Consistent description of quantum criticality of correlated electrons

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Outline

1. Introduction – thermodynamic phases (structural & magnetic)

2. Critical behavior: Thermodynamic approach
   - Classical criticality - Ising model
   - Quantum criticality of correlated electrons
   - Hubbard model
   - Thermodynamic consistency: Macroscopic conservation laws vs. microscopic dynamics

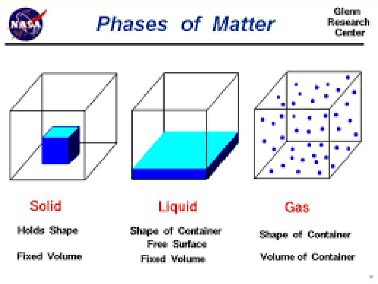
3. Towards consistent quantum criticality: Two-particle approach
   - Taming critical fluctuations – Linearized Ward identity
   - Example: Kondo behavior in single-impurity Anderson model – quantum criticality in spectral & thermodynamic functions

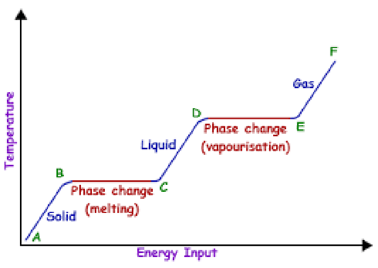
4. Conclusions

Equilibrium phases and phase transitions

Phases of matter
– differ in physical properties (shape & volume)

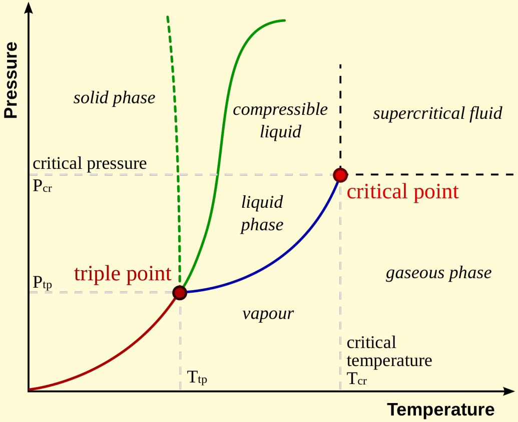
Phase transitions
– continuous or discontinuous changes of parameters





Structural phase diagram

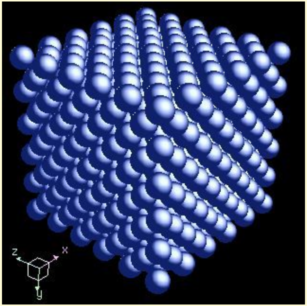
Structural phases – discontinuous transitions



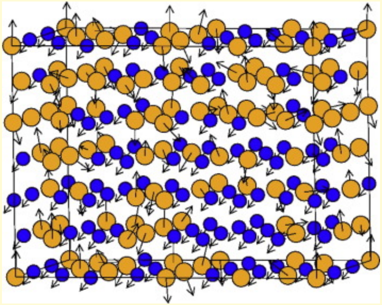
Response function diverges at the critical function

Magnetic properties of crystals

Regular lattice with a fixed structure

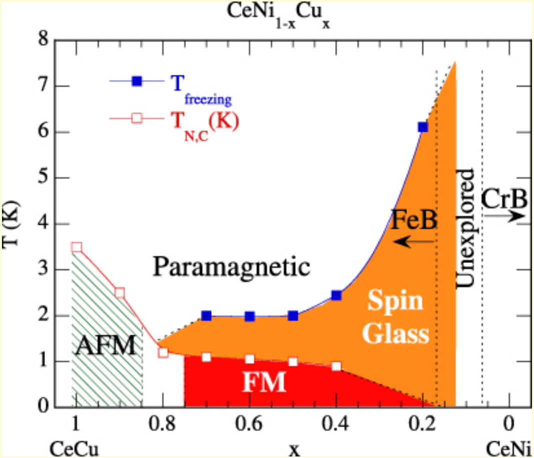


Spin properties



Magnetic phase diagram

Magnetic phases – continuous (critical) transitions



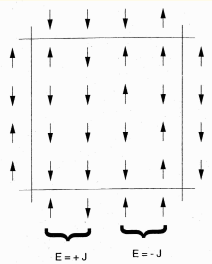
Microscopic models for critical transitions

- Model of interacting spins (Ising)

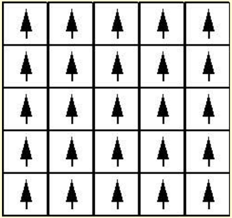
$$H[J, S, h] = -J \sum_{<ij>} S_i S_j - h \underbrace{\sum_i S_i}_{H_{ext}[S,h]}$$

- Classical spins with $S_i = \pm 1$ ($\hbar/2$ units)

Paramagnetic phase (high temperature)



Ferromagnetic phase (low temperature)



PM- FM – Critical phase transition for $h = 0$

Mean-field thermodynamics – self-consistent theory

- Full thermodynamic information in (Gibbs) free energy

$$-\beta F(T,h) = \ln \mathrm{Tr}_S \exp\left\{-\beta H[J,S,h]\right\}$$

$\beta = 1/k_B T$ and global magnetization

$$m(T,h) = -\frac{\partial f(T,h)}{\partial h} = \frac{1}{N}\,\frac{\sum_i \mathrm{Tr}_S S_i e^{-\beta H[J,S,h]}}{\mathrm{Tr}_S e^{-\beta H[J,S,h]}}$$

- Mean-field (Weiss) solution – long-range spin exchange
Legendre transform – Helmoholtz free energy in m

$$f(T,m) = \frac{1}{N} F(T,h) - mh = \frac{Jm^2}{2} - \frac{1}{\beta}\ln 2\cosh\left(\beta J m\right)$$

- Equilibrium state – magnetization minimizing $f(T,m)$

$$\frac{\partial f(T,m)}{\partial m} = 0 = J\left[m - \tanh(\beta J m)\right]$$

Critical point & symmetry breaking ($h = 0$)

- Critical point $\beta J = 1$ separates two phases
  - Paramagnetic: $m = 0$
  - Ferromagnetic: $1 \geq m^2 > 0$
- Magnetic susceptibility divergent at the critical point:

$$\chi = -\left.\frac{\partial^2 f(T,h)}{\partial h^2}\right|_{h=0} = \frac{\beta\left(1-\tanh(\beta J m)^2\right)}{1-\beta J(1-\tanh(\beta J m)^2)} \propto \left[\frac{\partial^2 f(T,m)}{\partial m^2}\right]^{-1} \geq 0$$

- Spin-reflection symmetry $H[J,S] = H[J,-S]$ broken in the ordered (ferromagnetic) phase
- Magnetic energy $H_{ext}[S,h] = -h\sum_i S_i$ lifts degeneracy – critical point circumvented

Susceptibility below T_c becomes negative in the paramagnetic state $m = 0$

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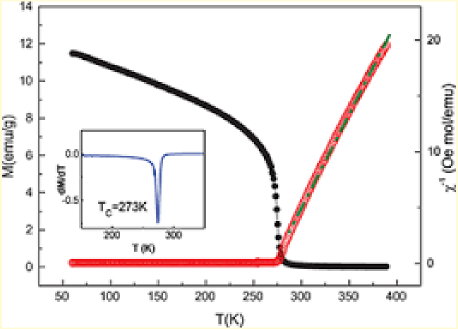
Thermodynamic consistency

Thermodynamic consistency at the critical point:

$$m(T) = \lim_{h\to 0} m(T,h)$$



Classical order parameter m has no internal dynamics:
Universality - critical & noncritical functions separated.

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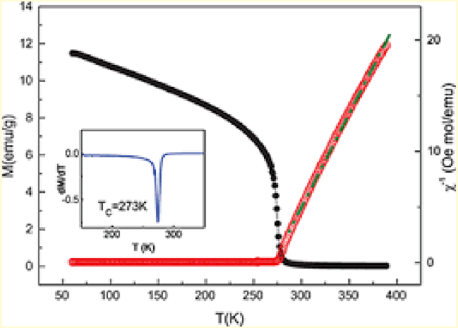

Divergence in the response function must enforce the emergence of an order to continue the solution beyond the critical point.

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Thermodynamic consistency

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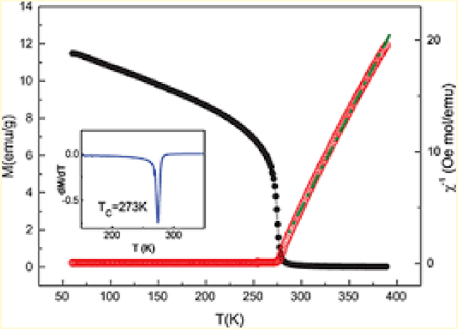

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Quantum statistical mechanics

- Equilibrium grand potential

$$\Omega(N,T,\mu) = -k_B T \log \mathrm{Tr}\left[\exp\left\{-\beta\left(\widehat{H}_0 + \widehat{H}_I - \mu\widehat{N}\right)\right\}\right]$$

  - Unperturbed Hamiltonian H_0
  - Perturbation due to interaction H_I
- Quantum character:

$$[\widehat{H}_0, \widehat{H}_I] \neq 0$$

- Second quantization – creation & annihilation operators
- Quantum fluctuations – Matsubara frequencies
- Thermal & quantum fluctuations mixed (non-zero temperatures)
- Zero temperature: only quantum fluctuations

Grand potential – does not contain full information
Dynamics introduced via Green functions

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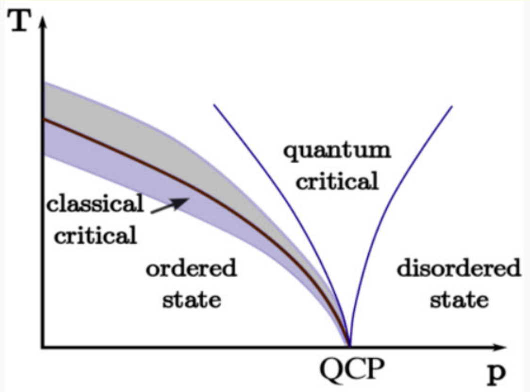
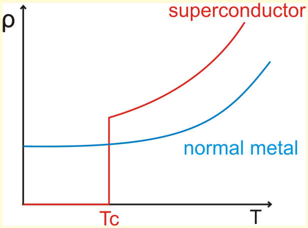
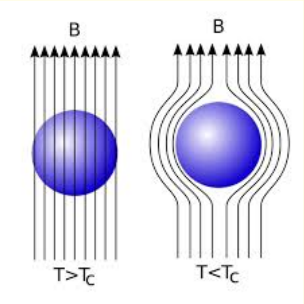
Quantum criticality



Quantum phases

- Superconductivity – persistent current & Meissner effect



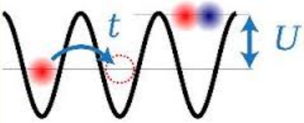


- Quantm phase without quantum critical point
- Condensate of (bound) Cooper electron pairs – pure quantum effect
- Ordered phase – does not conserve charge (nontrivial equilibrium)

Correlated electrons & quantum perturbations

Tight-binding description: Conduction electrons in a periodic lattice

Screened Coulomb



$$t c^{\dagger}_{i+1\sigma} c_{i\sigma} \qquad U n_{i\uparrow} n_{i\downarrow}$$

$$n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$$

Generic Hamiltonian with external perturbation

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

Normal & anomalous (non-classical, non-conserving) perturbations

$$\widehat{H}_{ext} = \int d1 d2 \left\{ \sum \eta^{||}_{\sigma}(1,2) c^{\dagger}_{\sigma}(1) c_{\sigma}(2) \right.$$ . . . conserves charge & spin

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$$+ \left[\bar{\xi}^\perp(1,2) c_\uparrow(1) c_\downarrow(2) + \xi^\perp(1,2) c^\dagger_\downarrow(2) c^\dagger_\uparrow(1)\right] \quad \text{... conserves spin}$$

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1P Green function & self-energy – order parameter

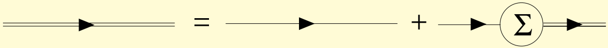
- Unperturbed Green function (no Coulomb repulsion)

$$G^{(0)}_\sigma(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu + \sigma h - \epsilon(\mathbf{k})}$$

- Fermionic Matsubara frequencies $\omega_n = (2n+1)\pi k_B T$
- Effect of electron correlations – self-energy $\Sigma_\sigma(\mathbf{k}, i\omega_n)$
- Dyson equation – full Green function (dynamical oder)

$$G_\sigma(\mathbf{k}, i\omega_n) = G^{(0)}_\sigma(\mathbf{k}, i\omega_n)\left[1 + \Sigma_\sigma(\mathbf{k}, i\omega_n) G_\sigma(\mathbf{k}, i\omega_n)\right]$$

diagrammatically



- Self-energy – 1P irreducible diagrams

Response & vertex functions

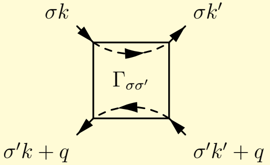
- Response function (susceptibility) – singular at the critical point

$$\chi(q) = -\frac{2}{(\beta N)^2}\sum_{k,k'} G(k)G(k+q)\left[\delta(k-k') + \Gamma(k,k';q)G(k')G(k'+q)\right]$$

from the full 2P vertex $\Gamma_{\sigma\sigma'}(k,k';q)$

- Thermodynamic energy-momentum notation
  $k = (\mathbf{k}, i\omega_n)$, $q = (\mathbf{q}, i\nu_{m})$, $\nu_m = 2\pi m k_B T$

- Charge and spin conservation in vertices:
  normal Γ and transposed Γ^t



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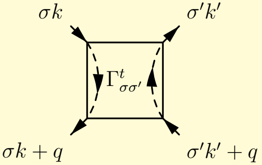
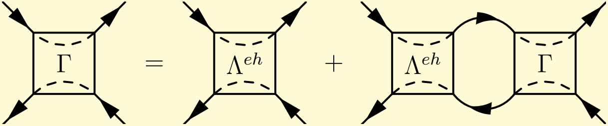


- Transposition symmetry: $\Gamma_{\sigma\sigma}(k,k';q) = -\Gamma^t_{\sigma\sigma}(k,k+q;k-k')$

Representing the full two-particle vetex

Bethe-Salpeter equations – nonequivalent representations of the full 2P vertex

- 2P self-energy – irreducible vertices Λ^{α}
  - Electron-hole multiple singlet scatterings



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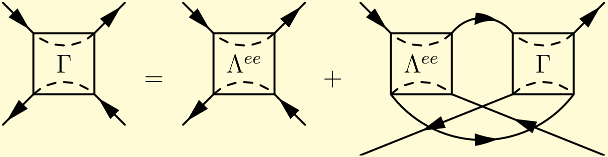
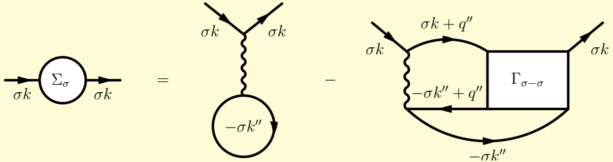


Vertex Γ divergent at the critical point

Consistency – 1P propagators related to 2P vertices

1P propagators in equilibrium are related to the 2P vertex

- Schwinger-Dyson equation: Microscopic quantum dynamics



- Integral Ward identity: Macroscopic mass conservation

How to introduce the Ward identity into perturbation theory?

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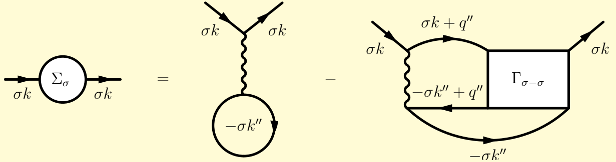

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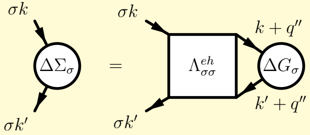

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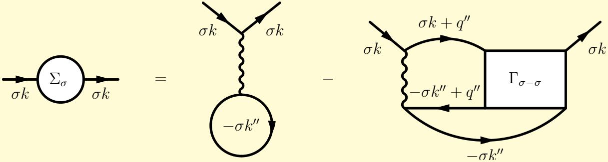

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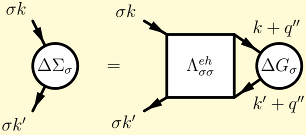

How to introduce the Ward identity into perturbation theory?

Conservation of charge source in correlated electrons

- Generating Luttinger-Ward functional $\Phi[U,G]$:

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

- Stationarity equations

$$\frac{\delta\Omega}{\delta\Sigma_\sigma(\mathbf{k},i\omega_n)} = \frac{\delta\Omega}{\delta G_\sigma(\mathbf{k},i\omega_n)} = 0 = \frac{\partial\Omega}{\partial n_\sigma}$$

- Consistency - dynamical charge conservation ($\delta U = \delta[e^2/r]$)

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

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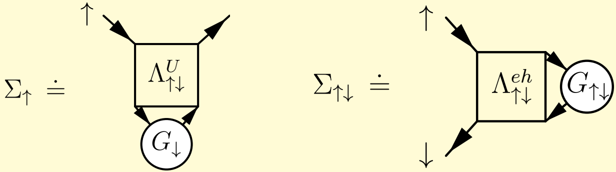
Ward identity and Schwinger-Dyson equation cannot be obeyed simultaneously

Linearized Ward identity

- WI resolved only linearly w.r.t. the symmetry-breaking field
- Irreducible vertex depends on even powers of the perturbing field
- Critical point in the spin-symmetric state ($G_\uparrow = G_\downarrow$)
- WI linearized in the external magnetic field



- Mathematical expression (normal state)

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

$$\Lambda(k,k';q) = (\Lambda_{\uparrow\downarrow}(k,k';q) + \Lambda_{\downarrow\uparrow}(k,k';q))/2$$

Thermodynamically consistent approach

Generating functional: Two-particle vertex $\Lambda\left[G^T\right]$
replacing Luttiner-Ward functional $\Phi[G]$

- Linearized WI determines the thermodynamic self-energy Σ^T from $\Lambda\left[G^T\right]$
- 1P propagators G^T renormalized with Σ^T via Dyson eq.
- Symmetry of the self-energy Σ^T broken at the divergence in Bethe-Salpeter equation with $\Lambda[G^T]$

Both self-energies Σ^T and Σ
share the same critical behavior

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Physical (spectral) self-energy from Schwinger-Dyson equation

$$\Sigma_{\uparrow}(k) = \frac{U}{\beta N}\sum_{k'} G^T_{\downarrow}(k')\left[1 - \frac{1}{\beta N}\sum_{k''} G^T_{\downarrow}(k'')G^T_{\uparrow}(k+k'-k'') \times \Gamma^T_{\uparrow\downarrow}(k'', k; k'-k'')\right]$$

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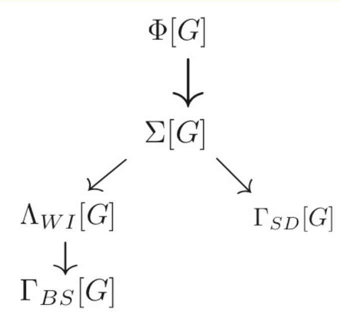
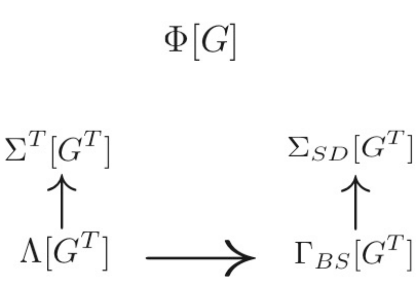
Standard vs. new approach

Baym-Kadanoff approach:
Luttinger-Ward functional Φ



single self-energy
two vertex functions
different criticaliities

Consistent criticality approach:
irreducible 2P vertex Λ



single two-particle vertex
two self-energies
(with the same criticality)
no thermodynamic potential

Single-impurity Anderson Model

Atom attached to metallic leads

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

Conduction electrons can be integrated out

$$\mathcal{Z} = \int \mathcal{D}\psi \mathcal{D}\psi^* \exp \left\{ \sum_n \psi^*_n \left[G_0(i\omega_n) \right]^{-1} \psi_n - U \int_0^{\beta} d\tau \, \widehat{n}^d_{\uparrow}(\tau) \widehat{n}^d_{\downarrow}(\tau) \right\}$$

Quantum criticality: Kondo effect - exponentially small scale $U \to \infty$

- Quasiparticle peak in the spectral function at FE (dynamics) $w_K = w \exp\{-\pi^2 U \rho_0 / 8\}$
- Saturation of the magnetic susceptibility (thermodynamics) at $T_K = \sqrt{U/\pi\rho_0} \exp\{-\pi^2 U \rho_0 / 8\}$

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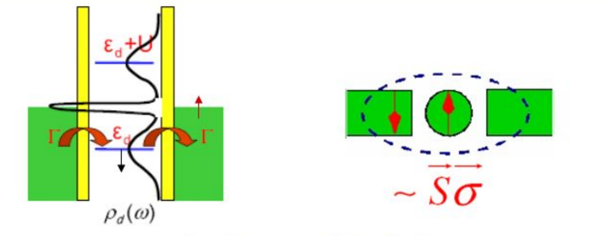

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Effective interaction approximation I

- Two-particle self-consistency from reduced parquet equations
  – static approximation on Λ
  – only diverging fluctuations dynamical

$$\Lambda^{eh}(i\omega_n, i\omega_{n'}; i\nu_m) \to \Lambda$$
$$\Gamma(i\omega_n, i\omega_{n'}; i\nu_m) \to \Gamma(i\nu_m)$$

- Effective interaction – generalization of HFA to strong coupling

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

with
$$\Psi_\sigma[\Lambda] = -\frac{\Lambda^2}{\beta}\sum_n \frac{\phi_\sigma(-i\omega_n)G_\sigma(i\omega_n)G_{-\sigma}(-i\omega_n)}{1 + \Lambda\phi_\sigma(-i\omega_n)}$$

where ($\Lambda = (\Lambda_\uparrow + \Lambda_\downarrow)/2$) and

$$\phi_\sigma(i\nu_m) = \frac{1}{\beta}\sum_n G_\sigma(i\omega_n)G_{-\sigma}(i\omega_n + i\nu_m)$$

Effective interaction approximation II

- Thermodynamic 1P Green function (auxiliary)

$$G_\sigma(\omega) = \int_{-\infty}^{\infty} \frac{d\epsilon \rho(\epsilon)}{\omega + i0^+ + \bar{\mu}_\sigma - \epsilon}$$

effective chemical potential $\bar{\mu}_\sigma = \mu + \sigma h - \frac{U - \Lambda}{2} - \Lambda n_\sigma^T$

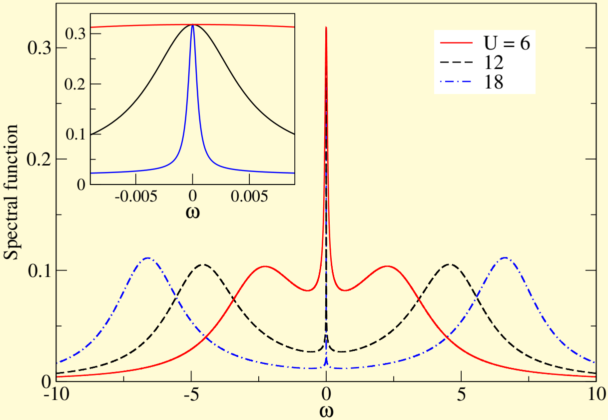
- Spectral (dynamical) self-energy (Schwinger-Dyson eq.)

$$\Sigma_\sigma^{sp}(\omega) = \frac{U\Lambda}{\pi} \int_{-\infty}^{0} dx \left\{ G_{-\sigma}(x+\omega) \Im \left[\frac{\phi_\sigma(x)}{1 + \Lambda \phi_\sigma(x)} \right] + \frac{\phi_\sigma^*(x-\omega)}{1 + \Lambda \phi_\sigma^*(x-\omega)} \Im G_{-\sigma}(x) \right\}$$

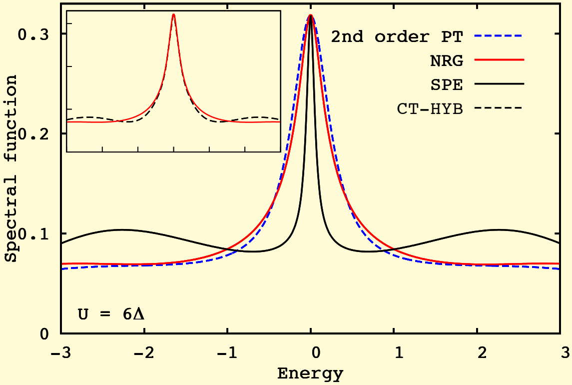
- 1P Green function (physical)

$$\mathcal{G}_\sigma(\omega) = \int_{-\infty}^{\infty} d\epsilon \frac{\rho(\epsilon)}{\omega + i0^+ + \mu + \sigma h - \epsilon - \frac{U}{2}\left(n - \sigma m^T\right) - \Sigma_\sigma^{sp}(k_n)}$$

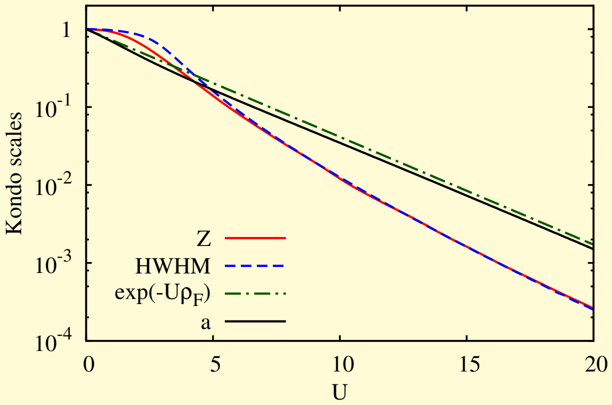
Spectral function of SIAM



Comparison with exact numetics

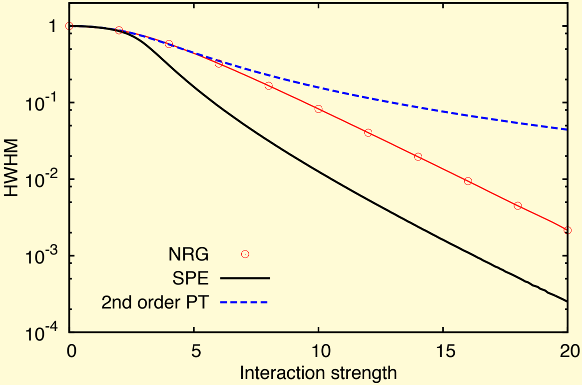


Exponential Kondo scales

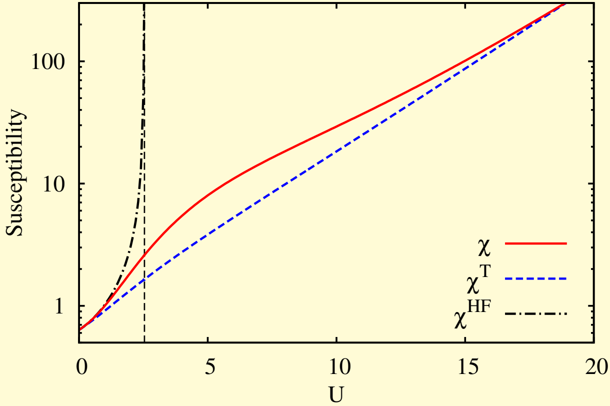


$$Z = [1 - \Sigma'(0)]^{-1}, \quad a = \Gamma(0)^{-1} = 1 - \lambda_0$$

Kondo scales compared with numerical simulations



Magnetic susceptibilities



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

Thermodynamic potential vs linearized WI I

1P approach: full 1P self-consistency

- 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

2P approach: Linearized Ward identity

- Vertex generating the approximation: $\Lambda_{\uparrow\downarrow}$
- Thermodynamic self-energy $\Sigma^{T}_{\sigma}(k) = \frac{1}{\beta N}\sum_{q}\Lambda(k,k;q)G_{-\sigma}(k+q)$
  – auxiliary to be used 1P propagators determining 2P functions
- Physical self-energy Σ 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