Isosbestic Points and Kinks: Fingerprints of Electronic Correlations

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“Localization and Interactions in Impure Metals”; Aspen, July 1981

Elihu Abrahams, Patrick Lee
Heavy Fermions and Valence Fluctuations/ Glassy Dynamics; Aspen, July 1985
Phil Anderson
Heavy Fermions and Valence Fluctuations / Glassy Dynamics; Aspen, July 1985
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Heavy Fermions and Valence Fluctuations / Glassy Dynamics; Aspen, July 1985
Phil Anderson
Strongly Correlated Electron Systems; Aspen, July 1988
Ravin Bhatt, Steve Kivelson
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Outline:

- Isosbestic points
- Kinks in the electronic dispersion

Characteristic energies/temperatures due to electronic correlations
1. Sharp crossing ("isosbestic") points

\[ \frac{\partial f(x, y)}{\partial y} \bigg|_{x^*(y)} = 0 \]

Eckstein, Kollar, DV (2007)
1. Sharp crossing ("isosbestic") points

\[ \frac{\partial f(x, y)}{\partial y} \bigg|_{x^*(y)} = 0, \quad x^*(y) = \text{const} \rightarrow \text{sharp crossing point} \]

"isosbestic" point

What do they tell us?

Eckstein, Kollar, DV (2007)
1) Isosbestic points in chemistry

**Isosbestic point:** “Specific wavelength at which two (or more) chemical species have the same extinction coefficient.”

Scheibe (1937)  
Cohen and Fischer (1962)

**Example:**
Solution of components A, B with concentrations $n_A$, $n_B$

A: 1,4-naphtaquinone diphenylhydrazone  
B: 4-dimethylaminoazobenzene

**Isosbestic:** from Greek *isos* “equal” + *sbestos*, verbal adj. from *sbennynai* “to quench, extinguish” = “equal attenuation”
2) Sharp crossing points in critical phenomena

Systems sizes $L=6-18$

Slevin et al. (2003)

Conductance distribution near the Anderson localization transition
3) Sharp crossing points in the specific heat of Fermi systems

\[ \frac{\partial C}{\partial P} > 0 \quad = 0 \quad < 0 \]

Greywall (1983)
3) Sharp crossing points in the specific heat of Fermi systems

Heavy fermion systems

4) Sharp crossing points in the dynamical conductivity

$T=10$ K spectra of the $\text{R}_2\text{Mo}_2\text{O}_7$ family

Kezsmarki et al. (2006)
5) Sharp crossing points in the spectral function

Hubbard model, 
$n=1, T=0,$ 
Bethe-DOS, 
DMFT(NRG)

Bulla, Hewson, Pruschke (1998)
Sharp crossing ("isosbestic") points:

Width of crossing regime?

- Sharp:
  - Linear superposition of two quantities,
  - Two-fluid model
  - Scaling behavior

- Approximate:
  - Smallness of a susceptibility, e.g., compressibility
  - Existence of a small parameter (1/Z)
  - Shape of band edges of spectral function

DV (1997)
Eckstein, Kollar, DV (2007)
II. Kinks in the electronic dispersion

a) Kinks

Byczuk, Kollar, Held, Yang, Nekrasov, Pruschke, DV; *Nature Phys.* (2007)

b) Waterfalls
Kinks at $\omega_\ast = 40$-70 meV
- Coupling of electrons to phonons or spin fluctuations?
- Coulomb interaction?

Valla et al. (1999)
Bogdanov et al. (2000)

Kordyuk et al. (2004)
Randeria et al. (2004)
Kakehashi, Fulde (2005)
Kinks due to electron-boson coupling

Kinks due to electron-electron hybridization
Kinks: Metal surfaces

Tungsten

Rotenberg et al. (2000)

ω* = 160 meV: Surface phonon

Kink due to electron-phonon coupling
Kinks: Metal surfaces

PES of quasi-1D electronic structures on Platinum(110) surface

300meV: too high for phonons

Menzel et al. (2005)

Kinks due to coupling of electrons to what?
Kinks: Graphene

Doping by potassium adsorption

- “Low energy” kinks at 200 meV
- “High energy” kinks at 400-900 meV (near X-ing of Dirac branches, $E_D$)
- coupling of electrons to plasmons?

Renormalization of LDA-bands by self-energy

Kinks at $\omega_* \approx 200$ meV

Yoshida et al. (2005)

Kinks at $\omega_* \approx 100$ meV

Origin of kinks in a purely electronic theory with one type of electron?
Strongly correlated paramagnetic metal


New energy scale?
\[ G(\omega) \xrightarrow{\text{DMFT}} \Sigma(\omega) = (\omega + \mu - \frac{1}{G(\omega)}) - \Delta[G(\omega)] \text{hybridization fct.} \]

linear for \(|\omega| \leq \Omega\)

For \( |\omega| \leq \omega_0 \propto G + O(G^2) \)

\[ \omega_0 = (\sqrt{2} - 1) Z_{FL} D_0 \]

\[ \Omega \sim \sqrt{Z_{FL}} \]


Electronic dispersion outside FL regime?
Electronic dispersion

- Spectral function: \( A(\mathbf{k}, \omega) \propto \text{Im} \frac{1}{\omega + \mu - \varepsilon_k - \Sigma(\mathbf{k}, \omega)} \)

\( \propto \) # excitations with \( \mathbf{k}, \omega \)

- Dispersion relation: \( E_k = \{ \omega \mid A(\mathbf{k}, \omega) = \text{max} \} \)

- Integrated spectral function: \( A(\omega) = \int d\mathbf{k} A(\mathbf{k}, \omega) \)
Fermi liquid dispersion
\[ E_k = Z_{FL} E_k^0 \]

Non-interacting dispersion
\[ E_k^0 \]

X-over

\[ E_k = \begin{cases} 
Z_{FL} E_k^0 ; & |E_k| \leq \omega_* \\
E_k^0 ; & |E_k| \geq \omega_* \gg U 
\end{cases} \]

1) Weak correlations: \( U=0.29W, Z_{FL}=0.8 \)

**E_k**: Hubbard model, cubic lattice, DMFT(NRG)
**E_k**: Hubbard model, cubic lattice, DMFT(NRG)

1) Strong correlations: \( U = 0.96W, Z_{FL} = 0.086 \)

Non-interacting dispersion
\[ E_k^0 \]

Fermi liquid dispersion
\[ E_k = Z_{FL} E_k^0 \]

Dispersion outside Fermi liquid regime
\[ E_k = Z' E_k^0 + c \]

\( Z' = \text{weight of central peak} > Z_{FL} = 0.135 \) (moderately correlated)

\( A(\omega) \): three-peak structure

- \( Z' \) = weight of central peak > \( Z_{FL} \)
  \[ = 0.135 \) (moderately correlated)
$E_k$: Hubbard model, cubic lattice, DMFT(NRG)

1) Strong correlations: $U=0.96W$, $Z_{FL}=0.086$
Properties of the kinks

E.g.: p-h symmetric case

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

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

  \Rightarrow \text{change in slope } Z'/Z_{FL} \text{ independent of interaction strength}

• curvature at the kink: \( \text{Im} \Sigma''(\omega_\star) \propto (Z_{FL})^2 \)
  \[ \Rightarrow \text{sharpness of kinks } \propto (Z_{FL})^{-2} \]
  \[ \Rightarrow \text{kinks get sharper with increasing interaction strength} \]
Conclusions

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

- robust mechanism based on local physics
- valid beyond DMFT