equation:

\[
\sum_{\sigma} (1, \bar{1}; \{\phi}\}) G_{\sigma} (\bar{1}, 2; \{\phi}\}) = -U \langle c_{-\sigma}^\dagger (1^+) c_{-\sigma} (1) c_{\sigma} (1) c_{\sigma}^\dagger (2) \rangle_{\phi}
\]

\[
\sum_{\sigma}^{(2)}(k) = U n_{\sigma} + \frac{U T}{8 N} \sum_q \left[ 3U_{sp}\chi_{sp}^{(1)}(q) + U_{ch}\chi_{ch}^{(1)}(q) \right] G_{\sigma}^{(1)}(k + q)
\]
A better approximation for single-particle properties (Ruckenstein)

Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. 33, 159 (1996);

N.B.: No Migdal theorem
Benchmarks for TPSC
\[ \xi \sim \exp\left( \frac{C(T)}{T} \right) \]

**Calc.:** Vilk et al. P.R. B 49, 13267 (1994)


Proofs...

$U = +4$
$\beta = 5$

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Thank you