Electron Correlations in Metals: Spectral function, magnetic susceptibility and specific heat of Anderson impurity

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FMFI UK Bratislava, February 15, 2017

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Outline

1. Electrons in metals - 1P approach
   - Models and static mean field
   - Dynamics: Baym-Kadanoff self-consistency
   - Schwinger-Dyson equation vs. Ward identity
2. Electron in metals - 2P approach
   - Bethe-Salpeter and parquet equations
   - Linearized Ward identity
   - Effective-interaction approximation
3. Numerical results in the Kondo regime of SIAM
4. Conclusions

Electron correlations – quantum criticality

- Electrons – Quantum statistics (Fermions & Pauli principle)
- Equilibrium static thermodynamic potential: incomplete
  - dynamical Green functions needed
- Quantum order parameters with nontrivial structure
  - complex phase (1P fermionic nonsingular GF)
- Response functions from 2P GF (bosonic singular)
- Critical (2P) & noncritical (1P) functions coupled
  non-universal behavior (bosonic & fermionic functions mixed up)

Macroscopic conservation laws (Ward identities)
not practically compatible with
microscopic dynamics (Schrödinger equation)

Hamiltonian & external perturbation

Tight-binding description: Conduction electrons in a periodic lattice

Screened Coulomb & external perturbation (nonequilibrium) $\widehat{H}_{ext}$

$$\widehat{H}_{\mu} = \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} \widehat{n}_{\mathbf{i}\uparrow} \widehat{n}_{\mathbf{i}\downarrow} - \sum_{\mathbf{i}\sigma} \mu_{\sigma} \widehat{n}_{\mathbf{i}\sigma} + \widehat{H}_{ext}$$

$$\widehat{H}_{SIAM} = \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \left(V_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} d_{\sigma} + H.c. \right) + E_d \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + U \widehat{n}^{d}_{\uparrow} \widehat{n}^{d}_{\downarrow}$$

$$\Omega[G^{(0)-1}, H] = -\beta^{-1} \log Tr \left[\exp \left\{ -\beta \left(\widehat{H}_0 - \mu \widehat{N} + \underbrace{\widehat{H}_I + \widehat{H}_{ext}}_{\text{perturbation}} \right) \right\} \right]$$

Hartree static mean-field approximation

- Generating functional

$$\frac{1}{N}\Omega[n_\uparrow, n_\downarrow] = -Un_\uparrow n_\downarrow - \frac{1}{\beta N}\sum_{\sigma,\omega_n,\mathbf{k}} e^{i\omega_n 0^+} \ln\left[i\omega_n + \mu + \sigma h - \epsilon(\mathbf{k}) - Un_{-\sigma}\right]$$

- Spectral function

$$G_\sigma(\omega) = \rho_0(\omega + \mu + \sigma h - Un_{-\sigma})$$

- Magnetic susceptibility (zero field, spin symmetric solution)

$$\chi = -\frac{2\phi(0)}{1 + U\phi(0)}$$

with $\phi(\omega) = -\int_{-\infty}^{\infty}\frac{dx}{\pi} f(x)\left(G(x+\omega) + G(x-\omega)\right)\Im G(x)$

- Total energy

$$E^{TOT} = -\sum_\sigma \int_{-\infty}^{\infty} f(\omega)\,(\omega + \mu)\,\Im G_\sigma(\omega) - Un_\uparrow n_\downarrow$$

Correlation effect only in susceptibility

Beyond mean-field - dynamical corrections

- Full vertex function from response function – Ward identity

$$\Gamma(\omega) = \frac{U}{1 + U\phi(\omega)}$$

- Spectral self-energy from Schwinger-Dyson equation

$$\Sigma(\omega) = U \int_{-\infty}^{\infty} \frac{dx}{\pi} \{ b(x) G(x+\omega) \Im [\phi(x)\Gamma(x)] - f(x)\phi^*(x-\omega)\Gamma^*(x-\omega)\Im G(x) \}$$

- Magnetic susceptibility with spectral self-energy

$$\chi = -2 \int_{-\infty}^{\infty} \frac{d\omega}{\pi} b(\omega) \Im \left[G(\omega - \Sigma(\omega))^2 \left(1 - \frac{UX(\omega)}{1 + U\phi(0)} \right) \right]$$

- Total energy

$$E^{TOT} = -2 \int_{-\infty}^{\infty} f(\omega)\omega \Im G(\omega - \Sigma(\omega)) - Un^2 - U \int_{-\infty}^{\infty} b(\omega) \Im \left[\phi(\omega)^2 \Gamma(\omega) \right]$$

1P self-consistent perturbation theory

- Renormalized generating Luttinger-Ward functional
  – "Legendre transform" of the thermodynamic potential

$$\Phi[G,H] = \Omega[G^{(0)-1},H] - \int d\,\bar{1}\left(G^{(0)-1}(1,\bar{1}) - G^{-1}(1,\bar{1})\right) G(\bar{1},1')$$

- 1P Green function and self-energy (equilibrium)

$$G^{\alpha}(12) = \left.\frac{\delta\Phi[G,H]}{\delta H_{\bar{\alpha}}(2,1)}\right|_{H=0}, \qquad \Sigma^{\alpha}(12) = \frac{\delta\Phi[G,0]}{\delta G_{\bar{\alpha}}(2,1)}$$

- 2P Green and irreducible vertex functions (equilibrium)

$$G^{\bar{\alpha}\alpha}(13,24) = \left.\frac{\delta^2\Phi[G,H]}{\delta H_{\alpha}(4,3)\delta H_{\bar{\alpha}}(2,1)}\right|_{H=0}, \quad \Lambda^{\bar{\alpha}\alpha}(13,24) = \frac{\delta^2\Phi[G,0]}{\delta G_{\alpha}(4,3)\delta G_{\bar{\alpha}}(2,1)}$$

- Diagrammatic expansion for $\Phi[G]$

Baym-Kadanoff thermodynamic consistency

- Generating stationary functional with electrons G and holes $\overline{G}$

$$\frac{2}{N}\Omega[\Sigma, G, \overline{\Sigma}, \overline{G}] = \Phi[U; G, \overline{G}] - \frac{1}{\beta N}\sum_{\sigma n,\mathbf{k}}\Big\{ e^{i\omega_n 0^+}\ln\left[i\omega_n + \mu_\sigma - \epsilon(\mathbf{k}) - \Sigma_\sigma(\mathbf{k}, i\omega_n)\right] + e^{-i\omega_n 0^+}\ln\left[-i\omega_n + \mu_\sigma - \epsilon(-\mathbf{k}) - \overline{\Sigma}_\sigma(-\mathbf{k}, -i\omega_n)\right] + G_\sigma(\mathbf{k}, i\omega_n)\overline{\Sigma}_\sigma(-\mathbf{k}, -i\omega_n) + \overline{G}_\sigma(-\mathbf{k}, -i\omega_n)\Sigma_\sigma(\mathbf{k}, i\omega_n)\Big\}$$

- Thermodynamic consistency: 1P and 2P irreducible vertices from the generating functional

$$\Sigma_\sigma[U; G, \overline{G}] = \frac{\delta\Phi[U; G, \overline{G}]}{\delta\overline{G}_\sigma} \quad , \quad \Lambda^{eh}_{\sigma-\sigma}[U; G, \overline{G}] = \frac{\delta\Sigma_\sigma[U; G, \overline{G}]}{\delta\overline{G}_{-\sigma}}$$

- Bethe-Salpeter equation for 2P vertex (equilibrium)

$$\Gamma_{\sigma-\sigma}[U; G, \overline{G}] = \Lambda^{eh}_{\sigma-\sigma}[U; G, \overline{G}] - \Lambda^{eh}_{\sigma-\sigma}[U; G, \overline{G}]G_\sigma\overline{G}_{-\sigma}\star\Gamma_{\sigma-\sigma}[U; G, \overline{G}]$$

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- Dyson equation for 1P GF

$$G^\alpha(1,2) = G^{(0)}(1-2) + \sum_{3,4} G^{(0)}(1-3)\Sigma^\alpha(3,4)G^\alpha(4,2)$$

- Bethe-Salpeter equation for 2P vertex (equilibrium)

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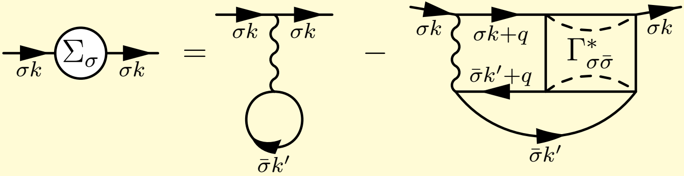
Schwinger-Dyson equation & alternative vertex

- Schwinger-Dyson equation – microscopic quantum dynamics

$$\Sigma_\sigma[U; G, \overline{G}] = U\left\langle \overline{G}_{-\sigma}\right\rangle - UG_\sigma \overline{G}_{-\sigma} \star \Gamma^*_{\sigma-\sigma}[U; G, \overline{G}] \circ G_{-\sigma}$$

- Diagrammatic representation



- Functional derivative - Ward identity & SDE

$$\Lambda^{eh}_{\sigma-\sigma} = \frac{\delta\Sigma_\sigma[U; G, \overline{G}]}{\delta \overline{G}_{-\sigma}} = U - U\left[1 + G_\sigma \overline{G}_{-\sigma}\Lambda^{eh}_{\sigma-\sigma}\star\right]^{-1} G_\sigma \left\{\Lambda^{eh}_{\sigma-\sigma} + \overline{G}_{-\sigma}\frac{\delta\Lambda^{eh}_{\sigma-\sigma}}{\delta\overline{G}_{-\sigma}}\right\}\left[1 + \star G_\sigma \overline{G}_{-\sigma}\Lambda^{eh}_{\sigma-\sigma}\right]^{-1} \circ G_{-\sigma}$$

Conservation of charge source in correlated electrons

- Coulomb repulsion: $U \sim e^2/R^{eff}$
- Charge carried by the present electrons: U and n related
- Sum rule (local compressibility & susceptibility)

$$\frac{\partial\Omega(U,\mu_{\mathbf{i}\sigma})}{\partial U} = \sum_{\mathbf{i}}\left[\frac{\delta^2\Omega}{\delta\mu_{\mathbf{i}\uparrow}\delta\mu_{\mathbf{i}\downarrow}} + \frac{\delta\Omega}{\delta\mu_{\mathbf{i}\uparrow}}\frac{\delta\Omega}{\delta\mu_{\mathbf{i}\downarrow}}\right] = \sum_{\mathbf{i}}\left\{\frac{T}{4}\left[\kappa_{\mathbf{ii}} - \chi_{\mathbf{ii}}\right] + n_{\mathbf{i}\uparrow}n_{\mathbf{i}\downarrow}\right\}$$

- Dynamical interaction $U(\mathbf{q}, i\nu_m)$
- Consistency - dynamical charge conservation ($\delta U = \delta[e^2/r]$)

$$\underbrace{\frac{\delta\Phi[U,G]}{\delta U(\mathbf{q}, i\nu_m)}}_{\text{Schwinger-Dyson}} = \underbrace{-\frac{1}{\beta N}\sum_{\mathbf{k},n}\frac{\delta G_\sigma(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_m)}{\delta\mu_{-\sigma}(\mathbf{k}, i\omega_n)}}_{\text{Ward}}$$

WI & SD may hold simultaneously in full exact but in no approximate (even asymptotically exact) theory

Thermodynamic consistency in quantum criticality

- Two definitions of response (correlation) functions:
  - Linear response function (disordered phase): $\delta\Omega/\delta U$
  - Derivative of the order parameter (ordered phase): $\delta^2\Omega/\delta\mu^2$
- Baym & Kadanoff thermodynamic consistency (paradigm):
  - Generating functional $\Phi[G]$
  - All quantities expressed in terms of the renormalized 1P propagator G (Dyson equation)
  - Equilibrium solution: Perturbation expansion for $\Sigma[G]$
  - Quantum criticality – singularity in vertex Γ from SDE
  - Charge not conserved: LRO in 1P self-energy (WI) does not emerge at the critical point of 2P vertex (SDE)
- Single self-energy in BK scheme leads to two vertex functions

Consistent quantum criticality with only a single divergent 2P vertex

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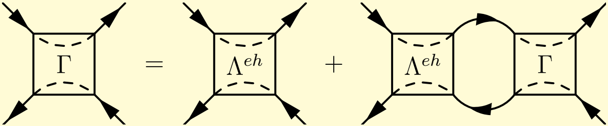
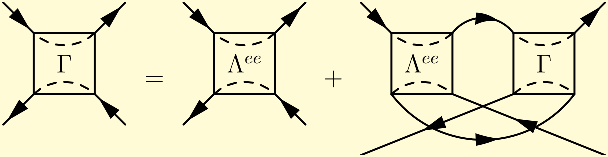
Fundamental scattering channels

Perturbation expansion for 2P vertex functions

- Multiple scatterings - electron-hole & electron-electron
  - Electron-hole multiple singlet scatterings



  - Electron-electron multiple scatterings



- Mixing the channels – 2P self-consistency

Vertex Γ divergent at the critical point

Parquet equations

- Channel-dependent decompositions of the full vertex:
  $\Gamma_{\sigma\sigma'} = \Lambda^{ee}_{\sigma\sigma'} + \mathcal{K}^{ee}_{\sigma\sigma'} = \Lambda^{eh}_{\sigma\sigma'} + \mathcal{K}^{eh}_{\sigma\sigma'}$
- Fully irreducible vertex (diagrammatically): $\mathcal{I} = \Lambda^{eh} \cap \Lambda^{ee}$
- Existence (applicability) of the parquet decomposition:

$$\mathcal{K}^{ee} \cap \mathcal{K}^{eh} = \emptyset$$

- Fundamental parquet decomposition:

$$\Gamma = \mathcal{I} \cup \mathcal{K}^{ee} \cup \mathcal{K}^{eh} = \Lambda^{eh} \cup \Lambda^{ee} \setminus \mathcal{I} = \mathcal{I} + \mathcal{K}^{eh} + \mathcal{K}^{ee} = \Lambda^{ee} + \Lambda^{eh} - \mathcal{I}$$

- Parquet equations:

$$\Lambda^{eh} = U - [\Lambda^{ee} GG] \circ [\Lambda^{eh} + \Lambda^{ee} - U]$$
$$\Lambda^{ee} = U - [\Lambda^{eh} GG] \star [\Lambda^{ee} + \Lambda^{eh} - U]$$

- Vertex Λ^{ee} may be divergent with repulsive interaction

Reduced parquet equations – 2P self-consistency

- Reduction of the parquet self-consistency in BS equations
- Nonsingular irreducible vertex (eh-channel)

$$\Lambda_{\uparrow\downarrow}(k,k';Q) = U - \frac{1}{\beta N}\sum_{k''} K_{\uparrow\downarrow}(k,k'';Q-k-k'') \times G_{\uparrow}(k'')G_{\downarrow}(Q-k'')\Lambda_{\uparrow\downarrow}(k'',k';Q)$$

- Singular reducible vertex (ee-channel)

$$K_{\uparrow\downarrow}(k,k';q) = -\frac{1}{\beta N}\sum_{k''}\Lambda_{\uparrow\downarrow}(k,k'';q+k+k'')G_{\uparrow}(k'')G_{\downarrow}(q+k'') \times \left[K_{\uparrow\downarrow}(k'',k';Q) + \Lambda_{\uparrow\downarrow}(k,k'';q+k''+k') - U\right]$$

- Full vertex

$$\Gamma_{\uparrow\downarrow}(k,k';q) = \Lambda_{\uparrow\downarrow}(k,k';q+k+k') + K_{\uparrow\downarrow}(k,k';q)$$

1P propagators in the 2P approach

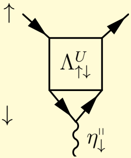
- Self energy from Schwinger-Dyson equation
  - Determines the microscopic dynamics
  - Self-energy from SDE does not break symmetry at critical points of Bethe-Salpeter equation
  - Solution breaks down beyond the critical point (singularity in Bethe-Salpeter equation)
- Self-energy from Ward identity
  - Controls macroscopic thermodynamics
  - Guarantees thermodynamic consistency between self-energy and Bethe-Salpeter equation
  - Full dynamical WI cannot be resolved – must be approximated

Qualitative consistency: LRO (1PGF) emerges at the critical point of 2P GF

Linearization in symmetry breaking field

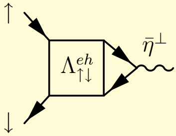
- Repulsive particle interaction – electron-hole scattering dominant
- Linear-response theory – weak external magnetic perturbation
- Longitudinal magnetic order (*eh* bubbles): normal self-energy

$\Sigma_{\uparrow}(\eta^{\shortparallel}_{\downarrow}) \doteq$



- Transversal (spin flip) magnetic order (*eh* ladders): self-energy anomalous only in the spin-polarized state

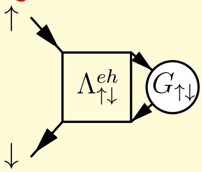
$\Sigma_{\uparrow\downarrow}(\bar{\eta}^{\perp}) \doteq$



Linearized Ward identity

- WI resolved only linearly w.r.t. the symmetry-breaking field
  - only normal component in disordered phase
- Irreducible vertex depends on even powers of the perturbing field
- Critical point in the spin-symmetric state ($G_\uparrow = G_\downarrow$)
- Linearized WI in the external magnetic field
  – thermodynamic self-energy

$\Sigma_{\uparrow\downarrow} \doteq$



- Mathematical expression

$$\Sigma^T_{\uparrow\downarrow}(k) = \frac{1}{\beta N} \sum_{k'} \Lambda(k, k'; k + k') G^T_{\uparrow\downarrow}(k')$$

with $\Lambda = (\Lambda_{\uparrow\downarrow} + \Lambda_{\downarrow\uparrow})/2$

Schwinger-Dyson equation - spectral self-energy

- Linearized WI: symmetry of the self-energy gets broken at the divergence in the BSE for a zero eigenvalue of

$$M_{k,k'} = \delta_{k,k'} + \Lambda(k, k'; k + k')G^T(k')G^T(k')$$

- 1P propagators should use Σ^T from LWI in all equations with 2P functions: BSE, SDE

Schwinger-Dyson equation with $\Gamma_{\sigma\sigma'}$ and G_σ from the Bethe-Salpeter equations determines the physical (spectral) self-energy

$$\Sigma_\uparrow(k) = -\frac{U}{\beta^2 N^2}\sum_{k'k''} G^T_\downarrow(k')G^T_\downarrow(k'')G^T_\uparrow(k+k'-k'')\Gamma^T(k'', k; k'-k'')$$

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Effective interaction – defining equations

- 1P propagator: $G_\sigma(\omega) = \left[\omega - E_d - \frac{U}{2} - \Lambda\left(\frac{1}{2} - n^T_{-\sigma}\right) + i\Delta\right]^{-1}$

  with $n^T_\sigma = -\int_{-\infty}^{\infty}\frac{d\omega}{\pi} f(\omega)\Im G_\sigma(\omega)$, $\quad \Lambda = (\Lambda_\uparrow + \Lambda_\downarrow)/2$
- Real effective interaction:

$$\Lambda_\sigma = \frac{U}{1 + \Psi_\sigma[\Lambda]}$$

- Screening factor

$$\Psi_\sigma[\Lambda] = \frac{\Lambda^2}{\pi}\int_{-\infty}^{\infty} d\omega \left\{ f(\omega)\Re\left[\frac{\phi_\sigma(-\omega - i\pi T)}{1 + \Lambda\phi_\sigma(-\omega - i\pi T)}\right]\Im\left[G_\sigma(\omega)G^*_{-\sigma}(-\omega)\right] \right.$$
$$\left. - b(\omega)\Im\left[\frac{\phi^*_\sigma(-\omega)}{1 + \Lambda\phi^*_\sigma(-\omega)}\right] \times \Re\left[G_\sigma(\omega - i\pi T)G_{-\sigma}(-\omega + i\pi T)\right]\right\}$$

- Electron-hole bubble

$$\phi_\sigma(E) = -\int_{-\infty}^{\infty}\frac{d\omega}{\pi} f(\omega)\left[G_{-\sigma}(\omega + E)\Im G_\sigma(\omega) + G_\sigma(\omega - E)\Im G_{-\sigma}(\omega)\right]$$

Effective interaction – spectral function

- Impurity Green function

$$\mathcal{G}_\sigma(\omega) = \frac{1}{\omega - E_d - Un_{-\sigma} + i\Delta - \Sigma_\sigma(\omega)}$$

- Particle density – HF self-consistency: $n_\sigma = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} f(\omega) \Im \mathcal{G}_\sigma(\omega)$
- Spectral (physical) self-energy

$$\Sigma_\sigma(\omega) - \frac{U\Lambda}{\pi} \int_{=\infty}^{\infty} dx \left\{ b(x) G_{-\sigma}(x+\omega) \Im \left[\frac{\phi_\sigma(x)}{1 + \Lambda \phi_\sigma(x)} \right] \right.$$
$$\left. - f(x) \frac{\phi^*_\sigma(x-\omega)}{1 + \Lambda \phi^*_\sigma(x-\omega} \Im G_{-\sigma}(x) \right\}$$

- Full 2P vertex

$$\Gamma_\sigma(\omega) = \frac{\Lambda}{1 + \Lambda \phi_\sigma(\omega)} \, .$$

Effective interaction – magnetic susceptibility

- Spin susceptibility ($h = 0$)

$$\chi = \frac{1}{\beta}\sum_n \left[\frac{\partial G_\uparrow(i\omega_n)}{\partial h} - \frac{\partial G_\downarrow(i\omega_n)}{\partial h}\right] = -\frac{2}{\beta}\sum_n G(i\omega_n)^2 \left[1 - \frac{\partial \Sigma_\uparrow(i\omega_n)}{\partial h}\right]$$

- Derivative of the (thermodynamic) self-energy

$$\left\{1 - \Lambda \int_{-\infty}^{\infty} \frac{d\omega}{\pi} f(\omega) \Im \left[G(\omega)^2\right]\right\} \frac{d\Sigma^T_\uparrow}{dh} = \Lambda\phi(0)$$

- Magnetic susceptibility

$$\chi = -\frac{2}{\beta}\sum_n \mathcal{G}(i\omega_n)^2 \left[1 - \frac{UX(i\omega_n)}{1 + \Lambda\phi(0)}\right]$$

- Quantum criticality: Kondo scale $a = 1 + \Lambda\phi(0) \ll 1$

Effective interaction – specific heat

- Total energy

$$E^{TOT} = -\sum_\sigma \int_{-\infty}^{\infty} f(\omega)(\omega - Un_{-\sigma})\Im\mathcal{G}_\sigma(\omega) + Un_\uparrow n_\downarrow - U\Lambda \int_{-\infty}^{\infty} b(\omega)\Im\left[\frac{\phi_\uparrow(\omega)^2}{1+\Lambda\phi_\uparrow(\omega)}\right]$$

- Correlation term via spectral self-energy

$$E^{TOT} = -\sum_\sigma \int_{-\infty}^{\infty} f(\omega)\omega\Im\mathcal{G}_\sigma(\omega) - Un_\uparrow n_\downarrow + \int_{-\infty}^{\infty} f(\omega)\Im\left[G_\uparrow(\omega)\Sigma_\uparrow(\omega)\right]$$

- Specific heat

$$C_V = \frac{\partial E^{TOT}(T)}{\partial T} = \gamma(T)T$$

Spectral function & specific heat share quantum criticality of magnetic susceptibility

Effective interaction – Kondo critical regime I

- Kondo asymptotics $a = 1 + \Lambda\phi(0) \ll 1$

$$K(\omega) \doteq \frac{\Lambda}{1 + \Lambda\phi(0) - i\Lambda\phi'\omega} ,$$

- Screening factor

$$\psi = -\Lambda \int_{-\infty}^{0} \frac{d\omega}{\pi} \Im \left[\frac{G(\omega) G^{*}(-\omega)}{a - i\Lambda\phi'\omega} \right] \doteq \frac{[\Im G(0)]^2 |\ln a|}{\pi\phi'} = |\ln a|$$

- Kondo asymptotics: $a = \exp\{-U\rho_0\}$

Effective interaction – Kondo critical regime II

- Spectral self-energy

$$\Re\Sigma^{(2)}(\omega) \doteq \frac{U}{\Lambda\pi^2\rho_0^2}\left[|\ln a|\,\Re G(\omega) + \arctan\left(\frac{\Lambda\pi\rho_0^2\,\omega}{a}\right)\Im G(\omega)\right]$$

$$\Im\Sigma^{(2)}(\omega) \doteq \frac{U}{2\Lambda\pi^2\rho_0^2}\ln\left[1 + \frac{\Lambda^2\pi^2\rho_0^4\,\omega^2}{a^2}\right]\Im G(\omega)$$

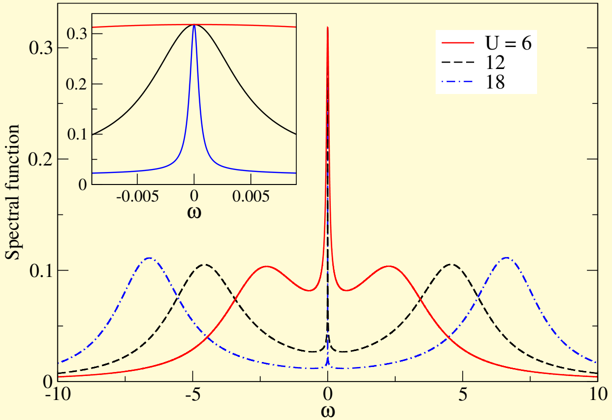
- Thermodynamic and spectral susceptibilities

$$\chi^T \doteq \frac{2}{a}\int_{-\infty}^{0}\frac{d\omega}{\pi}\Im\left[G(\omega)^2\right]$$

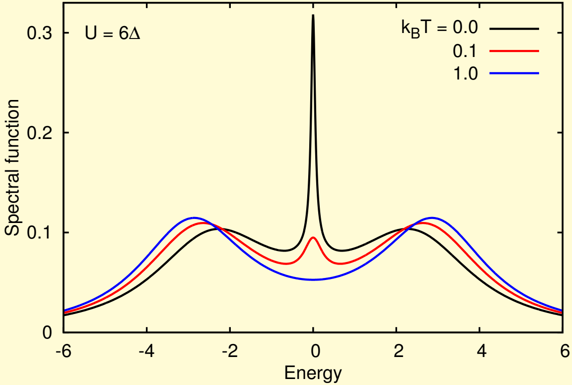
$$\chi \doteq -\frac{2U}{a}\int_{-\infty}^{0}\frac{d\omega}{\pi}\Im\left[\mathcal{G}(\omega)^2 X(\omega)\right]$$

- Specific heat coefficient: $\gamma = UZ/a$

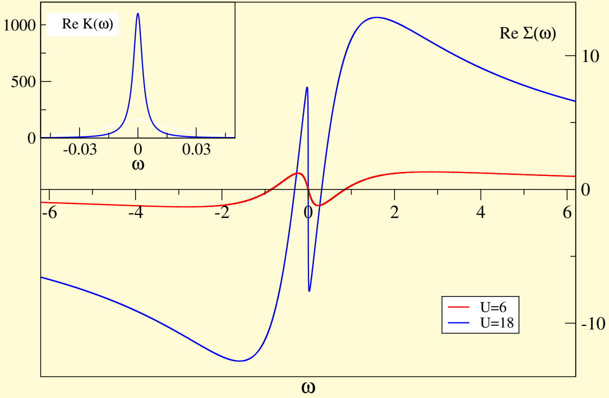
Spectral function of SIAM at half filling



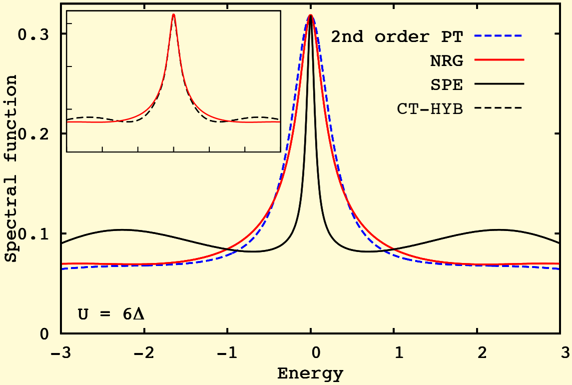
Spectral function of SIAM – temperature dependence



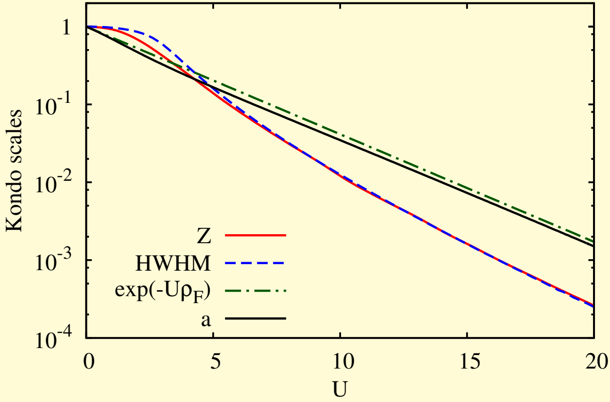
Self-energy and divergent vertex



Comparison with exact numetics

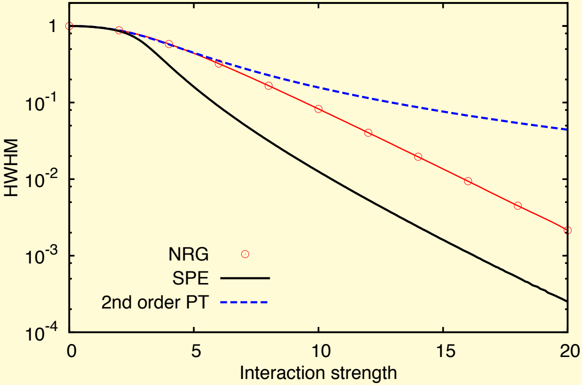


Exponential Kondo scales

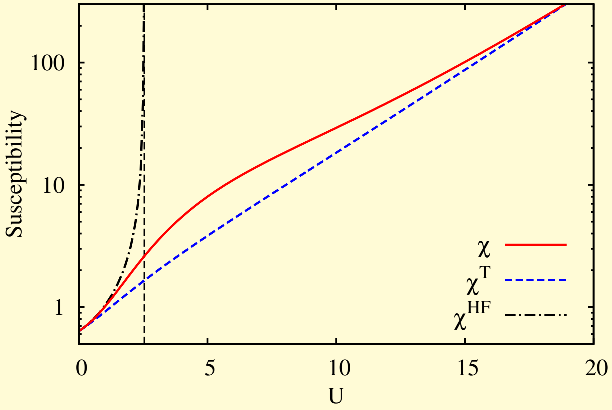


$$Z = [1 - \Sigma'(0)]^{-1}, \quad a = \Gamma(0)^{-1} = 1 - \lambda_0$$

Kondo scales compared with numerical simulations

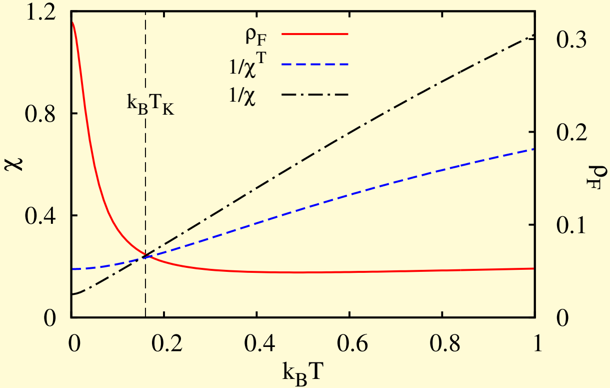


Magnetic susceptibilities



χ^{HF} – 1PGF with the Hartree-Fock self-energy (BK construction)

Saturation of Curie-Weiss law



$\chi(T) = \frac{C^2}{T+T_K}$, T_K from Bethe-ansatz solution

Thermodynamic potential vs linearized WI I

Baym thermodynamic construction: 1P approach

- Generating functional $\Phi[U, G]$
- Self-energy from stationarity equation:

$$\Sigma(\mathbf{k}, i\omega_n) = \frac{\delta\Phi[U, G]}{\delta G(\mathbf{k}, i\omega_n)}$$

  with SC condition $G(\mathbf{k}, i\omega_n) = [i\omega + \mu - \epsilon(\mathbf{k}) - \Sigma(\mathbf{k}, i\omega_n)]^{-1}$
- Two vertex functions: SDE (microscopic) & WI (macroscopic)
- Two-particle vertex in & SDE without thermodynamic meaning
- Scheme breaks down beyond the critical points:
  - No way to circumvent singularities in vertices
  - Long-range order does not match singularity at vertex function

Thermodynamic potential vs linearized WI II

Linearized Ward identity: 2P approach

- Vertex generating the approximation: $\Lambda = (\Lambda_{\uparrow\downarrow} + \Lambda_{\downarrow\uparrow})/2$
- Thermodynamic (static) self-energy from Ward identity
  $\Sigma^T_\sigma(k) = \frac{1}{\beta N}\sum_{k'} \Lambda(k, k'; 0) G_{-\sigma}(k')$
  – auxiliary to be used 1P propagators determining 2P functions
- Spectral (dynamical, beyond Hartree) self-energy $\Sigma(k)$ from Schwinger-Dyson equation
  – full dynamical structure , determines spectral properties
- LRO matches the poles in the vertex functions
  – Qualitatively correct description of quantum criticality
- Thermodynamic consistency – critical behavior qualitatively the same from spectral & thermodynamic functions