The standard model, from weak to intermediate coupling

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1. Motivation

- Here, \(-W < U < W\) with \((W = 8t)\)
  - Relevant for high \(T_c\) where \(U > W\)?
    - A question of threshold (and continuity)

- Importance of quantitative predictions
  - Location of QCP
  - No ferromagnetism
- Effective \(U < 0\) model may be not too strongly interacting
- Suppose we find new quasiparticles in strong coupling. How do we study residual interactions?
- Do we give up calculating Landau parameters?
  - How to predict when the theory is bad?
- Standard method gives qualitatively incorrect results
1. Motivation

2. The standard approach:
   - what it is
   - a qualitatively incorrect result
   - limitations of the approach

3. A non-perturbative approach ($U > 0$ and $U < 0$)
   - Proof that it works
   - How it works

4. Results:
   - Mechanism for pseudogap
   - Spectral weight rearrangement

5. Conclusion.
2. The standard approach:
- what it is (FLEX, self-consistent T-matrix ...)

\[
\Phi [G] = \begin{array}{c}
\begin{array}{c}
\rightarrow \quad \rightarrow \\
\circ \quad \circ
\end{array}
\end{array} + \frac{1}{2} \begin{array}{c}
\begin{array}{c}
\rightarrow \quad \rightarrow \\
\circ \quad \circ
\end{array}
\end{array} + \ldots
\]

\[
\Sigma [G] = \frac{\delta \Phi [G]}{\delta G} = \begin{array}{c}
\begin{array}{c}
\rightarrow \quad \rightarrow \\
\circ \quad \circ
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\rightarrow \quad \rightarrow \\
\circ \quad \circ
\end{array}
\end{array} + \ldots
\]

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\]
2. The standard approach:
- what it is (FLEX, self-consistent T-matrix ...)

- Thermodynamically consistent:
  \[ \frac{dF}{d\mu} = \text{Tr}[G] \]

- Satisfies Luttinger theorem
  (Volume of Fermi surface at \( T = 0 \) preserved)

- Satisfies Ward identities (conservation laws):
  \( G_2(1,1;2,3) \) appropriately related to \( G(1,2) \)
2. The standard approach:
- a qualitatively incorrect result

2. The standard approach:
- limitations of the approach

- Integration over coupling constant of potential energy does not give back the starting Free energy.

- The Pauli principle in its simplest form is not satisfied (It is used in defining the Hubbard model in the first place)

- There is an infinite number of conserving approximations (How do we pick up the diagrams?)

- Inconsistency:
  Strongly frequency-dependent self-energy, constant vertex

\[ \text{No Migdal theorem, so vertex corrections should be included} \]
\[ \Sigma (k_F, ik_n) \approx \frac{U}{4N} T \sum_q U_{sp} \chi_{sp} (q, 0) \frac{1}{ik_n - \tilde{\epsilon}_{k+q} - \Sigma (k_F+q, ik_n)} \]

\[ \Sigma (ik_n) = \frac{\Delta^2}{ik_n - \Sigma (ik_n)} \]

Re\[\Sigma^R(\omega) = \frac{\omega}{2} - \frac{\omega}{2|\omega|} \theta (|\omega| - 2\Delta) \left( \omega^2 - 4\Delta^2 \right)^{1/2} \]

Im\[\Sigma^R(\omega) = -\frac{1}{2} \theta (2\Delta - |\omega|) \left( 4\Delta^2 - \omega^2 \right)^{1/2} \]

Non Fermi-liquid but not singular at \( \omega = 0 \)

2. The standard approach:
   - problem...

   - We do not know how to properly solve even the «standard model» for heavy fermions (Coleman).

   - Lee-Rice-Anderson simpler approach seems qualitatively better, why?

   - GW approach to improve band structure calculations?
3. An approach for both $U > 0$ and $U < 0$
- Proofs that it works

Notes:
-F.L. parameters
-Self also Fermi-liquid

QMC + cal.: Vilk et al. P.R. B 49, 13267 (1994)
Proofs...

QMC: Bulut, Scalapino, White, P.R. B 50, 9623 (1994).
Proofs...

Proofs...

Moving to the attractive case....

Calc. : Kyung et al. cond-mat/0010001
QMC : Moreo, Scalapino, White, P.R. B. 45, 7544 (1992)

Proofs...

$U = -4$

| $|U| = 4$, $n = 0.87$ |
|----------------------|
| $T = 1/2$            |

| $T = 1/4$            |

| $T = 1/6$            |

| $T = 1/8$            |

$N(\omega)$
Proofs...

Calc.: Kyung et al. cond-mat/0010001
QMC: Trivedi and Randeria, P.R. L. 75, 312 (1995)

$U = -4$

$2^{nd}$ order perturbation theory

S.C. T-matrix
Proofs...

Kyung et al. cond-mat/0010001
3. An non-perturbative approach for both $U > 0$ and $U < 0$

Reminder: Generating function, with source field

$$Z [\phi] = \text{Tr} \left[ \mathcal{T}_\tau \left( e^{-\psi_\sigma^\dagger (\bar{1}) \phi_\sigma (\bar{1}, \bar{2}) \psi_\sigma (\bar{2})} \right) \right]$$

Propagator in the presence of the source field

$$G_\sigma (1, 2; \{\phi\}) = -\left\langle \psi_\sigma^\dagger (1) \psi_\sigma (2) \right\rangle_\phi = -\frac{\delta \ln Z [\phi]}{\delta \phi_\sigma (2, 1)}$$

Equation of motion and definition of self-energy

$$(G_0^{-1} - \phi) G = 1 + \Sigma G \ ; \ G^{-1} = G_0^{-1} - \phi - \Sigma$$

where, from the commutator of the interacting part of $H$:

$$\Sigma_\sigma (1, \bar{1}) G_\sigma (\bar{1}, 2) = -U \left\langle \psi_\sigma^\dagger (1^+) \psi_\sigma (1) \psi_\sigma (1) \psi_\sigma^\dagger (2) \right\rangle_\phi$$
Response functions:

\[GG^{-1} = 1\]

\[\frac{\delta G}{\delta \phi} G^{-1} + G \frac{\delta G^{-1}}{\delta \phi} = 0\]

Using \(G^{-1} = G_0^{-1} - \phi - \Sigma\)

\[\frac{\delta G}{\delta \phi} = -G \frac{\delta G^{-1}}{\delta \phi} G = G^{\ast} G + G \frac{\delta \Sigma}{\delta \phi} G\]

Legendre transform of \(Z\) is \(\Phi [G]\) and \(\Sigma [G] = \delta \Phi [G] / \delta G\). We have the RPA equation in particle-hole channel, (or Bethe-Salpeter in particle-particle)

\[\frac{\delta G}{\delta \phi} = G^{\ast} G + G \left[ \frac{\delta \Sigma}{\delta G} \frac{\delta G}{\delta \phi} \right] G\]
Vertices appropriate for spin and charge responses

\[ U_{sp} = \frac{\delta \Sigma_{\uparrow}}{\delta G_{\downarrow}} - \frac{\delta \Sigma_{\uparrow}}{\delta G_{\uparrow}} ; \quad U_{ch} = \frac{\delta \Sigma_{\uparrow}}{\delta G_{\downarrow}} + \frac{\delta \Sigma_{\uparrow}}{\delta G_{\uparrow}} \]
Hartree-Fock as an example of use of this formalism:

As an example, consider Hartree-Fock (N.B. all in external field $\phi$. Take $\phi = 0$ at the end only.)

\[ \Sigma^H_\sigma (1, \bar{1}) G^H_\sigma (\bar{1}, 2) = U G^H_{-\sigma} (1, 1^+) G_\sigma (1, 2) \]

\[ \Sigma^H_\sigma (1, 2) = U G^H_{-\sigma} (1, 1^+) \delta (1 - 2) \]

\[ \frac{\delta \Sigma \uparrow (1, 2)}{\delta G \downarrow (3, 4)} = U n_{-\sigma} \delta (1 - 2) \delta (3 - 1) \delta (4 - 2) \]
First step: Two-Particle Self-Consistent

\[ \Sigma^{(1)}_{\sigma} (1, \bar{1}) G^{(1)}_{\sigma} (\bar{1}, 2) = AG^{(1)}_{-\sigma} (1, 1^+) G^{(1)}_{\sigma} (1, 2) \]

where \( A \) depends on external field and is chosen such that the exact result

\[ \Sigma_{\sigma} (1, \bar{1}) G_{\sigma} (\bar{1}, 1^+) = U \left\langle n^\uparrow n^\downarrow \right\rangle \]

is satisfied. One finds

\[ A = U \frac{\left\langle n^\uparrow n^\downarrow \right\rangle}{\left\langle n^\uparrow \right\rangle \left\langle n^\downarrow \right\rangle} \]

Functional derivative of \( \left\langle n^\uparrow n^\downarrow \right\rangle / \left( \left\langle n^\uparrow \right\rangle \left\langle n^\downarrow \right\rangle \right) \) drops out of spin vertex

\[ U_{sp} = A = U \frac{\left\langle n^\uparrow n^\downarrow \right\rangle}{\left\langle n^\uparrow \right\rangle \left\langle n^\downarrow \right\rangle} \]
To close the system of equations, while satisfying conservation laws and the Pauli principle

\[
\left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \left\langle n_\uparrow \right\rangle + \left\langle n_\downarrow \right\rangle - 2\left\langle n_\uparrow n_\downarrow \right\rangle
\]

\[
\frac{T}{N} \sum_q \frac{\chi_0(q)}{1 - \frac{1}{2}U_{sp}\chi_0(q)} = n - 2\left\langle n_\uparrow n_\downarrow \right\rangle
\]

Recall

\[
U_{sp} = U \frac{\left\langle n_\uparrow n_\downarrow \right\rangle}{\left\langle n_\uparrow \right\rangle \left\langle n_\downarrow \right\rangle}
\]

To have charge fluctuations that satisfy Pauli principle as well,

\[
\frac{T}{N} \sum_q \frac{\chi_0(q)}{1 + \frac{1}{2}U_{ch}\chi_0(q)} = n + 2\left\langle n_\uparrow n_\downarrow \right\rangle - n^2
\]

(Bonus: Mermin-Wagner theorem)
Second step: improved self-energy

\[ \Sigma_\sigma \left( 1, \bar{1} \right) G_\sigma \left( \bar{1}, 2 \right) = -U \left\langle \psi^\dagger_{-\sigma} \left( 1^+ \right) \psi_{-\sigma} \left( 1 \right) \psi_\sigma \left( 1 \right) \psi^\dagger_\sigma \left( 2 \right) \right\rangle_\phi \]

\[ \Sigma_\sigma \left( 1, \bar{1} \right) G_\sigma \left( \bar{1}, 2 \right) = -U \left[ \frac{\delta G_\sigma \left( 1, 2 \right)}{\delta \phi_{-\sigma} \left( 1^+, 1 \right)} - G_{-\sigma} \left( 1, 1^+ \right) G_\sigma \left( 1, 2 \right) \right] \]

Last term is Hartree Fock (\( \lim \omega \to \infty \)). Multiply by \( G^{-1} \), replace lower energy part results of TPSC

\[ \Sigma_\sigma^{(2)} \left( 1, 2 \right) = U G_{-\sigma}^{(1)} \left( 1, 1^+ \right) \delta \left( 1 - 2 \right) - U G^{(1)} \left[ \frac{\delta \Sigma^{(1)} \delta G^{(1)}}{\delta G^{(1)} \delta \phi} \right] \]

Transverse+longitudinal for crossing-symmetry

\[ \Sigma_\sigma^{(2)} (k) = U n_{-\sigma} + \frac{U T}{8 N} \sum_q \left[ 3U_{sp} \chi^{(1)} (q) + U_{ch} \chi^{(1)} (q) \right] G_\sigma^{(1)} (k + q). \quad (4) \]
Results of the analogous procedure for $U < 0$

\[ U_{pp} = U \frac{\langle (1 - n^\uparrow)n^\downarrow \rangle}{\langle 1 - n^\uparrow \rangle \langle n^\downarrow \rangle}. \]  

(5)

\[ \chi^{(1)}_p(q) = \frac{\chi^{(1)}_0(q)}{1 + U_{pp} \chi^{(1)}_0(q)}. \]  

(6)

\[ \frac{T}{N} \sum_q \chi^{(1)}_p(q) \exp(-i q n^-) = \langle \Delta^\dagger \Delta \rangle = \langle n^\uparrow n^\downarrow \rangle. \]  

(7)

\[ \Sigma^{(1)} \simeq \frac{U}{2} - \frac{U_{pp} (1 - n)}{2}. \]  

(8)

\[ \Sigma^{(2)}_\sigma(k) = U n_{-\sigma} - U \frac{T}{N} \sum_q U_{pp} \chi^{(1)}_p(q) G^{(1)}_{-\sigma}(q - k). \]  

(9)
Satisfies Pauli principle and generalization of \( f \)-sum rule

\[
\int \frac{d\omega}{\pi} \text{Im} \chi^{(1)}(q, \omega) = \langle \left[ \Delta_q(0), \Delta_q^\dagger(0) \right] \rangle = 1 - n ; \quad \forall q
\]

\[
\int \frac{d\omega}{\pi} \omega \text{Im} \chi^{(1)}(q, \omega) = \left[ \frac{1}{N} \sum_k \left( \varepsilon_k + \varepsilon_{-k+q} \right) \left( 1 - 2 \langle n_{k\uparrow} \rangle \right) \right] \]
\[
-2 \left( \mu^{(1)} - \frac{U}{2} \right) (1 - n) ; \quad \forall q
\]

Internal accuracy check (For both \( U > 0 \) and \( U < 0 \)).

\[
\frac{1}{2} \text{Tr} \left[ \Sigma^{(2)} G^{(1)} \right] = \lim_{\tau \to 0^-} \frac{T}{N} \sum_k \Sigma^{(2)}_\sigma(k) G^{(1)}_\sigma(k) e^{-ikn\tau} = U \langle n_{\uparrow} n_{\downarrow} \rangle
\]

Check : \( \text{Tr} \left[ \Sigma^{(2)} G^{(1)} \right] \sim \text{Tr} \left[ \Sigma^{(2)} G^{(2)} \right] \)
4. Results:
- Mechanism for pseudogap
  - Enter the renormalized-classical regime.  
    N.B. $d = 2$
4. Results:

- Mechanism for pseudogap

- Pairing correlation length larger than single-particle thermal de Broglie wavelength ($v_F / T$)

\[ \xi \sim 1.3 \xi_{th} \]
Mechanism for pseudogap formation in the attractive model:

$U = -4$

$d = 2$ is crucial

4. Results:
- Spectral weight rearrangement
- Pseudogap appears first in total density of states
- Fills in instead of opening up
- Rearrangement over huge frequency scale compared with either $T$ or $\Delta T$. ($\Delta T \sim 0.03$, $T \sim 0.2$, $\Delta \omega \sim 1$)
4. Results:
- Crossover diagram

\[ U = -4 \]
5. Conclusion:

- Evidence against renormalized classical regime for spin fluctuations in pseudogap regime.

\[ U > 0 \]

Figure 2: Normalized imaginary part of the spin susceptibility at the AF wavevector in the normal state, at \( T = 100 \) K, for four oxygen contents in YBCO (\( T_c = 45, 55, 61, 61.5 \) K for \( x = 0.5, 0.85, 0.92, 0.97 \) respectively). These curves have been normalized to the same units using standard phonon calibration\(^{14}\) (100 counts in the vertical scale roughly correspond to \( \sim 350 \mu^2/\text{eV} \) in absolute units) \((\text{from}^{12})\).

Philippe Bourges cond-mat/0009373
- Quantum critical point, $d = 2$:
  - Instability at incommensurate $q$
  - Largest doping: $0.315$

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

- Decreases with increasing $U$
  - $U < W$
  - $U > W$

Freericks, Jarrell cond-mat/9405025
- Slightly Overdoped High-Tc Superconductor TlSr$_2$CaCu$_2$O$_{6.8}$
- Pseudogap in Knight shift and NMR relaxation strongly $H$ dependent, contrary to underdoped (up to 23 $T$).

- Underdoped in a range $\Delta T \sim 15 K$ near $T_c$ see evidence for renormalized classical regime ($KT$ behavior).

- Higher symmetry group creates large range of $T$ where there is a pseudogap.