André-Marie Tremblay

Sponsors:

CENTRE DE RECHERCHE SUR LES PROPRIÉTÉS ÉLECTRONIQUES DE MATÉRIAUX AVANCÉS

Université de Sherbrooke

CIAR The Canadian Institute for Advanced Research
Mathematics, Physics, and Computers: strongly correlated electrons in two dimensions as a case study.

I. All is not well with the theory of solids

II. A microscopic model

III. Inching our way up the weak-coupling regime.

IV. What was the competition up to?

V. Conclusion
I. All is not well with the theory of solids

Theory of solids

\[ H = \text{Kinetic} + \text{Coulomb} \]

- Many new ideas and concepts needed for progress (Born-Oppenheimer, H-F, Bands...)

- Successful program
  - Semiconductors, metals and superconductors
  - Magnets

- Is there anything left to do?
  - Unexplained materials: High Tc, Organics...
  - Strong correlations:
    strong interactions, low dimension
    strong fluctuations
The standard approaches:

Quasiparticles, Fermi surface and Fermi liquids
- LDA (Nobel prize 1998)

La$_2$CuO$_4$

Angle-Resolved Photoemission (ARPES)

\[ e_{\text{ph}} \pm \omega + \mu - W = \frac{k^2}{2m} \]

Quasi 2-d material
FIG. 1. ARPES intensity plot of the Mo(110) surface recorded along the $\overline{1} - \overline{N}$ line of the SBZ at 70 K. Shown in the inset is the spectrum of the region around $k_F$ taken with special attention to the surface cleanliness.

FIG. 2. Spectral intensity as a function of binding energy for constant emission angle, normalized to the experimentally determined Fermi cut-off. Data are symbols, while lines are fits to the Lorentzian peaks with a linear background. The dependence on the binding energy (a), temperature (b), and hydrogen exposure (c) is shown.

T. Valla, A. V. Fedorov, P. D. Johnson, and S. L. Hulbert
$n = 1$, Metal according to band AFM insulator in reality
Optimally doped BISCCO


- $d=2$ partial vanishing act of the Fermi surface away from $n = 1$. 

II. A microscopic model

κ-(BEDT)$_2$X
Simplest microscopic model for Cu O planes.

- Size of Hilbert space: $4^N$ ($N = 16$)
- Compute $\frac{\text{Tr}[Oe^{-H/k_B T}]}{\text{Tr}[e^{-H/k_B T}]}$
Hubbard model (Kanamori, Gutzwiller, 1963):

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

- Screened interaction $U$
- $U, T, n$
- $a = 1, t = 1, \hbar = 1$

- 2001 vs 1963: Numerical solutions to check analytical approaches
\[ A(k, \omega) \]

\[ U = 0 \]

\[ t = 0 \]

\[ A(k, \omega) \]

\[ -U/2 \quad U/2 \]

\[ \omega \]

\[ k \]

\[ -\pi/a \quad \pi/a \]

\[ \mu \quad U \]

\[ +U/2 \quad -U/2 \]

\[ t = 0 \]

\[ A(k, \omega) \]

\[ +U/2 \quad -U/2 \]

\[ \mu \]

\[ U \]

\[ -4t \quad +4t \]

\[ \omega \]

\[ k \]

\[ -\pi/a \quad \pi/a \]
Weak vs strong coupling

\[ A(k_F, \omega) \]

\[ \Delta \]

\[ U \]

\[ T \]

\[ \omega \]

\[ \omega \]

D. Sénéchal
III. Inching our way up the weak coupling regime

QMC
André Reid, Christian Boily, Hugues Nélisse

Liang Chen

Claude Bourbonnais

L. Chen, C. Bourbonnais, T. Li, and A.–M. S. Tremblay

FIG. 2. Feynman diagrams which lead to the renormalized $U$. The calculation is for the $Q=0$ structure factor (static susceptibility). The $S^+S^-$ susceptibility is on the first line. The vertex in the second line obeys the usual RPA equation except that the $Q_iQ_a$ dependence of the effective interaction in the last line is included. All external legs are shown only for labeling momenta and Matsubara frequencies.
• Problems:
  
  • Cannot compute charge structure factor with satisfactory accuracy
  
  • Predicts a finite $T$ antiferromagnetic phase transition in $d = 2$
  
  • Contradicts Mermin-Wagner theorem

\[
(\nabla \theta)^2 \rightarrow q^2 \theta_q \theta_q \rightarrow k_B T \quad \quad \langle \theta^2 \rangle \propto \int d^2 q \frac{k_B T}{q^2} \rightarrow \infty
\]
• Yury Vilk, 1993

• Forget diagrams

• Keep RPA form since satisfies conservation laws

• Determine renormalized interaction from sum-rule (Singwi)
  
  • (Double-occupancy determined self-consistently)

• Get the charge fluctuations from Pauli principle

⇒ • Mermin-Wagner theorem automatically satisfied
A non-perturbative approach for both $U > 0$ and $U < 0$

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

Proofs that it works

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

QMC: Bulut, Scalapino, White, P.R. B 50, 9623 (1994).
\[ S_{sp}(\pi, \pi) \]

**Monte Carlo**
- 4x4
- 6x6
- 8x8
- 10x10
- 12x12

\[ \xi \sim \exp(C(T)/T) \]

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

\[ O(N = \infty) \]
What about single-particle properties? (Ruckenstein)

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

N.B.: No Migdal theorem
Quantitative agreement with QMC

Fig. 1. – Comparison of our results for $G(k, \tau)$ (––––) with Monte Carlo data (o), FLEX (-- --), parquet (- - - -), and second-order perturbation theory (--- ---), all on $8 \times 8$ mesh with $U = 4$, $k_F = (\pi, 0)$. Monte Carlo data and results for FLEX and parquet are from ref. [4]. a) $n = 0.875$, $T = 0.25$; b) $n = 1$, $T = 0.17$. 
Qualitatively new result:
effect of critical fluctuations on particles (RC regime)

\[
\Sigma(k_F, ik_n) \propto T \int d^d q \frac{1}{q_\perp^2 + q_\parallel^2 + \xi^{-2}} \frac{1}{ik_n + \varepsilon_{-k+q}}
\]

\[
\text{Im} \Sigma^R(k_F,0) \propto -\frac{T}{\nu_F} \xi^{3-d}
\]

in 2D:
\[
\xi > \xi_{th} \quad (\xi_{th} \equiv \hbar \nu_F / \pi k_B T)
\]

\[
\Delta \varepsilon \approx \nabla \varepsilon_k \cdot \Delta k \approx \nu_F \hbar \Delta k = k_B T
\]

\[
\text{Im} \Sigma^R(k_F,0) \propto -U \xi / (\xi_{th} \xi_0^2) > 1
\]

in 3D:
\[
\Sigma^R(k_F,0) \propto -U (\ln \xi) / (\xi_{th} \xi_0^2)
\]

in 4D: quasiparticle survives up to \( T_c \)

Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. 33, 159 (1996);
IV. What was the competition up to?

**FLEX**

![Graph](image)

**QMC**

![Graph](image)

**Fig. 1.** (a) The spectral weight function \( A(p, \omega) \), evaluated at \( p = (\pi/2, \pi/2) \) for different lattice sizes for \( U = 4 \) and \( \beta = 5 \). (b) The Matsubara Green's function, \( G(p, \tau) \), for \( \beta = 5 \) with \( U = 4 \) for different lattice sizes with reference curves for comparison obtained from a narrow spectrum with no gap (dashed line), a broad spectrum with no gap (dotted line), a pseudogap (dashed-dotted line), and a full gap (dashed-double-dotted line).

J. J. Deisz, D. W. Hess, and J. W. Serene

State of the art analytical tools

\[ \Phi [G] = \langle \_ \rangle + \frac{1}{2} \langle \_ \rangle + \ldots \]

\[ \Sigma [G] = \frac{\delta \Phi [G]}{\delta G} = \langle \_ \rangle + \ldots \]

\[ \Gamma [G] = \frac{\delta \Sigma [G]}{\delta G} = \langle \_ \rangle + \ldots \]
Advantages

- 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):
  \[ G_2(1,1;2,3) \text{ appropriately related to } G(1,2) \]

Disadvantages

- 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

  No Migdal theorem, so vertex corrections should be included
How it works...

First step: Two-Particle Self-Consistent

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

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

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

is satisfied. One finds

\[
A = U \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle}
\]

Functional derivative of \( \langle n_\uparrow n_\downarrow \rangle / (\langle n_\uparrow \rangle \langle n_\downarrow \rangle) \) drops out of spin vertex

\[
U_{sp} = A = U \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle}
\]
How it works...

To close the system of equations, while satisfying conservation laws and the Pauli principle

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

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

(1)

Recall

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

(2)

To have charge fluctuations that satisfy Pauli principle as well,

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

(3)

(Bonus: Mermin-Wagner theorem)
How it works...

Second step: improved self-energy

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

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

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

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

Transverse+longitudinal for crossing-symmetry

\[ \Sigma_\sigma^{(2)} (k) = U n_{-\sigma} + \frac{U T}{8} \sum_q \left[ 3 U_{sp} \chi_{sp}^{(1)} (q) + U_{ch} \chi_{ch}^{(1)} (q) \right] G^{(1)}_\sigma (k + q). \quad (4) \]
Proof that generalization for $U < 0$ works

Kyung et al. cond-mat/0010001
Mechanism for pseudogap formation in the attractive model:

Even part of the pair susceptibility at $q = 0$, for different temperatures

$U = -4$

$d = 2$ is crucial

- Renormalized classical regime for spin fluctuations in pseudogap regime?

Figure 2: Normalized imaginary part of the spin susceptibility at the AF wavevector in the normal state, at $T = 100\,\text{K}$, for four oxygen contents in YBCO ($T_c=45.83,61.2,3.6,0.97$ K for $x=0.6,0.85,0.92,0.97$ respectively). These curves have been normalized to the same units using standard phonon calibration$^{14}$ (100 counts in the vertical scale roughly correspond to $\sim 350\,\mu\text{eV}^{-1}$ in absolute units) $^{15}$.
- 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.

**U < 0**

Pairing-fluctuation induced pseudogap
V. Conclusion

- What is happening now?
  - Methods for thermodynamics and for crossed channels.

- Computers:
  - Small sizes, not all relevant parameter regimes are accessible
- Analytical studies:
  - No small parameter, no perfect approximation
  - Limiting cases, physical intuition
  - Not always reliable
- How can we understand electronic systems that show both localized and extended character?
- Why do both organic and high-temperature superconductors show broken-symmetry states where mean-field-like quasiparticles seem to reappear?
- Why is the condensate fraction in this case smaller than what would be expected from the shape of the would-be Fermi surface in the normal state?
- Are there new elementary excitations that could summarize and explain in a simple way the anomalous properties of these systems?
- Do quantum critical points play an important role in the Physics of these systems?
- Are there new types of broken symmetries?
- How do we build a theoretical approach that can include both strong-coupling and \( d = 2 \) fluctuation effects?
- What is the origin of \( \text{d-wave} \) superconductivity in the high-temperature superconductors?