Generic ambiguity of the description of strongly correlated electrons

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Outline

1. Introduction - generic model
2. 1P approach - single 1P self-energy & two 2P vertex functions
   - Generating functional & Baym-Kadanoff self-consistency
   - Static mean field
   - Schwinger-Dyson equation vs. Ward identity
3. 2P approach - single 2P vertex & two 1P self-energies
   - Bethe-Salpeter and parquet equations
   - Linearized Ward identity
   - Effective-interaction approximation
4. Numerical results in the Kondo regime of SIAM
5. Conclusions

Strong 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 with bare part & perturbation

Tight-binding description: Conduction electrons in a periodic lattice

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

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

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

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

Bare propagator & external perturbation

Unperturbed Green function

$$G_\sigma^{(0)}(z,\mathbf{k}) = \frac{1}{z+\mu+\sigma h-\epsilon(\mathbf{k})}$$

Normal & anomalous perturbations

$$\begin{aligned}
\widehat{H}_{ext} = \int d1d2 \Bigg\{ & \sum_\sigma \eta_\sigma^{||}(1,2)c_\sigma^\dagger(1)c_\sigma(2) && \ldots \text{conserves charge \& spin} \\
+ & \sum_\sigma \left[\bar{\xi}_\sigma^{||}(1,2)c_\sigma(1)c_\sigma(2) + \xi_\sigma^{||}(1,2)c_\sigma^\dagger(1)c_\sigma^\dagger(2)\right] && \ldots \text{changes charge \& spin} \\
& + \left[\bar{\xi}^\perp(1,2)c_\uparrow(1)c_\downarrow(2) + \xi^\perp(1,2)c_\downarrow^\dagger(2)c_\uparrow^\dagger(1)\right] && \ldots \text{conserves spin} \\
& + \left[\eta^\perp(1,2)c_\uparrow^\dagger(1)c_\downarrow(2) + \bar{\eta}^\perp(1,2)c_\downarrow^\dagger(2)c_\uparrow(1)\right] && \ldots \text{conserves charge} \Bigg\}
\end{aligned}$$

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 $\Phi[G]$, better for $\Sigma[G]$

Baym-Kadanoff scheme I

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

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

- 1P irreducible vertex (self-energy) from the generating functional

$$\Sigma_\sigma[U; G, \overline{G}] = \frac{\delta\Phi[U; G, \overline{G}]}{\delta \overline{G}_\sigma}$$

Baym-Kadanoff scheme II

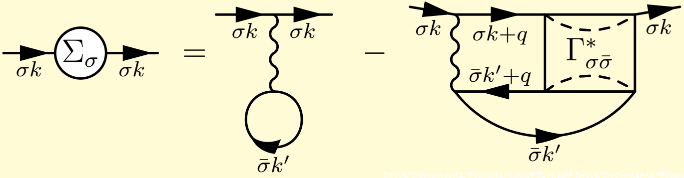
- Dyson equation for 1P GF

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

- Schwinger-Dyson equation – microscopic quantum dynamics introducing a two-particle vertex Γ:

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

- Diagrammatic representation



Baym-Kadanoff – conserving vertex

- Macroscopic conservation laws - not implied by the equation of motion (Schwinger-Dyson)
- Generalized Ward identity (thermodynamic consistency)

$$\Lambda^{\bar{\alpha}\alpha}(13,24) = \frac{\delta^2\Phi[U;G,\overline{G}]}{\delta G_\alpha(4,3)\delta\overline{G}_{\bar{\alpha}}(2,1)} = \frac{\delta\Sigma^\alpha(1,2)}{\delta G_\alpha(4,3)}$$

- Two-particle vertices not included in the Luttinger-Ward functional $\Phi[U;G,\overline{G}]$ (second derivatives thereof)
- Bethe-Salpeter equations for 2P vertex (equilibrium)

$$\Gamma^{\alpha\alpha'}(k,k';q) = \Lambda^{\alpha\alpha'}(k,k';q) + \left[\Lambda^{\alpha\alpha'} G_\alpha G_{\alpha'} \odot \Gamma^{\alpha\alpha'}\right](k,k';q)$$

- Two generic vertex functions:

$$\Gamma \neq \Gamma^*$$

Hartree approximation – 1P renoramlization

- Generating (Luttinger-Ward) functional

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

- Schwinger-Dyson equation ($\Gamma^* = 0$):

$$\Sigma_\sigma(\omega) = Un_{-\sigma}$$

- Renormalized 1P propagator

$$G_\sigma(\omega, \mathbf{k}) = \frac{1}{\omega + \mu + \sigma h - \epsilon(\mathbf{k}) - Un_{-\sigma}}$$

- Total energy free of vertex corrections

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

Hartree approximation – thermodynamics

- 2P irreducible vertex – Ward identity

$$\Lambda(\omega, \omega'; \Omega) = U$$

- Full vertex function from form Bethe-Salpeter equation (zero field, spin symmetric solution)

$$\Gamma(\omega, \omega'; \Omega) = \frac{U}{1 + U\phi(\Omega)}$$

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

- Magnetic susceptibility

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

Nontrivial thermodynamics – trivial spectral function

Hartree 1P renormalization – RPA spectral function

- Hartree renormalization of 1P propagators
- Spectral self-energy from vertex $\Gamma(\Omega)$ – SDE:

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

- Magnetic susceptibility with spectral self-energy

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

Nontrivial spectral function & Hartree thermodynamics
Two 1P self-energies to the single 2P vertex

Inability to obey simultaneously SDE & WI

- Schwinger-Dyson equation – with physical vertex

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

- Bethe-Salpeter equation

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

- WI used in SDE – integro-functional differential equation

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

Solution equals solving Schwinger field theory,
the same as summing all Feynman diagrams

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)

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

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

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

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)
  - 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

Renormalized perturbation expansion I

How to perform renormalizations in the perturbation expansion?

Using 1P self-energy & SDE

- Central object of renormalization is the self-energy
- SDE - a self-consistennt equation for the self-energy (1P self-consistency)
- Auxiliary 2P vertex Γ^* in SDE
- Conserving 2P vertex $\Gamma \neq \Gamma^*$ from WI
- Auxiliary vertex Γ^* diverges prior to Γ
- Ordered solution does not math the disordered one (at the transition)

Renormalized perturbation expansion II

Using 2PIR vertex & WI

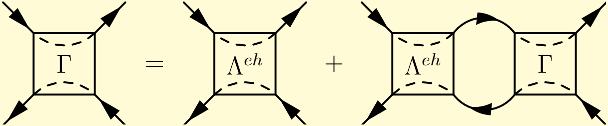
- Central object of renormalization a 2PIR vertex Λ of the singular BSE
- WI used to match thermodynamic self-energy Σ^T with vertex Λ
- Thermodynamic self-energy used to renormalize 1P propagators G
- Spectral self-energy Σ^{Sp} from SDE with thermodynamic propagators G (non-self-consistent)
- The spectral function from $\mathcal{G}$ with Σ^{Sp}
- Ordered solution matches the disordered one (at the transition)

2P self-consistency needed to avoid spurious critical behavior

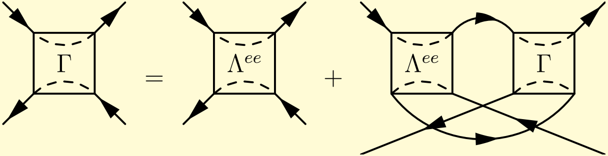
Fundamental scattering channels

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} becomes divergent with repulsive interaction
- Full parquets miss quantum criticality (SIAM)

Reduced parquet equations – 2P self-consistency

- Reduction of the parquet self-consistency in BS equations
- Nonsingular irreducible vertex ($\Lambda = \Lambda^{eh}$) – reduced equation with superdivergent term $[\Lambda^{ee} GG] \circ \Lambda^{ee}$ removed & $\Lambda^{ee} \gg U$

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

- Singular reducible vertex ($\Lambda^{ee} = K$)

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

- Full vertex ($q = Q - k - k'$)

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

Renormalized 1P propagators in the 2P approach

- Thermodynamic self-energy – from Λ via WI

$$\Lambda = \frac{\delta \Sigma^T}{\delta G}$$

(approximations needed!)

- Thermodynamic propagators $G(\omega) = G^{(0)}(\omega - \Sigma^T(\omega))$
- 2PIR vertex $\Lambda[G]$ – functional of the thermodynamic propagator
- Spectral self-energy $\Sigma^{Sp}[G]$ from SDE with thermodynamic propagators , no self-consistency in SDE
- Spectral function from $\mathcal{G} = G^{(0)}(\omega - \Sigma^{Sp}(\omega))$

$\Sigma^{Sp}[G]$ & $\Sigma^T[G]$ share the same critical behavior induced by the critical point in BSE generated by $\Lambda[G]$

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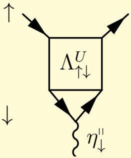
Linearization in symmetry breaking field

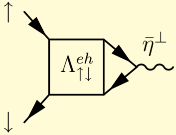
- Repulsive particle interaction – electron-hole scattering dominant
- Linear-response theory – weak external magnetic perturbation
- Longitudinal magnetic order (*eh* bubbles): normal self-energy

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



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

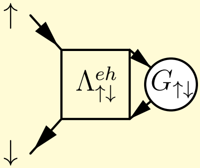
$\Sigma_{\uparrow\downarrow}(\bar{\eta}^{\perp}) \doteq$



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

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

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

$$M_{k,k'} = \delta_{k,k'} + \Lambda(k, k'; k + k')G(k')G(k')$$

- 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

$$\Sigma^{Sp}_{\uparrow}(k) = -\frac{U}{\beta^2 N^2} \sum_{k' k''} G_{\downarrow}(k')G_{\downarrow}(k'')G_{\uparrow}(k + k' - k'')\Gamma(k'', k; k' - k'')$$

Reduced parquet equations in quantum criticality

- Analytic structure of (reduced) parquet equations unknown
- Simplification in quantum criticality:
  Dominant polar contribution $\mathbf{q} \to \mathbf{q}_0$ & $\nu_m \to 0$

$$\Lambda(k, k') = \frac{U}{1 + \langle K(k', k; -q) G(k - q) G(k' + q) \rangle_q}$$

where $k' = k + Q$ and $\langle X(q) \rangle_q = (\beta N)^{-1} \sum_q X(q)$

  - Zero temperature: $k = k' = 0$ (Fermi surface)

$$K(q) = -\frac{\Lambda^2 \langle G(k) G(k+q) \rangle_k}{1 + \langle G(k) G(k+q) \rangle_k}$$

    $\Lambda(k, k') \to \Lambda$ – effective interaction

  - Non-zero temperatures: $|q| \ll k, k'$ with $k, k' \to 0$ in criticality
    $\Lambda(k, k')$ and $K(k, k'; q)$ fully analytically controlable

Effective interaction – Kondo critical regime I

- SIAM at zero temperature and half filling ($\Sigma^T = 0$)
- Kondo dimensionless scale $a = 1 + \Lambda\phi(0) \ll 1$

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

- Screening factor: $\Lambda = U/(1+\psi)$

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

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

  Bethe ansatz: $a = \exp\{-\frac{\pi^2}{9} U\rho_0\}$ (only Lorentzian DoS)

Effective interaction – Kondo critical regime II

- Spectral self-energy

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

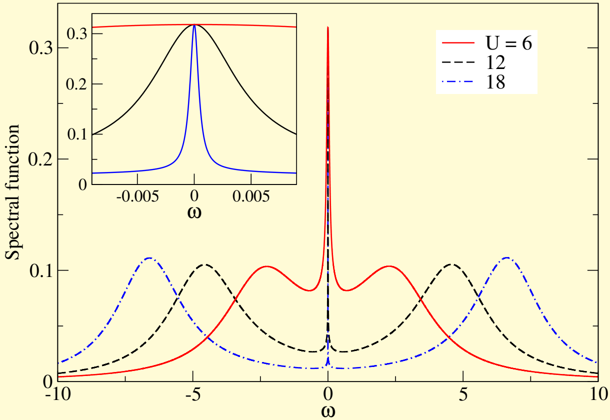
$$\Im\Sigma^{(Sp)}(\omega) \doteq \frac{U}{2\Lambda\pi^2\rho_0^2}\ln\left[1 + \frac{\Lambda^2\pi^2\rho_0^4\,\omega^2}{a^2}\right]\Im G(\omega)$$

- Thermodynamic and spectral susceptibilities

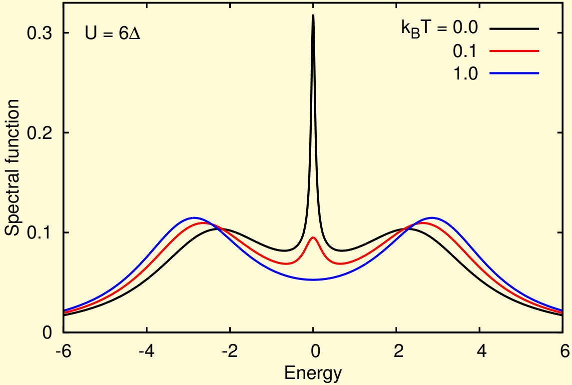
$$\chi^T \doteq \frac{2}{a}\int_{-\infty}^{0}\frac{d\omega}{\pi}\Im\left[G(\omega)^2\right]$$

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

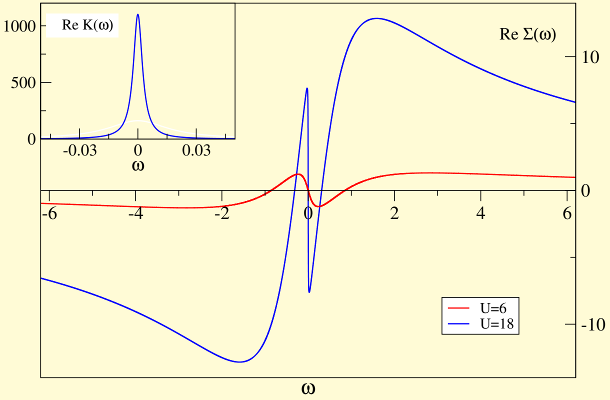
Spectral function of SIAM at half filling



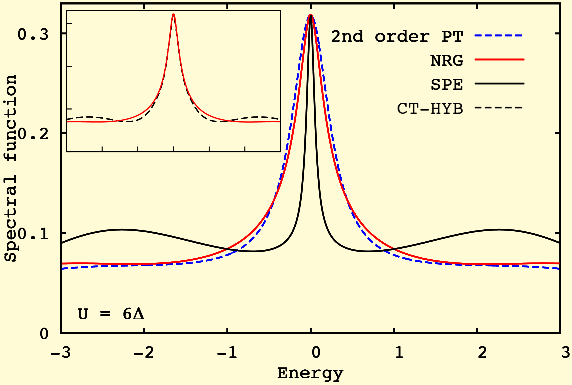
Spectral function of SIAM – temperature dependence



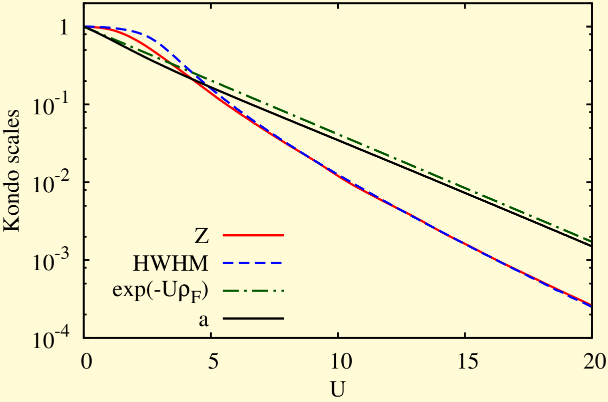
Self-energy and divergent vertex



Comparison with exact numetics

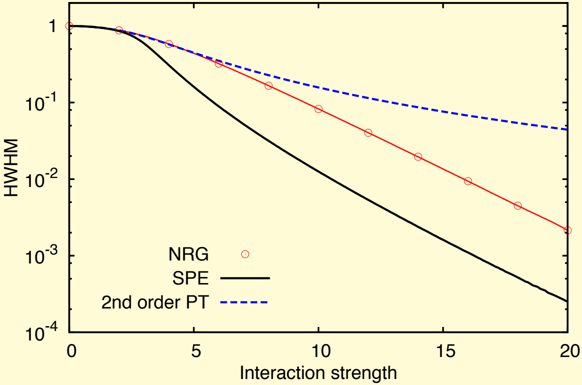


Exponential Kondo scales

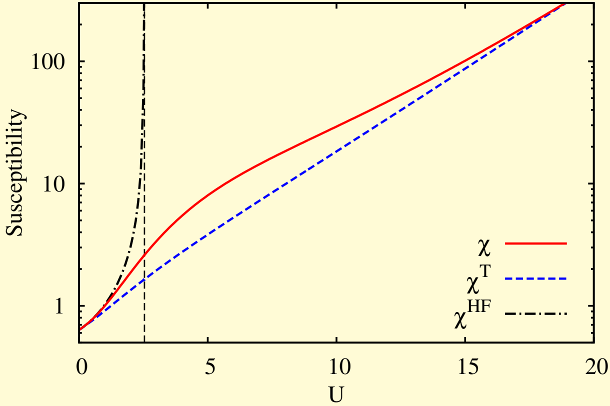


$Z = [1 - \Sigma'(0)]^{-1}, \quad a = \Gamma(0)^{-1} = 1 - \lambda_0$

Kondo scales compared with numerical simulations

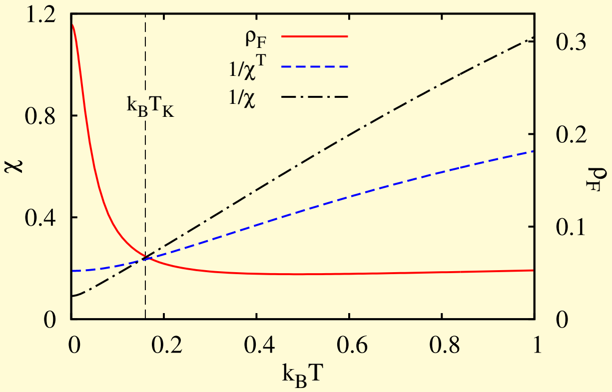


Magnetic susceptibilities



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

1P approach – self-energy & SDE central

- Unique self-energy $\Sigma[G]$ from the renormalized perturbation (diagrammatic) expansion with full G
- Φ-derivable approximation if a generating functional $\Phi[U, G]$ exists:

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

- Ambiguous vertex functions: from SDE $\Gamma^*[G]$ (dynamical) & from WI $\Gamma[G]$ (conserving) – do not coincide (qualitatively)
- Two-particle vertex in SDE without thermodynamic meaning
- Scheme breaks down beyond the critical points of Γ^*:
  - No way to circumvent singularities in vertices
  - Long-range order does not match singularity at vertex function

Thermodynamic potential vs linearized WI II

2P approach – 2PIR vertex & WI (linearized) central

- Unique generating 2P vertex: $\Lambda = (\Lambda_{\uparrow\downarrow} + \Lambda_{\downarrow\uparrow})/2$
  – from renormalized perturbation expansion
- Thermodynamic self-energy from (linearized) Ward identity
  $\Sigma^{T}_{\sigma}(k) = \frac{1}{\beta N}\sum_{k'} \Lambda(k, k'; 0) G_{-\sigma}(k')$
  – determining 1P self-consistency & thermodynamic properties
- Spectral (dynamical) self-energy $\Sigma^{Sp}(k)$
  from Schwinger-Dyson equation (non-self-consistent)
  – full dynamical structure & spectral properties
- Two self-energies with equivalent description of quantum phase transitions
- Thermodynamic consistency – critical behavior of the 2P vertex matches the symmetry breaking in both self-energies