Genesis of the Curie-Weiss law in strongly correlated electron systems

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Mark's interests in quantum many-body

Common denominator: Numerical complexity

- Numerical solution of the Kondo problem
- *1P approach* – Self-energy in DMFT
- Beyond DMFT – Cluster expansion & real materials
- *2P approach* – Vertex functions & parquet equations

PHYSICAL REVIEW E **87**, 013311 (2013)

Solving the parquet equations for the Hubbard model beyond weak coupling

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One-particle vs. two-particle approaches

One-particle approach

- Generating Luttinger-Ward functional $\Phi[U, G]$
- Perturbation theory for the self-energy $\Sigma[U, G]$
- Conserving approximations – Baym-Kadanoff $G[\Sigma]$

Two-particle approach

- Perturbation theory for 2PIR vertex $\Lambda[I[U], G]$
- Bethe-Salpeter equation for full vertex $\Gamma[\Lambda, G]$
- Schwinger-Dyson equation for $\Sigma[\Gamma, G]$

2P approach much more complicated than 1P theory.

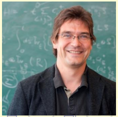
Recognition of two-particle approaches

When is 2P approach needed?
Renormalizations in response functions necessary.

- N. E. Bickers – parquet equations, numerical solution

- A. I. Lichtenstein – dual fermions, beyond DMFT

- K. Held – dynamical vertex, DMFT parquet equations



Magnetic response – insulators vs. metals

Spin magnetism

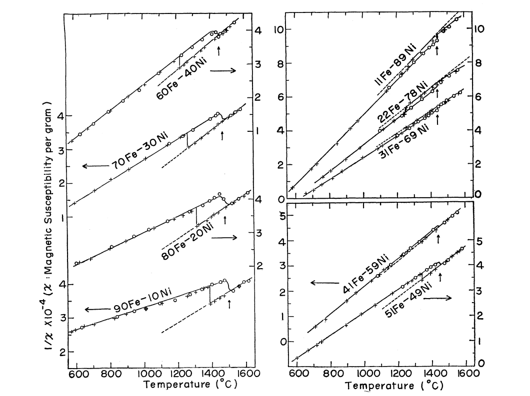
- Well defined local magnetic moment $g\mu_B\sqrt{S(S+1)}$
- Curie-Weiss susceptibility at low temperatures: $\chi = \frac{C}{T}$
- Curie constant: $C = ng^2\mu_B^2 S(S+1)/3k_B$

Itinerant magnetism

- Conduction electrons – no local moment
- Pauli paramagnet at low temperatures (Fermi liquid):
  $\chi_P = \mu_0\mu_B^2\nu(E_F)\left[1 - \frac{\pi^2}{12}\frac{k_B^2T^2}{E_F^2}\right]$
- No linear temperature dependence

Transition metals enigma

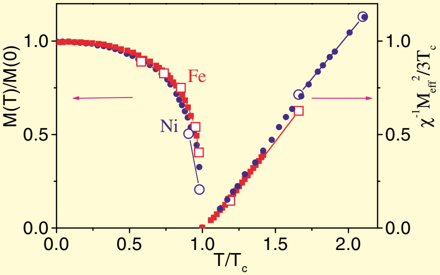
- Ferromagnetic critical temperature much lower than the mean-field value (Stoner)
- Curie-Weiss susceptibility above T_C



Y. Nagakawa, JPS J **12**, 700 (1957)

Metallic ferromagnetism

- Weak ferromagnets – Moriya theory (modified RPA)
- Strong coupling – DMFT ferromagnetic transition for Fe & Ni at high temperatures



A. I. Lichtenstein, M. Katsnelson, G. Kotliar, PRL **87**, 067205 (2001)

When can the Curie-Weiss law emerge at low temperatures in metals?

Generic Hamiltonians

Hubbard model

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

SIAM

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

Vertex functions & 2P approach

- Full 2P vertex

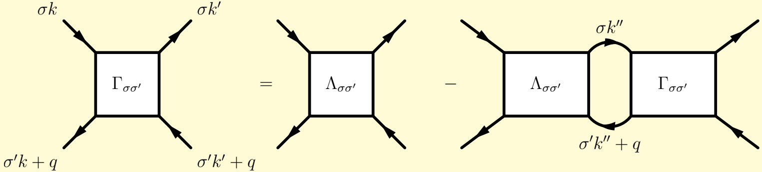
$$\Gamma_{\sigma\sigma'}(k,k';q) = \Lambda^{\alpha}_{\sigma\sigma'}(k,k';q) + \mathcal{K}^{\alpha}_{\sigma\sigma'}(k,k';q)$$

- 2P irreducible vertex in channel α: $\Lambda^{\alpha}_{\sigma\sigma'}(k,k';q)$
- 2P reducible vertex in channel α: $\mathcal{K}^{\alpha}_{\sigma\sigma'}(k,k';q)$
- Fully 2P irreducible vertex: $\mathcal{I}_{\sigma\sigma'}(k,k';q)$

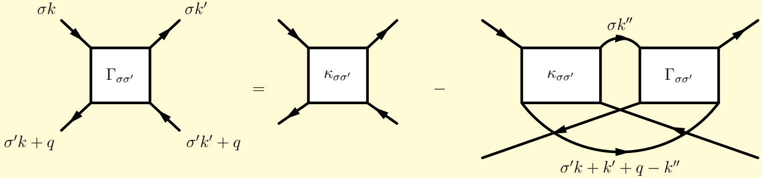
Bethe-Salpeter & parquet
equations to be aprroximated

Bethe-Salpeter equations I

- Electron-hole scattering channel (*eh*)

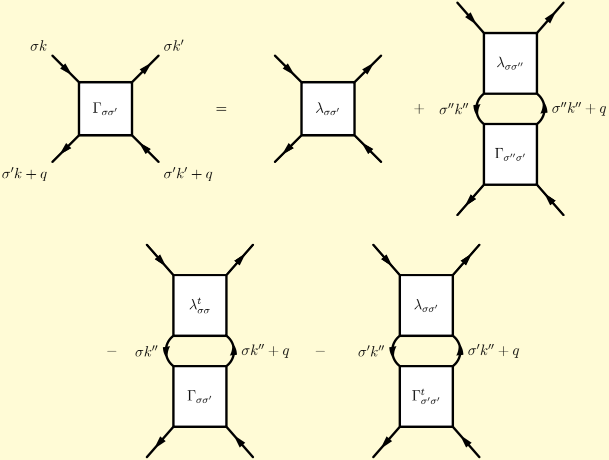


- Electron-electron scattering channel (*ee*)



Bethe-Salpeter equations II

- Vertical scattering channel (U)



Parquet equations

- Parquet equation with the reducible vertices

$$\Gamma = \mathcal{K}^{eh} + \mathcal{K}^{ee} + \mathcal{K}^{U} + \mathcal{I}$$

- Parquet equation for the irreducible vertices

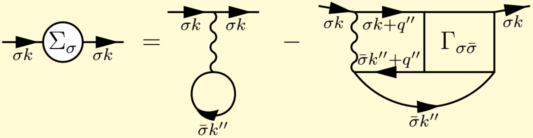
$$2\Gamma + \mathcal{I} = \Lambda^{eh} + \Lambda^{ee} + \Lambda^{U}$$

- Input to parquet equations: $\mathcal{I}(k, k'; q) = U$ and $G_\sigma(k)$
- Output: Self-consistently determined $\Lambda^{eh}, \Lambda^{ee}, \Lambda^{U}$

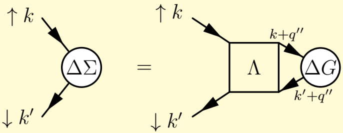
Renormalization of the interaction strength.
$\Rightarrow$ Only integrable singularities may exist!

SDE vs. WI in 2P approaches

- Schwinger-Dyson equation – from Luttinger-Ward



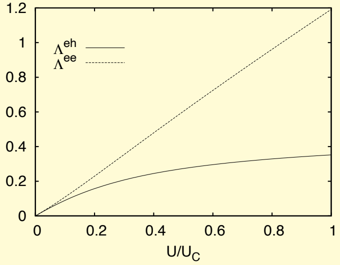
- *Ward identity* – additional consistency condition



They can never be satisfied simultaneously.

Problems of full parquet equations $(I = U)$

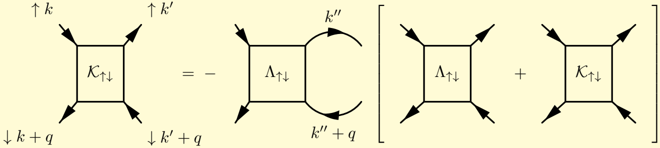
- Only in Matsubara frequencies
- No direct access to spectral properties
- No criticality – No Kondo behavior $(\Lambda^{eh} \nearrow U_c = U_{RPA})$



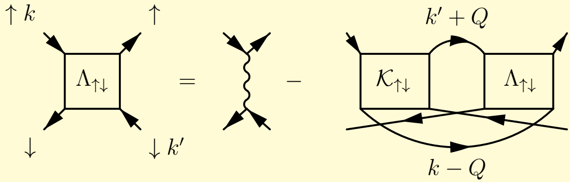
A balanced contribution from *ee* and *eh* multiple scatterings is needed.

Reduced parquet equations – definitions

- Full vertex decomposition: $\Gamma = \Lambda^{eh} + \mathcal{K}^{eh}$
- BSE in the *eh* channel – critical behavior



- Reduced BSE in the *ee* channel – *nonsingular* (screening of the interaction strength)



Reduced parquet equations – properties

Critical behavior from RPA with a renormalized interaction $U \to \Lambda$ extended to strong coupling

- *Analytic control of the critical behavior*
  – real frequencies & spectral properties
- No spurious transition to the magnetic state (pole in the eh BSE is nonintegrable)
- Anomalous & normal self-energies to reconcile WI & SDE

Qualitatively correct Kondo behavior

VJ, P. Zalom, V. Pokorný, and A. Klíč,
Phys. Rev. B **100**, 195114 (2019)

Mean-value approximation I

- *Static approximation* – decoupling of convolutions of fermionic Matsubara frequencies
- Self-consistent approximation for an effective interaction (renormalized RPA in eh channel)

$$\Lambda_{\uparrow\downarrow} = \frac{U}{1 - \Lambda_{\uparrow\downarrow}^2 \phi(0) X_{\uparrow\downarrow}(\Lambda_{\uparrow\downarrow})}$$

- eh bubble

$$\phi_{\uparrow\downarrow}(\Omega_+) = -\int_{-\infty}^{\infty} \frac{dx}{\pi} f(x) \left[G_\downarrow(x + \Omega_+) \Im G_\uparrow(x_+) \right.$$
$$\left. + \, G_\uparrow(x - \Omega_+) \Im G_\downarrow(x_+) \right]$$

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Mean-value approximation II

- Decoupling of integrals from ee channel: $X_{\uparrow\downarrow} = X_0 + \Delta X$
- Low-temperature contribution (*quantum fluctuations*)

$$X_0 = -\int_{-\infty}^{\infty} \frac{dx}{\pi} f(x) \Im \left[\frac{G_\uparrow(x_+) G_\downarrow(-x_+)}{1 + \Lambda_{\uparrow\downarrow}\phi_{\uparrow\downarrow}(-x_+)} \right]$$

- High-temperature contribution (*thermal fluctuations*)

$$\Delta X = \int_{-\infty}^{\infty} \frac{dx}{\pi} \frac{\Re\left[G_\uparrow(x_+) G_\downarrow(-x_+)\right]}{\sinh(\beta x)} \Im \left[\frac{1}{1 + \Lambda_{\uparrow\downarrow}\phi_{\uparrow\downarrow}(-x_+)} \right]$$

$$1/\sinh(\beta x) = f(x) + b(x)$$

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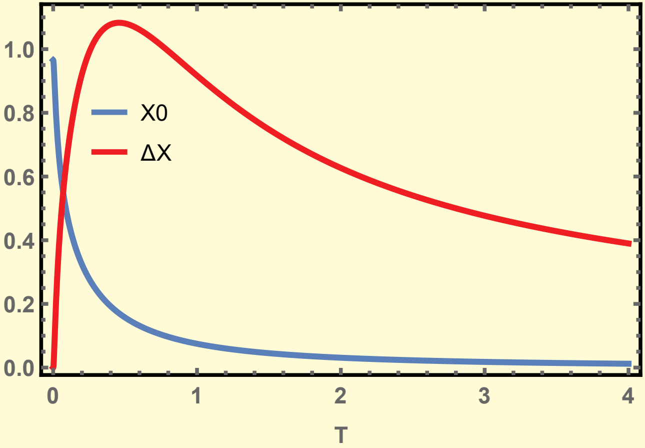
Thermal vs. quantum fluctuations



Kondo temperature: $X_0 = \Delta X$

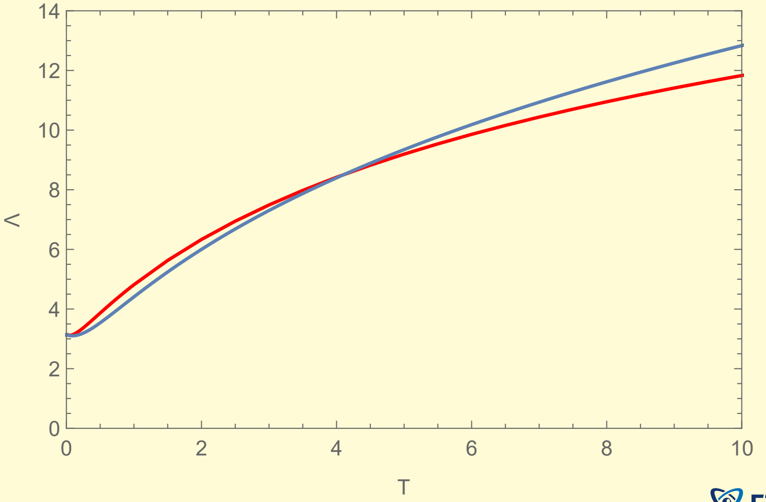
VJ and A. Klíč, arXiv:1909.02292 (2019)

Interpolating temperature scheme

$$\int_{-\infty}^{\infty} dx f(x) F(x) = \int_{0}^{\infty} dx \left[F_{+}(x) - \tanh\left(\frac{\beta x}{2}\right) F_{-}(x) \right]$$
$$\to \int_{0}^{\infty} dx F_{+}(x) - \frac{\beta}{2} \int_{0}^{2/\beta} dx\, x F_{-}(x) - \int_{2/\beta}^{\infty} dx F_{-}(x)\,,$$

$$\int_{-\infty}^{\infty} dx b(x) F(x) = - \int_{0}^{\infty} dx \left[F_{+}(x) - \mathrm{cotanh}\left(\frac{\beta x}{2}\right) F_{-}(x) \right]$$
$$\to - \int_{0}^{\infty} dx F_{+}(x) + \frac{2}{\beta} \int_{0}^{2/\beta} \frac{dx}{x} F_{-}(x) + \int_{2/\beta}^{\infty} dx F_{-}(x)$$

Exact vs. interpolating distributions



Critical (Kondo) regime

- Low-frequency approximation $1 + \Lambda\phi(\omega_+) \doteq a - i\omega D$
- Critical (Kondo) scale $a = 1 + \Lambda\phi(0) \to 0$
- Low-temperature limit $\beta \to \infty$

$$X_0 = \frac{1}{\pi D\Delta^2} \ln\left(\frac{D\Delta}{a}\right)$$

$$\Delta X = \frac{2}{\pi\Delta^2\beta a} \arctan\left(\frac{D}{\beta a}\right)$$

- Two regimes: $\Delta\beta a \gg 1$ & $\Delta\beta a \ll 1$

Zero temperature $(\Delta X = 0)$

- No critical point $a > 0$ for finite U
- Strong-coupling solution $(U \to \infty)$

$$\phi(0) = -\frac{1}{\pi\Delta}\,, \qquad D_0\Delta = \frac{\Lambda_0}{\pi\Delta}$$

$$X_0 = \frac{1}{\pi\Delta(D_0\Delta - a)^2}\left[D_0\Delta \ln\left(\frac{D_0\Delta}{a}\right) - D_0\Delta + a\right]$$

$$a = 1 - \frac{\Lambda_0}{\pi\Delta}\,, \qquad \Lambda_0 = \sqrt{\frac{U}{(1-a)X_0}}$$

- Exponential Kondo scale $a = \exp\{-U/\pi\Delta\}$

Temperature crossover $(\Delta X = X_0)$

- Low temperature limit $\beta a \to \infty$ (Fermi liquid)

$$\delta_T \phi(0) = \frac{4}{3\pi}\frac{1}{\beta^2\Delta^3}\,, \qquad \delta_T(D\Delta) = -\frac{8\Lambda_0}{3\pi\Delta}\frac{1}{\beta^2\Delta^2}$$

$$\delta_T X_0 = -\frac{2D_0\Delta}{3\pi\Delta}\frac{1}{\beta^2\Delta^2 a^2}\,, \quad \Delta X = \frac{2D_0\Delta}{\pi\Delta}\frac{1}{\beta^2\Delta^2 a^2}$$

- Above Kondo temperature $\beta a \ll 1$ and $\Delta X/X_0 > 1$

$$D = \frac{D_0}{\pi}\sqrt{\frac{U\beta a}{(1-a)}}\,, \qquad \Lambda = \Delta\sqrt{\frac{U\beta a}{(1-a)}}$$

$$(1-a)^3 = \phi(0)^2\Delta^2 U\beta a$$

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Genesis of the Curie-Weiss susceptibility I

- Magnetic susceptibility & Kondo scale

$$\chi \doteq -\frac{2\phi(0)}{1+\phi(0)\Lambda} = -\frac{2\phi(0)}{a}$$

- Critical behavior at low temperatures ($a \to 0$)

$$\frac{\chi}{\chi_0} = \frac{1}{T}\,\frac{U\Delta^2\beta^2}{4\pi^2 k_B}\arctan^2\left(\frac{2}{\Delta\beta}\right)$$

- Curie constant (temperature dependent):

$$C = U\Delta^2\beta^2\arctan^2\left(2/\Delta\beta\right)/4\pi^2 k_B$$

Genesis of the Curie-Weiss susceptibility II

- Limits on temperature for the Curie-Weiss behavior

$$\frac{U}{\pi^2} \gg k_B T \gg \frac{U}{\pi^2} e^{-U/\pi\Delta}$$

- Lower limit on the interaction strength

$$U \gg \frac{8\pi^2\Delta}{\beta\Delta \arctan\left(\frac{2}{\Delta\beta}\right)\left[\beta\Delta \arctan\left(\frac{2}{\Delta\beta}\right) + \frac{2\Delta^2\beta^2}{4+\Delta^2\beta^2}\right]}$$

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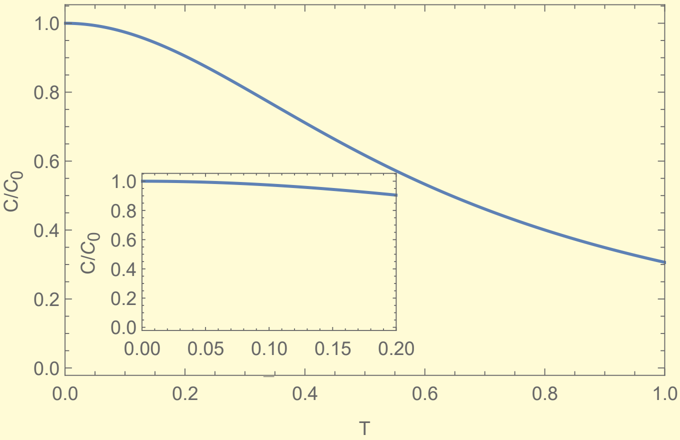
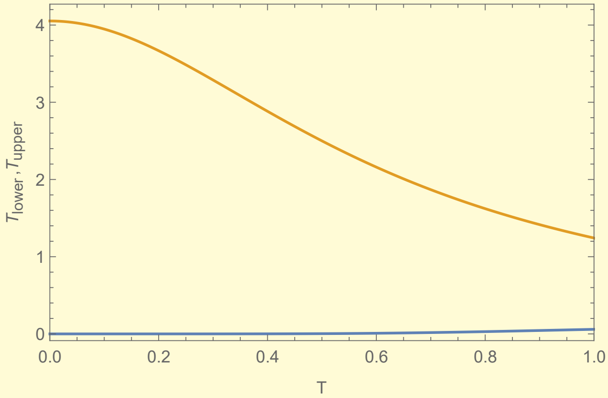
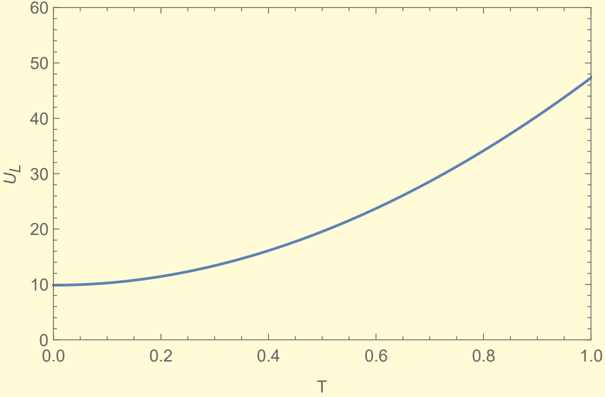
Curie constant – temperature dependence



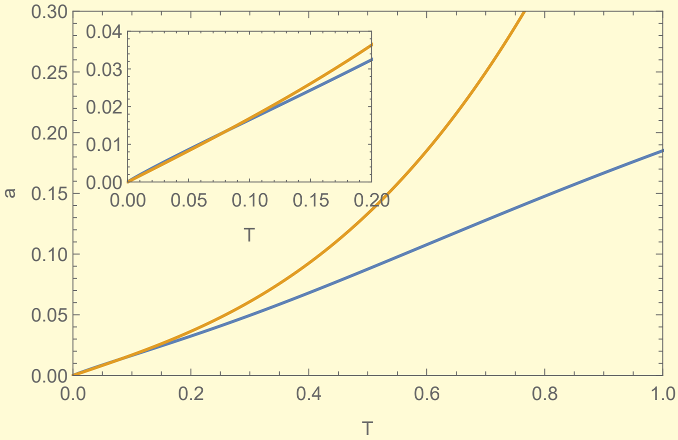
Temperature limits



Lower interaction limit



Curie-Weiss regime ($U = 60\Delta$)



Conclusions

Curie-Weiss law in metallic systems

- Only in strongly correlated metals
- *Low-temperatures* –quantum (dynamical) fluctuations
- Non-Fermi-liquid regime
- Critical region: $\Delta \beta a \ll 1$
- *Spatial fluctuations* –increase the Curie-Weiss temperature region

Renormalization of the interaction strength is a necessary condition!

Memory of Mark from Prague 2014 – RIP

Drive/Documents/Figures/FZU-L-CMYK.pdf Drive/Documents/Figures/FZU-L-CMYK.pdf