Strongly correlated electrons: Mass and charge renormalization

V. Janiš
Institute of Physics AS CR, Prague

FZÚ, 21/03/2006

Collaborator: Pavel Augustinský (PhD student)

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Outline

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Three regimes of correlated electrons in metals

- Low-energy & low temperature physics ($T = 0$)
- Conduction electrons – kinetic energy (band structure, hopping t)
- Screening – short-range interaction (Coulomb interaction U)

Interplay between extended kinetic energy t and local interaction U

Naive (static) classification

- $U \ll t$ – weak coupling
- $U \approx t$ – intermediate coupling
- $U \gg t$ – strong coupling

Interaction acts dynamically due to quantum fluctuations – static classification affected by spatial diemensionality

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Fermi liquid

Adiabatic (continuous) transition from Fermi gas

- Dominance of Fermi energy – the only relevant energy scale
- Elementary excitations – quasiparticles near the Fermi surface
- Particle interaction – weak scattering of quasiparticles
- Renormalization of Fermi-gas parameters (densities), inherent mass renormalization, no space for charge renormalization

Intermediate coupling

Presence of strong dynamical fluctuations

- Emergence of new energy (length) scales – long-range correlations
- Quantum critical behavior – with or without (classical) long-range order
- Cooperative phenomena – avalanche-type changes in equilibrium state
- Actual interaction – dynamical and strongly renormalized
- Vertex function – critical, vertex corrections & charge renormalization indispensable

Strong coupling

Long-range scales

- Heavy-fermion liquid — no critical point from weak coupling
  — *Kondo strong-coupling asymptotics* (impurity models, SIAM)
- Electron-hole liquid — critical transition from weak copupling (MIT or magnetic LRO)
  — insulator with satellite bands (lattice models, 1d Hubbard)

Outline

Ultimate objective of theoretical research

Theoretical challenge

Construct an approximation that qualitatively

- reproduces Fermi-liquid properties in weak coupling,
- captures dominant dynamical fluctuations due to electron correlations,
- controls analytically emerging singularities,
- *reproduces the Kondo asymptotics in SIAM.*

The resulting theory must be

- thermodynamically consistent and controllable,
- viable with available analytic-numerical methods,
- universal – applicable to various models and dimensions.

Most suitable framework: Renormalized diagrammatic perturbation theory

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Hubbard & Single Impurity Anderson Models

One-band model Hamiltonian

$$\widehat{H}_H = \sum_{\mathbf{k}\sigma} (\epsilon(\mathbf{k}) - \mu + \sigma B)\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} \widehat{n}_{\mathbf{i}\uparrow} \widehat{n}_{\mathbf{i}\downarrow}$$

Single-impurity Anderson Model

$$\widehat{H}_{SIAM} = \sum_{\mathbf{k}\sigma} (\epsilon(\mathbf{k}) - \mu)\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + E_d \sum_{\sigma} d^\dagger_\sigma d_\sigma + \sum_{\mathbf{k}\sigma} \left(V_{\mathbf{k}}\, d^\dagger_\sigma c_{\mathbf{k}\sigma} + V^*_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma} d_\sigma \right) + U \widehat{n}^d_\uparrow \widehat{n}^d_\downarrow$$

Calculational simplifications: $\mu = E_d = -U/2, \quad n^d = 1,$

$$\Delta(\epsilon) = \pi \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \delta(\epsilon - \epsilon(\mathbf{k})) = \Delta$$

Conduction electrons can be integrated out
– single-site theory with dynamical fluctuations

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Many-body perturbation theory

Grand partition sum

$$\mathcal{Z} = \int \mathcal{D}\psi \mathcal{D}\psi^* \exp\left\{ \sum_n \psi^*_n (i\omega_n + i\,\mathrm{sign}(\omega_n)\Delta)\psi_n - U \int_0^\beta d\tau\, \widehat{n}^d_\uparrow(\tau)\widehat{n}^d_\downarrow(\tau) \right\}$$

- Perturbation expansion in the interaction strength U
- Bare propagator

$$G_0(x+iy) = \frac{1}{x + i\,\mathrm{sign}(y)(\Delta + |y|)}$$

- *Grand potential* – (huge) sum of connected diagrams

$$\Omega = -k_B T \ln \mathcal{Z} = \Omega[G_0, U]$$

Renormalization of perturbation expansion –
reorganization of the sum of elementary diagrams

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Renormalization of perturbation expansion – reorganization of the sum of elementary diagrams

Outline

Equations of motion

- Dyson equation – full one-particle propagator via the self-energy (one-particle vertex)

$$G(k) = G_0(k)\left[1 + \Sigma(k)G(k)\right]$$

four-vector notation: $k = (\mathbf{k}, i\omega_n)$

- Bethe-Salpeter equations – full two-particle vertex via irreducible vertices (channel dependent), generically

$$\Gamma(k;q,q') = \Lambda(k;q,q') - \left[\Lambda GG \odot \Gamma\right](k;q,q')$$

- Schwinger-Dyson equation – Schrödinger equation for Green functions – connects 1P & 2P vertices

$$\Sigma_\sigma(k) = \frac{U}{\beta N}\sum_{k'} G_{-\sigma}(k') - \frac{U}{\beta^2 N^2}\sum_{k'q} G_\sigma(k+q)G_{-\sigma}(k'+q)\Gamma_{\sigma-\sigma}(k+q;q,k'-k)G_{-\sigma}(k')$$

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Mass renormalization – Baym-Kadanoff approach I

Perturbation expansion in renormalized quantities only (one-particle level)

Free energy

$$\Omega\left\{G^{(0)-1},U\right\} = -\beta^{-1}\ln\left[Z\left\{J;G^{(0)-1},U\right\}\right]$$
$$= -\beta^{-1}\ln\int \mathcal{D}\varphi\mathcal{D}\varphi^{*}\exp\left\{\varphi^{*}\left[G^{(0)-1}-J\right]\varphi+U\left[\varphi,\varphi^{*}\right]\right\}$$

Replacement in PT: $G^{(0)-1}\longrightarrow G^{-1}+\Sigma$, (Dyson equation) in Ω

Variational approach: new functional $\Psi[G,\Sigma]$ defined from

$$\frac{\delta\beta\Psi}{\delta\Sigma} = \frac{\delta\beta\Omega}{\delta G^{(0)-1}}+\left[G^{(0)-1}-\Sigma\right]^{-1}$$
$$\frac{\delta\beta\Psi}{\delta G} = \frac{1}{G^{2}}\frac{\delta\beta\Omega}{\delta G^{(0)-1}}-G^{-1}$$

Mass renormalization – Baym-Kadanoff approach II

Explicit functional

$$\Psi[G,\Sigma,U] = \Omega\left\{G^{-1}+\Sigma, U\right\} - \beta^{-1}\mathrm{tr}\ln G - \beta^{-1}\mathrm{tr}\ln\left[G^{(0)-1}-\Sigma-J\right]$$

Variational conditions:

$$\frac{\delta\Psi[G,\Sigma]}{\delta G} = 0 \qquad \frac{\delta\Psi[G,\Sigma]}{\delta\Sigma} = 0$$

Approximations expressed entirely in terms of renormalized quantities G,Σ

Dynamical Mean-Field Theory (one particle)

Separation of **site** diagonal and off-diagonal parts

$$G = G^{diag}\left[d^0\right] + G^{off}\left[d^{-1/2}\right], \qquad \Sigma = \Sigma^{diag}\left[d^0\right] + \Sigma^{off}\left[d^{-3/2}\right]$$

Mean-field functional

$$\Psi[G,\Sigma] = \Omega\left\{G^{diag\,-1} + \Sigma^{diag}\right\} - \beta^{-1}\mathrm{tr}\ln G^{diag} - \beta^{-1}\mathrm{tr}\ln\left[G^{(0)-1} - \Sigma^{diag} - J\right]$$

where $G(\mathbf{k}, i\omega_n) \longrightarrow G^{diag}(i\omega_n)$, $\Sigma(\mathbf{k}, i\omega_n) \longrightarrow \Sigma^{diag}(i\omega_n)$

Only **local** correlations matter in the generating functional
– all irreducible vertices local in DMFT

Problems with two-particle functions – ambiguous way to define nonlocal correlation functions

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Three types of two-particle irreducibility

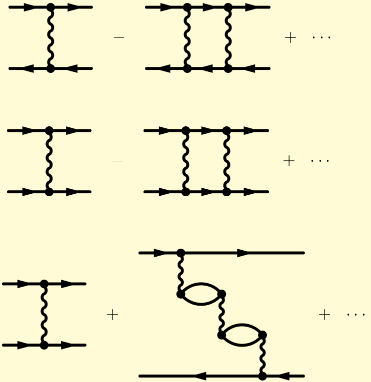
Ambiguity in the choice of the relevant Bethe-Salpeter equation with the local mean-field irreducible vertex

2P irreducibility – three (independent) two-particle scattering channels
– beyond static local theory (atomic limit)

eh ladders

ee ladders

eh bubbles



Three elementary Bethe-Salpeter equations

- Ring diagrams (GWA) $\quad (\Lambda^{U}_{\uparrow\downarrow} = U)$

$$\Gamma^{GWA}_{\uparrow\downarrow}(k, k', q) = \frac{U}{1 - U^2 X_{\uparrow\uparrow}(q) X_{\downarrow\downarrow}(q)}$$

$$X_{\sigma\sigma'}(q) = \frac{1}{\beta\mathcal{N}} \sum_{k''} G_{\sigma}(k'') G_{\sigma'}(k'' + q)$$

- Ladder diagrams (RPA, TMA) $\quad \Lambda^{eh}_{\uparrow\downarrow} = U \quad \vee \quad \Lambda^{ee}_{\uparrow\downarrow} = U$

$$\Gamma^{RPA}_{\uparrow\downarrow}(k, k'; q) = \frac{U}{1 + U X_{\uparrow\downarrow}(k - k'')}$$

$$\Gamma^{TMA}_{\uparrow\downarrow}(k; q; q) = \frac{U}{1 + U Y_{\uparrow\downarrow}(k + k' + q')}$$

$$Y_{\sigma\sigma'}(q) = \frac{1}{\beta\mathcal{N}} \sum_{k''} G_{\sigma}(k'') G_{\sigma'}(q - k'')$$

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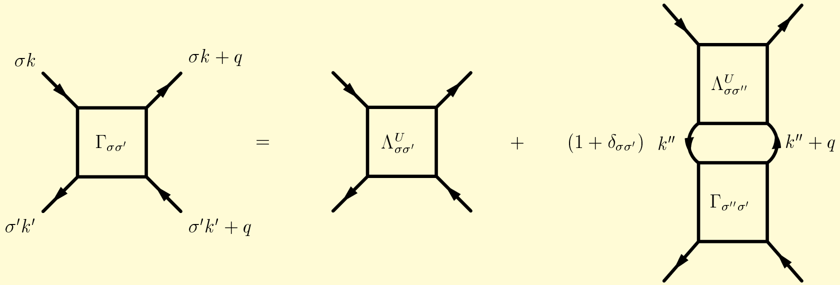
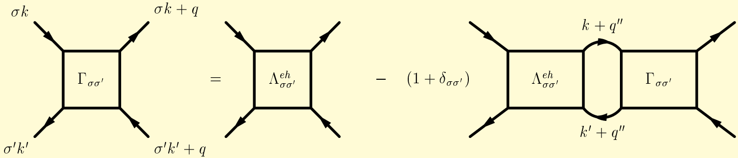
Full Bethe-Salpeter equations I

Vertical electron-hole scattering channel (GWA)

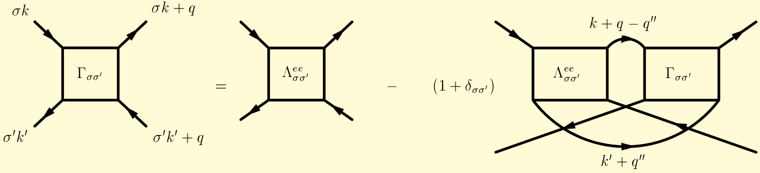


Full Bethe-Salpeter equations II

Horizontal electron-hole scattering channel (RPA)



Horizontal electron-electron scattering channel (TMA)



Beyond FLEX – two-particle selfconsistency

- Completely 2P irreducible function I: irreducible in all 2P channels (disconnected by cutting at least three fermion lines)
- *Parquet approach*: I determined diagrammatically, Λ^a from defining equations
- Topological nonequivalence of different 2P channels (beyond local static theory, atomic limit)

$$\Gamma = \Lambda^a + \mathcal{K}^a, \qquad \Lambda^a = I + \sum_{a' \neq a} \mathcal{K}^{a'}$$

- *Parquet equations* – Reducible functions $\mathcal{K}^a$ replaced by the solutions of the respective Bethe-Salpeter equations
- *Genuine charge renormalization* $U \longrightarrow \Lambda$ in perturbation theory:

$$\Lambda^a = L^a\left[I[U;G,\Lambda];\Lambda,G\right]$$

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Hatree & GWA

- *Static mean-field* spin-polarized solution : $\Sigma_\sigma = \sigma U m/2$

$$\langle n_\sigma \rangle = \frac{1}{\pi}\int_{-\infty}^{0} d\omega \, \frac{\Delta}{(\omega + \sigma \frac{U}{2} m)^2 + \Delta^2}$$

$$m = \frac{2}{\pi} \arctan\left(\frac{Um}{2\Delta}\right)$$

- Critical interaction strength $U_c = \pi\Delta$ – *unphysical* in SIAM
- Satellite split bands: $\pm Um/2$ – no Fermi liquid in weak coupling, insulator in strong coupling
- *GWA vertex function* $\Lambda^U = U$ (Hartree 1P propagators)

$$\Gamma_{\uparrow\downarrow}(z) = \frac{U}{1 - U^2 \chi_{\uparrow\uparrow}(z)\chi_{\downarrow\downarrow}(z)}$$

$$\chi_{\sigma\sigma'}(z) = \int_{-\infty}^{0} \frac{d\omega}{\pi}\left[G_{\sigma'}(\omega + z)\Im G_\sigma(\omega_+) + G_\sigma(\omega - z)\Im G_{\sigma'}(\omega_+)\right]$$

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FLEX-type approximations (1P self-consistency)

- Intermediate coupling – dynamical fluctuations shift the spurious MIT to $U_c = \infty$
- DOS at the Fermi energy (half filling) *does not depend on interaction* (Fermi liquid)
- Electron-electron channel (TMA) – noncritical, bounded 2P vertex
- Electron-hole channels (RPA, GWA) – *critical, diverging 2P vertex*

FLEX-type self-energy $\quad C(z) := \chi_{\uparrow\downarrow}(z)\Gamma_{\uparrow\downarrow}(z)$

$$\Re\Sigma(\omega_+) = -\frac{U^2}{2}\int_{-\infty}^{0} dx \left\{\rho(x)\Re\left[C(x-\omega_+) - C(x+\omega_+)\right] + \frac{1}{\pi}\Im C(x_+)\Re\left[G(x-\omega_+) - G(x+\omega_+)\right]\right\},$$

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$$\Im\Sigma(\omega_+) = U^2\int_{0}^{|\omega|} dx \rho(x-|\omega|)\Im C(x_+)$$

FLEX-type approximations (1P self-consistency)

- Intermediate coupling – dynamical fluctuations shift the spurious MIT to $U_c = \infty$
- DOS at the Fermi energy (half filling) does not depend on interaction (Fermi liquid)
- Electron-electron channel (TMA) – noncritical, bounded 2P vertex
- Electron-hole channels (RPA, GWA) – critical, diverging 2P vertex

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Strong-coupling asymptotics in FLEX I

Low-frequency behavior of 2P vertex Γ decisive (electron-hole part dominant)

$$\Gamma(\omega_+) = \frac{U}{1 + U\chi(0) - i\pi U\rho_0^2\omega}$$

Self-energy for $a = 1 + U\chi(0) \longrightarrow 0$

$$\Re\Sigma(\omega_+) = \frac{\mathrm{sign}(\omega)\Im G(\omega_+)}{\pi^2\rho_0^2}\ \arctan\left(\frac{\pi U\rho_0^2 D}{a}\right) + \frac{\Re G(\omega_+)}{2\pi^2\rho_0^2}\ \ln\left[1 + \left(\frac{\pi U\rho_0^2\omega}{a}\right)^2\right]$$

$$\Im\Sigma(\omega_+) = \frac{\Im G(\omega_+)}{2\pi^2\rho_0^2}\ \ln\left[1 + \left(\frac{\pi U\rho_0^2\omega}{a}\right)^2\right]$$

$$G(\omega_+) = \frac{1}{\omega - \Re\Sigma(\omega) + i(\Delta - \Im\Sigma(\omega))}$$

Strong-coupling asymptotics in FLEX II

- Solution: for $\omega/\Delta \gg a$, $\pi^2\rho_0^2 w^2 = \ln \frac{\pi U \rho_0^2 D}{a}$

$$G(\omega_+) = \frac{1}{w}\left[\frac{\omega}{w} - i\sqrt{1 - \frac{\omega^2}{w^2}}\right]$$

- Electron-hole bubble $\chi(0) = \frac{1}{\pi}\int_{-w}^{0} d\omega \Im G(\omega_+) \Re G(\omega) \longrightarrow -\frac{2}{3\pi w}$
- Critical interaction strength

$$1 = \frac{2U}{3\pi w} = \frac{2}{3}\frac{U\rho_0}{\sqrt{\ln\left[\frac{\pi U \rho_0^2 D}{a}\right]}}, \qquad a = \pi U \rho_0^2 D \exp\left\{-\left(\frac{2}{3}U\rho_0\right)^2\right\}$$

Neither Kondo asymptotics nor satellite peaks

What is wrong with FLEX?

Positive features

- Dynamical fluctuations & mass renormalization included
- Fermi liquid & quasiparticles in weak coupling
- No spurious MIT in SIAM

Drawbacks

- No Kondo asymptotics
- Quasiparticle peak either too narrow (RPA, GWA) or too broad (TMA))
- MIT removed only due to mass renormalization
- No charge renormalization & screening of electron-hole scatterings (bare 2P irreducible vertex U)

Outline

Need for a charge renormalization

What is needed in strong coupling

- Electron-hole scatterings to drive the system toward MIT
- Electron-hole scatterings must be screened by electron-electron sctatterings
- Two-particle self-consistency – *eh* and *ee* scatterings self-consistently mixed up

What is sufficient in strong coupling

- Two-channel parquet approximation – RPA (GWA) & TMA channels
- Irreducible vertices Λ^{eh} and Λ^{ee} determined self-consistently from nonlinear equations

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Two-channel parquet approximation

- Electron-hole Bethe-Salpeter equation

$$\Gamma_{\uparrow\downarrow}(n,n';m) = \Lambda^{eh}_{\uparrow\downarrow}(n,n';m) - \frac{1}{\beta}\sum_{n''}\Lambda^{eh}_{\uparrow\downarrow}(n,n'';m)G_{\uparrow}(n'')G_{\downarrow}(n''+m)\Gamma_{\uparrow\downarrow}(n'',n';m)$$

- Electron-electron Bethe-Salpeter equation

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Parquet equation to exclude vertex $\Gamma_{\uparrow\downarrow}$:

$$\Gamma_{\uparrow\downarrow} = \Lambda^{eh}_{\uparrow\downarrow} + \Lambda^{ee}_{\uparrow\downarrow} - U$$

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Simplified parquet equations

- Singulariry in the two-particle vertex only in Bethe-Salpeter equations
- Only electron-hole scatterings contribute to the singularity (due to the combination of the summed frequency)
- $\Lambda^{ee}_{\uparrow\downarrow} \longrightarrow \Lambda(\omega)$ diverges at $\omega = 0$ – remains dynamic, frequency-dependent
- $\Lambda^{eh}_{\uparrow\downarrow} \longrightarrow \overline{U}$ finite – replaced by a static effective interaction

Simplified parquet equations (zero temperature & half filling)

$$\overline{U} = \frac{U}{1 + \langle \Lambda G_\uparrow G_\downarrow \rangle}, \qquad \langle \Lambda G_\uparrow G_\downarrow \rangle = \frac{1}{\pi}\int_{-\infty}^{0} d\omega\, \Im\left[\Lambda(\omega_+) G(\omega_+)^2\right]$$

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Strong-coupling asymptotics I

Low-frequency singularity in the vertex $\Lambda(\omega)$

$$\Lambda(\omega) \doteq \frac{\overline{U}}{a - i\pi\overline{U}\rho_0^2\omega}$$

with $a = 1 + \overline{U}\chi(0) = 1 - \overline{U}/\pi\Delta \to 0$, $\rho_0 = 1/\pi\Delta$ independent of U

Solution

$$\langle \Lambda G_\uparrow G_\downarrow \rangle = \ln\left[\frac{\overline{U}}{\pi\Delta a}\right]$$

$$\Re\chi(\omega) = -\frac{4\Delta^2}{\pi\omega(4\Delta^2+\omega^2)}\arctan\frac{\omega}{\Delta} + \frac{\Delta}{\pi(4\Delta^2+\omega^2)}\ln\left(1+\frac{\omega^2}{\Delta^2}\right)$$

$$\Im\chi(\omega) = -\frac{2\Delta^2}{\pi\omega(4\Delta^2+\omega^2)}\ln\left(1+\frac{\omega^2}{\Delta^2}\right) - \frac{2\Delta}{\pi(4\Delta^2+\omega^2)}\arctan\frac{\omega}{\Delta}$$

Strong-coupling asymptotics II

Kondo asymptotics

$$a = \frac{\overline{U}}{\pi\Delta} \exp\left\{ -\frac{U}{\overline{U}} \right\} \doteq \exp\left\{ -\frac{U}{\pi\Delta} \right\}$$

Compare with the exact (Bethe-ansatz) solution

$$a = \exp\left\{ -\frac{\pi^2}{8} \frac{U}{\pi\Delta} \right\}$$

Full vertex function

$$\Gamma(\omega_+) = \overline{U} + \Lambda(\omega_+) - U = \overline{U} + \frac{\overline{U}}{1 + \overline{U}\chi(\omega_+)} - U$$

Self-energy and 1P propagator in the parquet approach I

Self-energy from 2P vertex – non-self-consistent Schwinger-Dyson equation with bare 1P propagators

$$\Re\Sigma(\omega_+) = \frac{U}{\pi}\int_{-\infty}^{0} dx \left\{\Im\left[\left(G(x_+ + \omega) - G(x_+ - \omega)\right)\Lambda(x_+)\chi(x_+)\right]\right.$$
$$\left. -\Im\left[\Lambda(x_+)\chi(x_+)\right]\Re\left[G(x_+ - \omega) - G(x_+ + \omega)\right]\right\}$$
$$\Im\Sigma(\omega_+) = -\frac{U}{\pi}\int_{0}^{|\omega|} dx \Im G(x_+ - |\omega|)\Im\left[\Lambda(x_+)\chi(x_+)\right]$$

Analytic approximation with an interpolated bubble

$$\chi(\omega + i\sigma 0) \approx -\frac{1}{\pi\Delta}\frac{1}{1 - i\sigma\omega/\Delta}$$
$$G(x + i\sigma 0) = \frac{1}{\Delta}\frac{1}{\omega/\Delta + i\sigma}$$

Self-energy and 1P propagator in the parquet approach II

Explicit solution for the self-energy

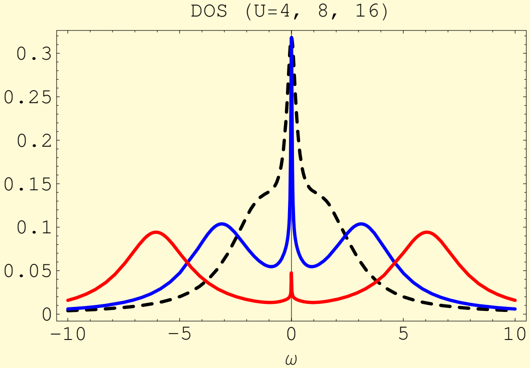
$$\Im\Sigma(\omega_+) = -\frac{U(1-a)}{2\pi}\left(\frac{\Delta^2}{\Delta^2(1-a)^2+\omega^2}+\frac{\Delta^2}{\Delta^2(1+a)^2+\omega^2}\right) \times\left[\frac{1}{2}\ln\left(\left(1+\frac{\omega^2}{a^2\Delta^2}\right)\left(1+\frac{\omega^2}{\Delta^2}\right)\right)+\frac{\omega}{\Delta}\arctan\frac{\omega}{\Delta}\right]$$

$$\Re\Sigma(\omega_+) = -\frac{U(1-a)}{2\pi}\sum_{\sigma=\pm1}\frac{\Delta^2}{\Delta^2(1-\sigma a)^2+\omega^2} \times\left[\frac{\omega}{2\Delta}\left(\ln\frac{a^2\Delta^2}{\omega^2+\Delta^2}+\sigma\ln\left(\frac{\omega^2}{\Delta^2}+a^2\right)\right)+(1-\sigma a)\left(\arctan\frac{\omega}{a\Delta}-\arctan\frac{\omega}{\Delta}\right)\right]$$

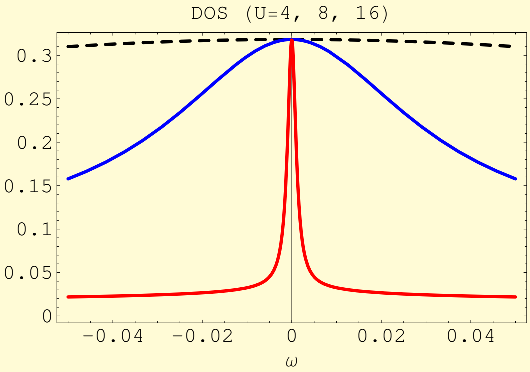
Kondo asymptotics (not in FLEX!) : $a = \exp\left\{-\frac{U}{\pi\Delta}\right\}$

Full 1P propagator $G(\omega_+) = \left[\omega - \Re\Sigma(\omega_+) + i(\Delta - \Im\Sigma(\omega_+))\right]^{-1}$

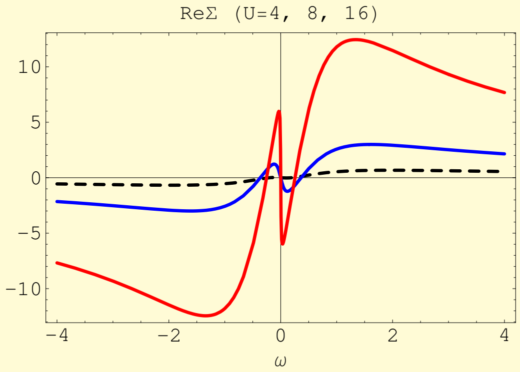
Self-energy and 1P propagator in the parquet approach III



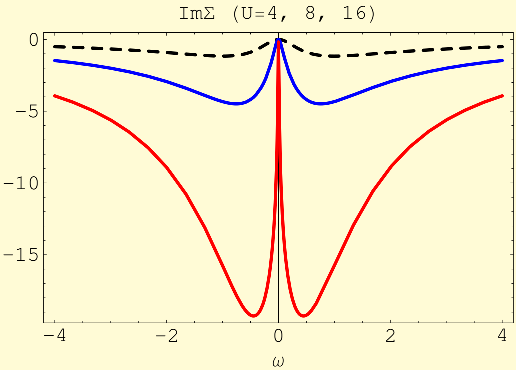
Self-energy and 1P propagator in the parquet approach IV



Self-energy and 1P propagator in the parquet approach V

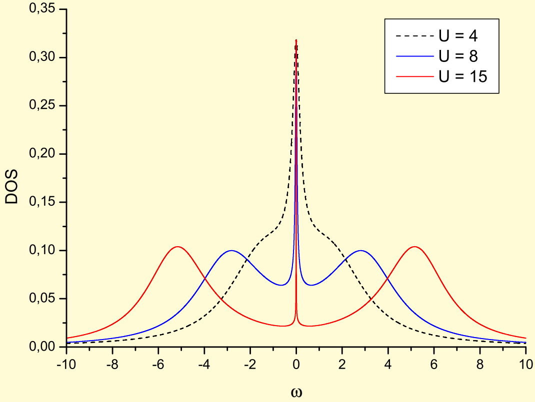


Self-energy and 1P propagator in the parquet approach VI



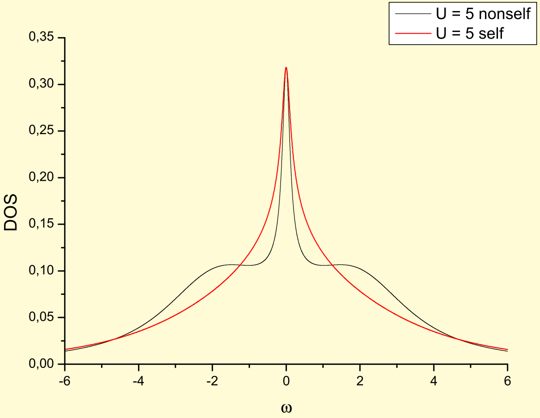
Numerical solution – non-self-consistent

Numerical solution with the full form of the two-particle bubble



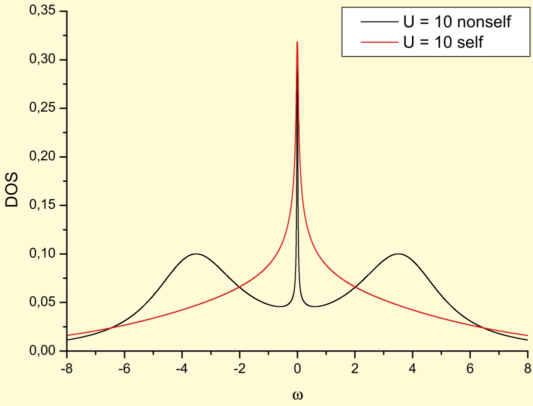
Numerical solution – 1P self-consistency I

Bare 1P propagator in the parquet equations is replaced by the renormalized one $G(z) \longrightarrow G(z - \Sigma(z))$



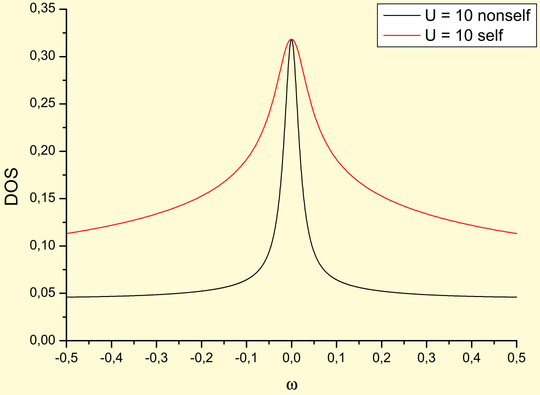
Numerical solution – 1P self-consistency II

1P self-consistency smears out the satellite peaks



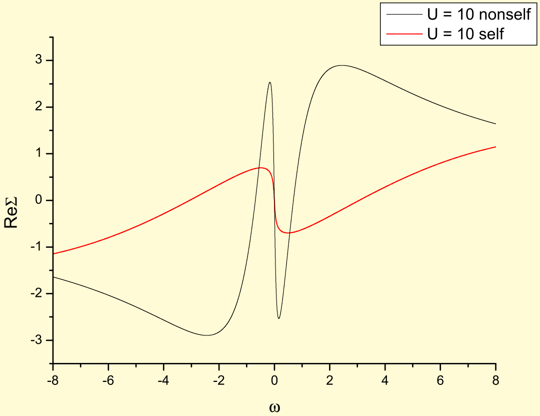
Numerical solution – 1P self-consistency III

Quasiparticle peak magnified



Numerical solution – 1P self-consistency IV

The weight of the low-frequency states is suppressed – electrons expelled from the Fermi surface



Outline

Two-particle scatterings in strong coupling

What is relevant for the Kondo asymptotics?

- Electron-hole scatterings
  - Irreducible vertex Λ^{eh} regular – effective interaction $\overline{U}$
  - Only low-energy behavior of the electron-hole bubble matters

$$\chi(\omega_+) \sim \chi(0) + i\pi\rho_0^2\omega$$

  - One-particle density ρ_0 does not depend on interaction (Fermi liquid)
- Electron-electron scatterings
  - Irreducible vertex singular due to eh scatterings

$$\Lambda^{ee}(\omega_+) = \frac{\overline{U}}{1 + \overline{U}\chi(\omega_+)}$$

  - Effective interaction from electron-electron scatterings

$$\overline{U} = \frac{U}{1 + \langle \Lambda^{ee} G_\uparrow G_\downarrow \rangle}$$

Self-energy & one-particle self-consistency

Self-energy & one-particle self-consistency

- Self-energy from the Schwinger-Dyson equation with bare or full 1P propagators
- Asymptotic algebraic fit of the self-energy for low & high frequencies ($\omega \gg a\Delta$ – Kondo peak irrelevant)

$$\Sigma(\omega_+) \doteq \frac{U\Delta}{\omega + i\Delta}\left[|\ln a| - \frac{i\pi}{2} \mathrm{sign}\, \frac{\omega}{\Delta} \right]$$

where $a = 1 + \overline{U}\chi(0) \to 0$

- One-particle and two-particle critical behavior interconnected
- General trend of 1P self-consistency:
  - Slows down the drift to the two-partical criticality
  - Smears out the satellite peaks

What is missing yet?

What yet influences the critical Kondo behavior?

- Inclusion of the vertical electron-hole channel (GWA) – triplet scatterings of virtual electron-hole pairs drive the system toward MIT
- One-particle self-consistency – changes the low-frequency behavior of 1P propagator – slows down the drift toward MIT
- Electron-hole asymmetric case – ρ_0 depends on interaction
- Lattice models (DMFT) – 1P propagator must be renormalized
- Beyond the (simplified) parquet approximation – electron-hole & electron-electron scatterings in a balanced manner

Outline

Conclusions

Correct extrapolation to the strong-coupling limit

- Singularity in the electron-hole Bethe-Salpeter equations
- Two-particle vertex – only low frequency behavior relevant
- Mass renormalization only (FLEX) – insufficient
- Charge renormalization needed – self-consistent binding of electron-hole amd electron-electron scatterings
- Three relevant static parameters – ρ_0, $\chi(0)$, $\langle \Lambda GG \rangle$
- Simplified parquet equations – capture the proper strong-coupling Kondo asymptotics within the complexity comparable with FLEX

Simplified parquet approximation – a manageable impurity solver interpolating qualitatively correctly between the Fermi-liquid and the strong-coupling regimes

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Simplified parquet approximation – a manageable impurity solver interpolating qualitatively correctly between the Fermi-liquid and the strong-coupling regimes

Outlook

What do we plan to do next

- Add the vertical (GWA) channel
- Clear (analytically) the role of 1P self-consistency onto the Kondo behavior
- Hubbrad model in $d = \infty$ – existence of the Mott-Hubbard MIT
- Electron-hole asymmetric situation & general band structure
- Multi-band Hubbard & other models of strongly correlated electrons
- Parquet approximation in low spatial dimensions – beyond mean field