Kinks in the dispersion of correlated electrons

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Outline

1. Kinks in the dispersion relation
   - in high-$T_c$ cuprates
     - low-energy kinks at 40-70 meV
     - high-energy kinks at 300-400 meV (“waterfalls”)
   - in various correlated metals

2. A purely electronic mechanism for kinks
   - weakly vs. strongly correlated metals
   - generation of kink energy scale $\omega_*$
   - dispersion $E_k$ beyond $\omega_*$
Dispersion of correlated electrons

Dispersion relation $E_k$:

- spectral function:
  \[ A(k, \omega) \propto \text{Im} \frac{1}{\omega + \mu - \epsilon_k - \Sigma(k, \omega)} \]
  \[ \propto \text{# excitations with } k \text{ and } \omega \]

- $E_k = \{ \omega \text{ where } A(k, \omega) = \max \}$

experimentally:

- $k$-resolved: $A(k, \omega)$ from ARPES
- integrated: $A(\omega) = \int A(k, \omega) \, dk$ from PES
1a. Kinks in high-$T_c$ cuprates
Electronic dispersion in high-$T_c$ cuprates

Kinks at $\omega_\star = 40$-70 meV:

- possible origins:
  - electron-phonon coupling
    Lanzara et al. (2001); ...; Zhou et al. (2005); ...
  - electron-electron interaction
    Manske et al. (2001), ... → seminar talk by D. Manske
    Kordyuk et al. (2004, 2005), Borisenko et al. (2006), ... → workshop talk by A. Kordyuk
    Randeria et al. (2004)
    Kakehashi & Fulde (2005)
Proposed electronic mechanisms

Kinks due to Coulomb interaction of electrons because of:

  coupling of quasiparticles to spin fluctuations [FLEX]

- Kordyuk et al. (2004, 2005), Borisenko et al. (2006), ...
  Kramers-Kronig relations in electronic self-energy

- Randeria, Paramekanti, Trivedi (2004)
  effect on nodal quasiparticle dispersion:
  \[ E_{k}^{\text{high}} = \epsilon_k + k \frac{\partial}{\partial k} \text{Re}\Sigma \quad \text{and} \quad E_{k}^{\text{low}} = Z_{\text{FL}} E_{k}^{\text{high}} \]

- Kakehashi & Fulde (2005)
  coupling of quasiparticles to magnetic excitations [SCPM]
Electronic dispersion in high-$T_c$ cuprates

“Waterfalls”: kinks at $\omega_\star \approx 300$-$400$ meV

- kink energy **too high** for phonons
- electronic origins? Wang et al. (2006); Macridin et al. (2007); Zhu et al. (2007) → workshop talk by M. Jarrell
- matrix element effect? Kordyuk et al. (2007); Insosov et al. (2007) → poster by D. Insosov

see also Valla et al. (2006)
Pan et al. (2006)
Chang et al. (2006)
Meevasana et al. (2006)
1b. Kinks in various correlated metals
Electronic dispersion in graphene

graphene: low- and high-energy kinks

- kinks at $\omega_\ast \approx 200 \text{ meV}$ attributed to coupling of electrons to phonons
- kinks at $\omega_\ast \approx 400 - 900 \text{ meV}$ (near crossing of Dirac branches) attributed to coupling of electrons to plasmons

Bostwick et al. (2007) → workshop talk by E. Rotenberg
Electronic dispersion at metal surfaces

(3x1)-Br/Pt(110) surface

- kinks at $\omega_\star \approx 300\text{meV}$
- too high for phonons
- kinks due to coupling of electrons to what?

Menzel et al. (2006)
see also:
Valla et al. (1999)
Schäfer et al. (2004)
Electronic dispersion in a correlated metal

**SrVO$_3$**

**LDA+DMFT**

Nekrasov et al. (2006)

- $E_k$ crosses over from $Z_{FL}\epsilon_k$ to $Z'\epsilon_k$ at $\omega_{\star} \approx \pm 0.25$ eV
- kinks in purely electronic system?

spectral function $A(\omega)$ has three peaks

ARPES

Yoshida et al (2005)

kinks at $\omega_{\star} \approx 0.1$ eV
2. A purely electronic mechanism for kinks

- weakly vs. strongly correlated metals
- generation of kink energy scale $\omega_\star$
- dispersion $E_k$ beyond $\omega_\star$
Weakly vs. strongly correlated metals

Fermi liquids: \( E_k = Z_{FL} \epsilon_k \) for Landau quasiparticles up to \( \omega_{\star} \)

- weakly correlated system, \( Z_{FL} \lesssim 1 \)
  small interaction, \( U \ll D \approx \omega_{\star} \)

\[
E_k = \begin{cases} 
Z_{FL} \epsilon_k & \text{for } |E_k| \lesssim \omega_{\star} \\
\epsilon_k & \text{for } |E_k| \gtrsim \omega_{\star} \gg U
\end{cases}
\]

\( \Rightarrow \) essentially free at large energies

- strongly correlated system, \( 0 < Z_{FL} \ll 1 \)
  large interaction: \( U \gg D \gg \omega_{\star} \)

\[
E_k = \begin{cases} 
Z_{FL} \epsilon_k & \text{for } |E_k| \lesssim \omega_{\star} \\
Z' \epsilon_k & \text{for } \omega_{\star} \lesssim |E_k| \ll U
\end{cases}
\]

\( \Rightarrow \) intermediately correlated at large energies
Hubbard model and DMFT

Hubbard model:

\[ H = -t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^+ c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Dynamical mean-field theory:

- \( \Sigma(k, \omega) \equiv \Sigma(\omega) \), mapped onto single site
- exact in limit of large dimensions
- Mott transition in paramagnetic phase

\[ Z \]

Bulla (1999)

\[ A(\omega) \]

Metzner & Vollhardt (1989)
Georges & Kotliar (1992)
Jarrell (1992)
Weakly correlated system

Hubbard model, cubic lattice, DMFT(NRG), $U=0.29W$, $Z_{FL}=0.8$

- $E_k$ crosses over from Fermi-liquid dispersion $Z_{FL}\epsilon_k$ to free dispersion $\epsilon_k$
- outside FL regime: electrons are essentially free
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Strongly correlated system

Hubbard model, cubic lattice, DMFT(NRG), $U=0.96W$, $Z_{FL}=0.086$

\[E_k = \begin{cases} 
Z_{FL} \epsilon_k & \text{if } |\omega| < \omega_* \\
Z' \epsilon_k \pm c & \text{if } |\omega| > \omega_* 
\end{cases} \]

- outside FL regime: electrons are moderately correlated (here: $Z'=0.135$)

- three peaks in $A(\omega)$
  $Z'$ = weight of central peak
Strongly correlated system

Hubbard model, cubic lattice, DMFT(NRG), $U=0.96W$, $Z_{FL}=0.086$

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$Z' = \text{weight of central peak}$
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- Outside FL regime: electrons are moderately correlated (here: $Z'=0.135$)

- Three peaks in $A(\omega)$
  - $Z'$ = weight of central peak
Origin of electronic kinks

- $A(\omega) = \text{three-peak structure}$
- new energy scale from Kramers-Kronig:
  $\omega_{\text{max}} \approx Z_{\text{FL}}D_0$
- obtain kink energy $\omega_\star \approx 0.4 \omega_{\text{max}}$ and dispersion $Z'\epsilon_k \pm c$
  (with only $Z_{\text{FL}}$ and $\epsilon_k$ as input)
- Fermi-liquid regime extends only to $|\omega| \leq \omega_\star \propto Z_{\text{FL}}$
- intermediate-energy regime extends up to $\sim \Omega \sim \sqrt{Z_{\text{FL}}}$
Origin of electronic kinks

\[ A(\omega) = \frac{-\text{Im } G(\omega)}{\pi} \]

- \( A(\omega) = \) three-peak structure
- new energy scale from Kramers-Kronig:
  \[ \omega_{\text{max}} \approx Z_{FL} D_0 \]
- obtain kink energy
  \[ \omega_* \approx 0.4 \omega_{\text{max}} \]
  and dispersion \( Z' \epsilon_k \pm c \)
  (with only \( Z_{FL} \) and \( \epsilon_k \) as input)
- Fermi-liquid regime extends only to
  \[ |\omega| \leq \omega_* \propto Z_{FL} \]
- intermediate-energy regime extends up to
  \[ \sim \Omega \sim \sqrt{Z_{FL}} \]
Finding the kinks

Input:

- $\epsilon_k = \text{free dispersion}$ \implies $G_0(\omega) = \int \frac{dk}{\omega - \epsilon_k + i0}$
- $Z_{FL} = \text{Fermi-liquid parameter}$

Finding the kinks:

- $G(k, \omega) = \frac{1}{\omega + \mu - \epsilon_k - \Sigma(k, \omega)}$, $G(\omega) = \int dk\ G(k, \omega)$
- close to Fermi level: $\Sigma(\omega) = (1 - 1/Z_{FL})\omega + ...$
  \[ \implies G(\omega) = \frac{Z'}{\omega - \omega_0 + i(\gamma + \gamma'\omega)} + O(\omega^2) \]
- obtain $Z'$, $\omega_0$, $\gamma$, $\gamma'$ from $\epsilon_k$, $Z_{FL}$
- obtain $\Sigma(\omega)$ from $G(\omega)$
Correlated dispersion

Extract the dispersion:

- use $\Sigma(\omega) = \omega + \mu - \frac{1}{G} - \Delta[G(\omega)]$ with approximate $G(\omega)$
  - linear in central peak
  - $\approx (m_2 - m_1^2) G(\omega) \Rightarrow$ kinks at $\omega^*$

- self-energy: $\Sigma(\omega) \approx \begin{cases} (1 - 1/Z_{FL}) \omega & \text{if } |\omega| < \omega^* \\ (1 - 1/Z') \omega \pm c & \text{if } |\omega| > \omega^* \end{cases}$

- correlated dispersion: $E_k \approx \begin{cases} Z_{FL} \epsilon_k & \text{if } |\omega| < \omega^* \\ Z' \epsilon_k \pm c & \text{if } |\omega| > \omega^* \end{cases}$
Properties of the kinks

Analytical results: (for p-h symmetry)

- kink energy:
  \[ \omega^\star = 0.41 \cdot Z_{FL} \cdot \left[ \frac{\text{Im}(1/G_0)}{\text{Re}(G'_0/G_0^2)} \right]_{\omega=E_F^0} \]\n  inside central peak

- intermediate-energy regime:
  \[ Z' = Z_{FL} \cdot \left[ \frac{1}{\text{Re}(G'_0/G_0^2)} \right]_{\omega=E_F^0} = \text{weight of central peak in } A(\omega) \]

  ⇒ change in slope \( Z'/Z_{FL} \) independent of interaction strength

- curvature at the kink: \( \text{Im} \Sigma''(\omega^\star) \propto (Z_{FL})^2 \)
  ⇒ sharpness of kinks \( \propto (Z_{FL})^{-2} \)
  ⇒ kinks get sharper with increasing interaction strength
Away from half-filling

Hubbard model, cubic lattice, DMFT(NRG), $U=1.2W$, $Z_{FL}=0.26$, $n=0.8$

- kinks persist away from half-filling
- here: kink missing below Fermi energy
- doped Mott insulator: LHB not well-separated from central peak
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Beyond DMFT

Dynamical cluster approximation:

$$\tilde{G}(K, \omega) = \frac{N_c}{N} \sum_{\tilde{k}} \left[ G_0^{-1}(K + \tilde{k}, \omega) - \Sigma_c(K, \omega) \right]^{-1}$$

by same token: three-peak structure in some $A(k, \omega)$

$$\Rightarrow$$ kinks in $\Sigma(k, \omega)$

Recent DCA results: Macridin et al. (2007)
Conclusion

Kinks in the electronic dispersion

- generic for strongly correlated electrons
- purely electronic mechanism
- three-peak $A(\omega)$ sufficient
- new energy scale $\omega_\star$ inside central peak

- kinks at end of FL regime: $\omega_\star = Z_{FL} \cdot (\text{bare energy scale})$
- intermediate-energy regime with $Z' > Z_{FL}$

- robust mechanism based on local physics
- valid beyond DMFT

→ workshop talk by D. Vollhardt
→ poster by K. Byczuk