Curie-Weiss susceptibility in strongly correlated electron systems

Václav Janiš, Antonín Klíč, and Jiawei Yan
Institute of Physics, The Czech Academy of Sciences, Na Slovance 2, CZ-18221 Praha 8, Czech Republic
(Dated: June 22, 2020)

The genesis of the Curie-Weiss magnetic response observed in most transition metals that are Fermi liquids at low temperatures has been an enigma for decades and has not yet been fully explained from microscopic principles. We show on the single-impurity Anderson model how the quantum dynamics of strong electron correlations leads to the Curie-Weiss magnetic susceptibility sufficiently above the Kondo temperature. Such a behavior has not yet been demonstrated and can be observed only when the bare interaction is substantially screened (renormalized) and a balance between quantum and thermal fluctuations is kept. We set quantitative criteria for the existence of the Curie-Weiss law.

PACS numbers: 72.15.Qm, 75.20.Hr

Introduction

The Curie law for paramagnetic low-temperature susceptibility $\chi = C/T$ was derived by using the concept of local magnetic moments $[1]$. Later on, Weiss extended the Curie law to $\chi = C/(T - T_c)$ by introducing an interaction between atomic magnetic moments in order to cover transitions to the ferromagnetic state at $T_c$ $[2]$. This Curie-Weiss law well reproduces the magnetic response of insulating materials with fixed spin moments and no relevant charge fluctuations.

The metallic (itinerant) magnetism was first described by Bloch in terms of electron waves $[3]$ to which Stoner later added a mean-field description of electron correlations $[4]$. Such a static, weak-coupling theory with no local moments leads to Pauli paramagnetism at low temperatures and cannot account for the Curie-Weiss behavior when the critical temperature lies below the Fermi energy of the degenerate Fermi gas $[5]$.

A wave of efforts arose to understand the origin of the Curie-Weiss magnetic response in systems without the apparent presence of local magnetic moments $[6]$. First theory that qualitatively correctly reproduced the Curie-Weiss law in weak ferromagnetic metals was proposed by Moriya and collaborators. They introduced a self-consistent theory for the local magnetic susceptibility by including static spin fluctuations $[7][14]$. Although the theory was able to interpolate between the weak ferromagnetic and local moment pictures of itinerant magnetism, it missed the strong-coupling limit and did not provide a consistent thermodynamic and conserving approximation. Neither did it clearly explain the microscopic origin of the Curie-Weiss behavior.

The modern approach to strongly correlated electrons based on the dynamical mean-field theory (DMFT) was used to derive an implicit form of the Curie-Weiss law from local dynamical fluctuations $[15]$ and in combination with the local density functional also reproduced the critical behavior around the ferromagnetic transition of iron and nickel $[16]$. Although DMFT suggested that local dynamical fluctuations may be responsible for the Curie-Weiss law, the microscopic mechanism behind it has not been disclosed.

The reason for the failure of DMFT to identify the origin of the Curie-Weiss law is the lack of two-particle renormalization, that is, a self-consistent determination of the screening of the bare interaction. The simplest systematic theory with two-particle renormalizations is the parquet construction $[17][18]$. It is in its full generality, however, not analytically controllable and it does not reproduce the strong-coupling Kondo limit of the single-impurity Anderson model (SIAM) correctly $[19][20]$.

The way out from this trap of complexity with little analytic control is to reduce the parquet scheme. One has to keep its substantial part, the two-particle self-consistency, so that to interpolate qualitatively correctly between the weak- and strong-coupling regimes in a controlled way. One of the present authors has developed such an analytically controllable scheme qualitatively correctly interpolating between the weak and strong coupling in SIAM $[18][22][24]$. Since the parquet approach leads to Fermi liquid at low temperatures of SIAM, it is necessary to extend this approach properly to higher temperatures and beyond the Fermi-liquid regime. We succeeded to do so and introduced the Kondo temperature as a point at which the thermal fluctuations equal the quantum, zero-temperature ones and above which the Fermi-liquid description breaks down $[4]$.

The aim of this Letter is to disclose the origin of the Curie-Weiss law in strongly correlated electron systems. We show that local dynamical fluctuations due to strong electron correlations generate the Curie-Weiss magnetic response in metallic systems. The necessary constituents of the explanation of the Curie-Weiss law in itinerant systems are i) two-particle self-consistency renormalizing the interaction strength, ii) reliable interpolation between weak and strong coupling, and iii) balance between local quantum and thermal fluctuations. All these conditions...
are met in our reduced parquet scheme \[3\] \[4\]. We apply it to SIAM as the generic model to demonstrate how the dynamical forming of the local magnetic moment in strong coupling together with thermal fluctuations lead to a non-Fermi-liquid behavior and the Curie-Weiss susceptibility above the Kondo temperature. Our findings have the general relevance and hold for extended systems with critical magnetic fluctuations as well. We prove that the Curie-Weiss law is generally caused by local dynamical fluctuations while the spatial fluctuations affect the region of its validity.

Reduced parquet equations

The strong-coupling limit of the spin and charge symmetric state of SIAM at low temperatures (Kondo limit) stands for a model situation of the dynamical forming of the local magnetic moment. The spectral function displays a three-peak structure with an exponentially narrow central quasiparticle peak. The width of the central peak is proportional to the inverse lifetime of the pair of the electron with a given spin and the hole with the opposite spin. That is why the Kondo limit of SIAM is the simplest situation where the long-lived local magnetic moment can lead to the Curie-Weiss magnetic response.

The Hamiltonian of SIAM is

\[
\hat{H}_I = \sum_{k\sigma} \epsilon(k) c_{k\sigma}^\dagger c_{k\sigma} + E_d \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma} + \sum_{k\sigma} \left( V_k d_{\sigma}^\dagger c_{k\sigma} + V_k^* c_{k\sigma}^\dagger d_{\sigma} + U n_{\uparrow} n_{\downarrow} \right). \tag{1}
\]

The conduction electrons can be projected out, which leads to a band of energy states on the impurity. The effect of the conduction electrons can be approximated by a shift \( \Delta = 2\pi V^2 \rho_c \) of the imaginary part of the bare impurity propagator, where \( \rho_c \) is the density of states of the conduction electrons at the Fermi energy.

One has to directly approach the two-particle response and vertex functions when looking for a specific behavior of the magnetic susceptibility. We hence use the diagrammatic perturbation theory for the full two-particle vertex

\[
\Gamma(i\omega_n,i\omega_{n'};\nu_m) = \Lambda(i\omega_n,i\omega_{n'+m}) + \mathcal{K}(i\omega_n,i\omega_{n'};i\nu_m), \tag{2}
\]

where \( \Lambda \) and \( \mathcal{K} \) are irreducible and reducible vertices in a specific two-particle scattering channel, respectively. We use this decoupling in the singlet electron-hole channel with non-singular \( \Lambda \) and possibly singular \( \mathcal{K} \) in the strong-coupling limit.

We need to use a non-perturbative approximation for the irreducible vertex \( \Lambda \) to control the critical behavior of \( \mathcal{K} \). It will be achieved via a two-particle self-consistency of the parquet equations. Their complete form contains three coupled two-particle scattering channels and their solution can be reached only numerically in the Matsubara formalism \[21\] \[27\] \[30\]. The electron-hole singlet and triplet channels generate the same singularity in the two-particle vertex. We can hence neglect one of them without qualitatively affecting the critical behavior of the two-particle vertex. This is why we can resort only to two-channel parquet equations. Neither the three channel nor the two-channel parquet equations lead to to the Kondo behavior in their unrestricted form \[31\]. They also fail to guarantee that the strength of the electron repulsion is determined only by the present charge densities \[32\]. There is hence no urgent need to solve the parquet equations exactly, since they represent an approximate solution. That is why we introduced a reduced set of the two-channel parquet equations with the singlet electron-hole and electron-electron multiple scatterings. The corresponding Bethe-Salpeter equation in the electron-hole channel is graphically represented in Fig. 1. To reach the critical region of the weak-coupling pole of the random-phase approximation (RPA) in \( \mathcal{K} \) we reduce the Bethe-Salpeter equation for the irreducible vertex \( \Lambda \) in the electron-electron channel to an equation represented diagrammatically in Fig. 2 \[3\]. Only in this way the two-particle self-consistency is maintained and we can analytically continue the weak-coupling critical behavior to the strong-coupling Kondo regime.

Mean-value approximation

The reduced parquet equations represented in Figs. 1 \[2\] can be solved with unrestricted frequency dependence of the vertices only numerically in the Matsubara formalism. Since we are mainly interested in the crit-
tical behavior of the two-particle vertex we can simplify its frequency dependence. We can neglect all finite non-critical fluctuations and keep only the dominant critical dynamics of the reducible vertex $\mathcal{K}$. In the spirit of the mean-value theorem we can simplify the reduced parquet equations to a mean-field like self-consistent equation for the static irreducible vertex in the electron-hole channel $\Lambda$, an effective screened interaction, \[ \Lambda = \frac{U}{1 - \Lambda^2 \phi(0) X} \] where the electron-hole bubble is \[ \phi(\omega_+) = -\int_{-\infty}^{\infty} \frac{dx}{2\pi} f(x) \left[ G(x + \omega_+) + G_\sigma(x - \omega_+) \right] \times \Im G(x_+), \quad (4) \] and $\omega_+ = \omega + i0^+$ denotes the way the real axis is reached from the complex plane. The electron-electron multiple scatterings from vertex $\mathcal{K}$ contribute to the screening of the interaction strength via integral $X$ that we decompose into quantum and thermal contributions, $X_0$ and $\Delta X$, respectively

\[ X_0 = -\int_{-\infty}^{\infty} \frac{dx}{\pi} \Im [G(x_+) G(-x_-) \frac{G(-x_+)}{1 + \Lambda \phi(-x_-)}], \quad (5a) \]

\[ \Delta X = \int_{-\infty}^{\infty} \frac{dx}{\pi} \Re \left[ G_\sigma(x_+)^2 G_{-\sigma}(-x_-)^2 \sinh(\beta x) \right] \times \Im \left[ \frac{1}{1 + \Lambda \phi(-x_-)} \right]. \quad (5b) \]

We used an equality $f(x) + b(x) = 1/\sinh(\beta x)$. We straightforwardly used analytic continuations of summations over Matsubara frequencies to spectral integrals with Fermi, $f(x) = 1/(e^{\beta x} + 1)$ and Bose, $b(x) = 1/(e^{\beta x} - 1)$, distributions. We use the bare Green function of SIAM $G(\omega \pm) = 1/(\omega - E_F - U n/2 \pm i \Delta)$, where $n$ is the charge density. We showed that we reproduce the exact Kondo limit qualitatively correctly with this propagator [2, 3]. The Kondo strong-coupling criticality is manifested at half filling, that is $n = 1$ and $E_F = -U/2$, to which we resort.

The resulting approximation with the renormalized interaction $\Lambda$ has a well established analytic structure. It is easily numerically solvable for the whole range of the interaction strength and leads to thermodynamic and spectral properties defined analogously as in RPA. The major difference to RPA is that the renormalized vertex $\Lambda$ significantly decreases the critical interaction of RPA, $U_c = \pi \Delta$, and never crosses it in SIAM. Its strong-coupling asymptotics at zero temperature is $\Lambda = \pi \Delta \left[ 1 - \exp\left(-U/\pi \Delta \right) \right]$ [33]. This approximation also qualitatively correctly interpolates between the low and high temperatures [34]. Although the effective interaction $\Lambda$ is a constant, it was not derived from a static approximation. It can be seen from Eq. (3) where the value of $\Lambda$ is determined from the zero-frequency limit of the dynamical electron-hole bubble $\phi(\omega)$. The dynamical part of this bubble significantly renormalizes the multiple scatterings in the electron-electron scattering channel in integral $X$ from Eq. (5). That is why this approximation contains the dominant dynamical fluctuations in the critical region of the singularity of the full two-particle vertex.

The static thermodynamic susceptibility in this approximation has a simple, mean-field-like representation

\[ \chi = -\frac{2 \phi(0)}{\mu_B \mu_0} \left[ 1 + \frac{\pi \Delta}{U X} \right], \quad (6) \]

where $\mu_0$ is the permeability of vacuum and $\mu_B$ is the Bohr magneton. We introduce a dimensionless Kondo scale $a$, the denominator of the susceptibility that measures the distance from the critical point at which it would vanish. The equations for the Kondo scale and the effective interaction from Eq. (3) then are

\[ a = 1 + \phi(0) \Lambda, \quad (7a) \]

\[ \Lambda = \frac{1}{2X(1 - a)} \left[ \sqrt{1 + 4(1 - a)UX} - 1 \right]. \quad (7b) \]

The approximation defined by Eqs. (7) with Eqs. (4)-(5) leads to a Fermi liquid at low temperatures as explicitly demonstrated in the Supplemental Material (SM) [33]. The Curie-Weiss susceptibility may hence be observed only at higher temperatures. The full numerical solution of these equations at non-zero temperatures is unsuitable for identifying the microscopic origin of the Curie-Weiss magnetic susceptibility. To find it with its limits of validity we approximate the integrals with the Fermi and Bose distribution functions via simple algebraic forms in low ($|\omega| < 2/\beta$) and high ($|\omega| > 2/\beta$) frequency regions, see Eqs. (4) in [33]. We obtain explicit expressions with this approximation for all the needed frequency integrals. The electron-hole bubble explicitly is

\[ \phi(0) = -\frac{\beta}{2\pi} \arctan \left( \frac{2}{\beta \Delta} \right). \quad (8) \]

We further approximate the dynamical electron-hole bubble via its low-frequency asymptotics and use $1 + \Lambda \phi(\omega_+) = a - i\omega A/\Delta$ to obtain also explicit representations for the X-integrals. This approximation is justified in the critical region of the Kondo limit, $a \ll 1$. Using the same simplification of the frequency integral with the Fermi function we obtain a self-consistent equation for the expansion parameter $A$, see [33].

\[ A = \frac{\Lambda}{4\pi \Delta} \left[ \beta \Delta \arctan \left( \frac{2}{\beta \Delta} \right) + \frac{2\beta^2 \Delta^2}{4 + \beta^2 \Delta^2} \right]. \quad (9) \]
All the two-particle parameters used in this approximation, $\Lambda$, $A$, and $X$ are functions of the Kondo scale $a$ determined at the end from Eq. (10a). Its temperature dependence is decisive for the determination of the Curie-Weiss behavior. Both the temperature and the Kondo scale must be small. The full expressions for the integrals $X_0$ and $\Delta X$ are given in [33]. They reduce in the Kondo limit $a \to 0$ and in the leading order of $T \to 0$ to

$$\Delta X \simeq 2 \pi a \Delta^2 \arctan \left( \frac{A}{\beta a \Delta} \right), \quad (10a)$$

$$X_0 \simeq \frac{1}{\pi A \Delta} \ln \left( \frac{A}{a} \right). \quad (10b)$$

The low-temperature asymptotics in the Kondo limit depends on the behavior of parameter $A/\beta a \Delta$. It is evident from Eq. (10a) that the Fermi-liquid regime corresponds to the low-temperature limit $\beta a \Delta \gg A$ with $A \to 1$ for $\beta \Delta \to \infty$. More interesting is, however, the other limit $\beta a \Delta \ll A$ that may lead to a linear dependence of the Kondo scale on temperature and to the Curie-Weiss behavior. The Kondo scale at non-zero temperatures becomes small and $\beta a \Delta \ll 1$ only if

$$U \gg \frac{8 \pi \Delta}{\beta \Delta \arctan \left( \frac{2}{\beta \Delta} \right)} \left[ \beta \Delta \arctan \left( \frac{2}{\beta \Delta} \right) + \frac{2 \beta \Delta^2}{4 + \beta^2 \Delta^2} \right], \quad (11)$$

as derived in [33]. The lower bound $U_L$ on the interaction strength increases significantly with increasing temperature as shown in Fig. 3.

The low-temperature magnetic susceptibility above the Kondo temperature can in this regime be approximated by an asymptotic formula, [33],

$$\frac{X}{\mu_0 \mu_B^2} = \frac{U \beta^3 \Delta^2}{4 \pi^4 k_B} \arctan^3 \left( \frac{2}{\beta \Delta} \right) \frac{1}{T + \frac{2 \beta \Delta^2}{4 \pi^2 k_B} \arctan^2 \left( \frac{2}{\beta \Delta} \right) U e^{-U/\pi \Delta}, \quad (12)$$

which reduces to the Curie-Weiss form if the effective local moment $C = \mu_0 \mu_B^2 \Delta^2 \arctan^3 \left( \frac{2}{\beta \Delta} \right) / 4 \pi^3 k_B$ only weakly depends on temperature. It is the case if $\beta \Delta \gg 2$, which defines the order of the upper limit on the validity of the Curie-Weiss law. The lower bound for the validity of the Curie-Weiss law is the Kondo temperature $T_K$ defined from equality of quantum and thermal fluctuations expressed by an equation $\Delta X = X_0$ [3]. The magnetic susceptibility is then well approximated by the Curie-Weiss law if $\Delta X \gg X_0$, which sets the lower temperature bound. The order-of-magnitude temperature bounds on the validity of the Curie-Weiss law in SIAM are

$$\frac{\Delta}{2} \gg k_B T \gg \frac{U}{\pi^2} e^{-U/\pi \Delta}. \quad (13)$$

The Curie-Weiss susceptibility exists only in strongly correlated systems and sufficiently above the Kondo temperature but still at low temperatures, small fractions of the bandwidth, as demonstrated in Fig. 4. We can see a very good agreement of the asymptotic expression from Eq. (12) and the full numerical solution for interactions $U > 20 \Delta$. Although we may observe almost linear temperature dependence of the inverse susceptibility also at rather high temperatures, its origin there is no longer in the critical behavior of the magnetic transition at which the Kondo scale vanishes, $a = 0$.

**Extended systems**

The reduced parquet approximation can straightforwardly be extended to lattice systems. The dynamics of the two-particle functions is then determined not only by frequency but also momentum fluctuations. That is, the
The susceptibility transforms to $1 + \Lambda$ dependent, $\omega$ from constant $C$ in a interval of temperatures on which the effective Curie magnet is inversely proportional to the spatial correlation length $\xi$ critical point. The Kondo scale in extended systems is generalized Kondo scale $\Lambda$ which is the magnetic critical and $T_c$. The Curie-Weiss behavior in metallic systems and magnetic transitions with $a = 0$ at non-zero temperatures may occur in dimensions $d > 2$. The Curie-Weiss behavior can be observed on an interval of temperatures on which the effective Curie constant $C_d$ does not change much from its value at the critical point. The Kondo scale in extended systems is inversely proportional to the spatial correlation length $\xi$, $a = \Delta^2/\xi^2$. The results for extended systems are compatible with the Mermin-Wagner theorem [34]. No long-range order exists for dimensions $d = 1, 2$, which makes the reduced parquet equations a suitable and affordable approximation for studying critical instabilities in realistic systems.

Conclusions

There is no transition to the magnetic state in SIAM and that is why the Curie-Weiss law sets only for extremely strong interaction strengths, above the Kondo temperature, and beyond the Fermi-liquid regime. It is also the reason why the Curie-Weiss law has not yet been demonstrated in SIAM. The strong-coupling Kondo limit of SIAM is, however, a paradigm for the explanation of the Curie-Weiss magnetic response in metals. Our analysis has therefore a general significance beyond the impurity models. We can draw general conclusions if we appropriately interpret the scales used in SIAM. The Kondo scale is generalized to $a_c = (T - T_c)/T_F$, where $T_c$ is the magnetic critical and $T_F$ the Fermi temperature. Further on, $\Delta \sim k_BT_F$ and $A \sim \Delta_N$ with $N_F$ the density of states at the Fermi energy. The critical magnetic response in metallic systems is controlled by the generalized Kondo scale $a_c$. The smaller the ratio $T_c/T_F$ is, the longer is the temperature interval with the Curie-Weiss susceptibility above the critical temperature. The Curie constant $C$ is proportional to the bare interaction $U$ while the critical temperature $T_c$ to the renormalized vertex $\Lambda$. The Curie-Weiss behavior in metallic systems is hence most pronounced for broad-band systems with strong but significantly screened electron interaction.

ACKNOWLEDGMENT

The research was supported by Grant No. 19-13525S of the Czech Science Foundation.

[1] P. Langevin, Annales De Chimie Et De Physique 5, 70 (1905).
[2] P. Weiss, J. Phys. Theor. Appl. 6, 661 (1907).
[3] F. Bloch, Zeitschrift Fur Physik 57, 545 (1929).
[4] E. C. Stoner, Proceedings of the Royal Society of London Series a-Mathematical and Physical Sciences 165, 0372 (1938).
[5] Y. Nakagawa, Journal of the Physical Society of Japan 12, 700 (1957).
[6] C. Herring, Exchange interactions among itinerant electrons (Academic Press, New York, 1966), vol. 4 of Magnetism, chap. 9.
[7] T. Moriya and A. Kawabata, Journal of the Physical Society of Japan 34, 639 (1973).
[8] K. Ueda and T. Moriya, Journal of the Physical Society of Japan 39, 605 (1975).
[9] T. Moriya and Y. Takahashi, Journal of the Physical Society of Japan 45, 397 (1978).
[10] Y. Takahashi and T. Moriya, Journal of the Physical Society of Japan 46, 1451 (1979).
[11] T. Moriya, Spin Fluctuations in Itinerant Electron Magnetism, vol. 56 of Springer Series in Solid-State Sciences (Springer Verlag, Berlin Heidelberg, 1985).
[12] Y. Takahashi, Journal of the Physical Society of Japan 55, 3553 (1986).
[13] T. Moriya, Journal of Magnetism and Magnetic Materials 100, 261 (1991).
[14] T. Moriya, Proceedings of the Japan Academy Series B-Physical and Biological Sciences 82, 1 (2006).
[15] K. Byczuk and D. Vollhardt, Physical Review B 65, 134433 (2002).
[16] A. I. Lichtenstein, M. I. Katsnelson, and G. Kotliar, Physical Review Letters 87, 067205 (2001).
[17] C. D. Dominicis, Journal of Mathematical Physics 3, 983 (1962).
[18] C. D. Dominicis, Journal of Mathematical Physics 4, 255 (1963).
[19] N. E. Bickers and S. R. White, Physical Review B 43, 8044 (1991).
[20] N. Bickers, International Journal of Modern Physics B 05, 253 (1991).
[21] V. Janiš and P. Augustinský, Physical Review B 75, 165108 (2007).
[22] V. Janiš and P. Augustinský, Physical Review B 77, 085106 (2008).
[23] V. Janiš, A. Kauch, and V. Pokorný, Physical Review B 95, 045108 (2017).
[24] V. Janiš, V. Pokorný, and A. Kauch, Physical Review B 95, 165113 (2017).
[25] V. Janiš, P. Zalom, V. Pokorný, and A. Klíč, Physical Review B 100, 195114 (2019).
[26] V. Janiš and A. Klíč, Japan Physical Society Conference Proceedings 30, 011124 (2020).
[27] S. X. Yang, H. Fotso, J. Liu, T. A. Maier, K. Tomko, E. F. D’Azevedo, R. T. Scalettar, T. Pruschke, and M. Jarrell, Physical Review E 80, 046706 (2009).
[28] G. Li, N. Wentzell, P. Pudleiner, P. Thunström, and K. Held, Physical Review B 93, 165103 (2016).
[29] G. Li, A. Kauch, P. Pudleiner, and K. Held, Computer Physics Communications 241, 146 (2019).
[30] C. J. Eckhardt, C. Honerkamp, K. Held, and A. Kauch, Physical Review B 101, 155104 (2020).
[31] V. Janiš, Condens. Matter Physics 9, 499 (2006).
[32] V. Janiš, Journal of Physics: Condensed Matter 10, 2915 (1998).
[33] V. Janiš, A. Klíč, and J. Yan, *Curie-weiss susceptibility in strongly correlated electron systems - supplemental material.*
[34] N. D. Mermin and H. Wagner, Physical Review Letters 17, 1133 (1966).
Curie-Weiss susceptibility in strongly correlated electron systems
Supplementary Material

Václav Janiš*, Antonín Klíč, and Jiawei Yan
Institute of Physics, The Czech Academy of Sciences, Na Slovance 2, CZ-18221 Praha 8, Czech Republic
(Dated: June 22, 2020)

Low-frequency approximation

We need to evaluate integrals in Eqs. (4) and (5) of the main text. We use the low-frequency approximation in calculating the electron-hole bubble \( \phi(\omega_{\pm}) \) in the Kondo regime, where the Kondo scale \( a = 1 + \phi(0) \Delta \ll 1 \). We then replace \( 1 + \phi(\omega_{\pm}) \Delta \approx a + i \Delta \omega / \Delta \). Such an approximation is well justified in the critical region of a singularity for \( a = 0 \) with the pole in the Bethe-Salpeter equation in the electron-hole channel.

We denote
\[
g = \phi(0) = \int_0^\infty \frac{dx}{\pi} \frac{\tanh (\beta x / 2)}{2} \Im [G(x_{\pm})^2] . \quad \text{S1}
\]
We use the bare Green function \( G(x_{\pm})=1/(i x + i \Delta) \) to evaluate the integrals defining the parameters to be determined in the reduced parquet equations. We showed in our previous publications that the unperturbed Green function used in the perturbation expansion gives the best and qualitatively correct estimate for the Kondo strong-coupling asymptotics in SIAM [S1][S3]. The results for the \( X \) integrals from Eqs. (5) of the main text in the low-frequency approximation \( 1 + \Lambda \phi(\omega_{\pm}) \equiv a - i \omega A / \Delta \) are
\[
X_0 = - \int_0^\infty \frac{dx}{\pi} \frac{\tanh (\beta x / 2)}{2} \Re [G(x_{\pm})^2] A r + \Im [G(x_{\pm})^2] a / a^2 + A^2 x^2 / \Delta^2 . \quad \text{S2a}
\]
and
\[
A = - \frac{2A}{\pi} \int_0^\infty \frac{dx}{\sinh (\beta x / 2)} a^2 / A^2 x^2 / \Delta^2 . \quad \text{S2b}
\]
The expansion parameter of this low-frequency approximation is
\[
A = \frac{\beta \Lambda \Delta}{2\pi} \int_0^\infty \frac{dx}{\cosh^2 (\beta x / 2)} |G(x_{\pm})|^2 . \quad \text{S3}
\]
These integrals are the input for the self-consistent Eqs. (7) of the main text.

Temperature behavior

The integrals to be evaluated contain trigonometric functions preventing us from obtaining explicit analytic results. We can use interpolation formulas with linear fractions replacing the spectral functions in the regions of low and high frequencies. We use the following approximation
\[
\int_{-\infty}^\infty dx f(x) F_x(x) = \int_0^\infty dx [F_+(x) - \tanh (\beta x / 2) F_-(x)] \rightarrow \int_0^\infty dx F_+(x) - \frac{\beta}{2} \int_0^{\infty} \frac{dx}{\sinh x} F_-(x) - \int_0^{\infty} \frac{dx}{\sinh x} F_-(x) , \quad \text{S4a}
\]
for the Fermi integral and
\[
\int_{-\infty}^\infty dx b(x) F_x(x) = - \int_0^\infty dx [F_+(x) - \cotanh (\beta x / 2) F_-(x)] \rightarrow - \int_0^\infty dx F_+(x) + \frac{2}{\beta} \int_0^{\infty} \frac{dx}{\sinh x} F_-(x) + \int_0^{\infty} \frac{dx}{\sinh x} F_-(x) , \quad \text{S4b}
\]
for the Bose integrals. We introduced symmetric and antisymmetric functions, \( F_+(x) = \frac{1}{2} [F(x) + F(-x)] \) and \( F_-(x) = \frac{1}{2} [F(x) - F(-x)] \). These approximate formulas well reproduce the integrals with the Fermi and Bose distribution functions from low to high temperatures, see Fig. [S1].

The explicit approximate analytic expressions for the integrals in Eqs. (S1)-(S3) are
\[
g \doteq \frac{2\pi}{\beta} \arctan \left( \frac{2}{\beta \Delta} \right) , \quad \text{S5a}
\]
\[
A \doteq \frac{A}{4\pi^2 \Delta} \left[ \beta \Delta \arctan \left( \frac{2}{\beta \Delta} \right) + \frac{2\beta^2 \Delta^2}{4 + 2\beta^2 \Delta^2} \right] , \quad \text{S5b}
\]
\[
X_0 = \frac{1}{2\pi (A - a)} \left\{ \frac{A}{\Delta} \ln \frac{A^2 (4 + \beta^2 \Delta^2)}{4A^2 + \beta^2 a^2 \Delta^2} + \beta a \left[ \arctan \left( \frac{2}{\beta \Delta} \right) - \arctan \left( \frac{2A}{\beta a \Delta} \right) \right] \right\} \quad \text{S6a}
\]
and
\[
\Delta X = \frac{2A}{\pi \Delta (A^2 - a^2)} \left[ \frac{A^2 + a^2}{A^2 - a^2} \frac{A}{\beta a \Delta} \arctan \left( \frac{A}{\beta a \Delta} \right) \right] - \frac{2A^2}{A^2 - a^2} \frac{1}{\beta \Delta} \arctan \left( \frac{1}{\beta \Delta} \right) - \frac{1}{1 + 2\beta^2 \Delta^2} , \quad \text{S6b}
\]
The algebraic approximation for the Fermi and Bose distribution functions used to reach the above analytic expressions proves to be very accurate, in particular in the Kondo limit \( a \ll 1 \) as shown in Fig. S2 for integrals \( X_0 \) and \( \Delta X \).

We are interested in the low-temperature, \( \beta \Delta \to \infty \), together with the strong-coupling, \( a \to 0 \), limit. It follows from the above expressions that the quantity deciding how this limit looks like is \( \beta a \Delta \). We find two asymptotic regimes, \( \beta a \Delta \to \infty \) and \( \beta a \Delta \to 0 \). The former limit leads to Fermi liquid, while the latter to a magnetic criticality with the Curie-Weiss susceptibility. The Fermi liquid is recovered for \( \Delta X \ll X_0 \) while the Curie-Weiss for the opposite limit, \( \Delta X \gg X_0 \) for sufficiently low temperatures.

**Fermi-liquid regime**

The zero-temperature solution in the analytic low-frequency approximation is

\[
g_0 = -\frac{1}{\pi \Delta}, \quad \Lambda_0 = \frac{\Lambda_0}{\pi \Delta}, \quad X_0 = \frac{1}{(\Lambda_0 - \pi a \Delta)^2} \left[ \Lambda_0 \ln \left( \frac{\Lambda_0}{\pi a \Delta} \right) - (\Lambda_0 - \pi a \Delta) \right], \quad \Lambda_0 = \frac{1}{2(1-a)X_0} \left[ \sqrt{1 + 4(1-a)U X_0} - 1 \right], \quad a_0 = 1 - \frac{\Lambda_0}{\pi \Delta};
\]

\( g, X = X_0 + \Delta X, A, a, \Lambda \). We obtain

\[
\delta_T g = \frac{4}{3} \frac{1}{\beta^2 \Delta^3}, \quad \delta_T A = -8 \left. A_0 \right| \frac{1}{3 \pi \Delta \beta^2 \Delta^2}, \quad \delta_T X = -4 (\Lambda_0 - \pi a \Delta) \frac{1}{3 \pi^2 \Delta^2} \beta^2 \Delta^2 a^2.
\]

To add the temperature dependence of the self-consistent parameters we need to evaluate partial derivatives, all taken at \( T = 0 \). We use the derivatives with respect to the Kondo scale \( a \) and the effective interaction \( A \). Parameter \( A \) can be determined explicitly and does not enter the self-consistency at low-temperatures. The derivatives of the \( X \) integral are

\[
\frac{\delta X_0}{\delta a} = \frac{\pi \Delta}{(\Lambda_0 - \pi a \Delta)^3} \times \frac{\pi a \Delta}{\Lambda_0 \ln \left( \frac{\Lambda_0}{\pi a \Delta} \right) - (\Lambda_0 - \pi a \Delta)^2}, \quad \frac{\delta X_0}{\delta \Lambda_0} = -\frac{1}{(\Lambda_0 - \pi a \Delta)^3} \times \left[ (\Lambda_0 - \pi a \Delta) \ln \left( \frac{\Lambda_0}{\pi a \Delta} \right) - 2(\Lambda_0 - \pi a \Delta) \right].
\]

We will also need the derivatives of the right-hand side of Eq. (7b) of the main text with respect to parameters \( a \) and \( X \),

\[
\frac{\delta \Lambda}{\delta X} = \frac{1}{X_0} \frac{U - \Lambda_0}{\sqrt{1 + 4 (1-a_0) U X_0}}, \quad \frac{\delta \Lambda}{\delta a} = -\frac{X_0 \delta \Lambda}{1 - a_0 \delta X};
\]

The total temperature variations of \( A \) and the Kondo scale \( a \) are fully determined by the non-self-consistent
We determine the variation of the effective interaction by putting together the above partial derivatives. The result is

\[
\frac{\delta \Lambda}{\delta X} = \Lambda_0 \delta_T g + g_0 \delta \Lambda. \tag{S12}
\]

The temperature variation of the effective interaction is positive, that is, it increases with temperature and the renormalization of the bare interaction decreases. In the Kondo strong-coupling limit \( U \to \infty \) and \( a \to 0 \) we obtain

\[
\delta \Lambda = \frac{4 \pi}{3 \Delta} e^{U/\pi \Delta} k_B T^2. \tag{S14}
\]

The effective interaction is, however, not a strictly monotonic function of temperature. Its slope changes around the Kondo temperature at which the thermal fluctuations start to dominate and the low-temperature Fermi-liquid behavior goes over into the Curie-Weiss regime. If we use a dimensionless parameter

\[
\alpha = \frac{1}{2} \left[ \frac{\Delta \beta}{2} \arctan \left( \frac{2}{\beta \Delta} \right) + \frac{\beta^2 - \Delta^2}{4 + \beta^2 \Delta^2} \right], \tag{S15}
\]

then \( A = \Lambda \alpha/\pi \Delta \) and the \( X \) integrals in this limit are

\[
X_0 = \frac{1}{\Lambda \alpha} \ln \left( \frac{\Lambda \alpha}{\pi a \Delta} \right), \tag{S16a}
\]

\[
\Delta X = \frac{2}{\pi \beta a \Delta^2} \arctan \left( \frac{\Lambda \alpha}{\beta \alpha \Delta^2} \right). \tag{S16b}
\]

Assuming further \( \Lambda \alpha \gg \pi b a \Delta^2 \) we obtain

\[
X = X_0 + \Delta X = \frac{1}{\Lambda \alpha} \ln \left( \frac{\Lambda \alpha}{\pi a \Delta} \right) + \frac{1}{\beta a \Delta^2}. \tag{S18}
\]

The equations for the effective interaction and the Kondo scale \( a \ll 1 \) reduce to

\[
\Lambda = \sqrt{\frac{U}{X}}, \tag{S19}
\]

\[
1 = \frac{U g^2}{X}. \tag{S20}
\]

We determine \( X \) and \( \Lambda \) from the above equations and are left with a single equation for the Kondo scale

\[
U g^2 = \frac{|g|}{\alpha} \ln \left( \frac{\alpha}{a |g| \Delta} \right) + \frac{1}{\beta a \Delta^2}. \tag{S21}
\]

The second term on the right-hand side of this equation should dominate the first one to reach the Curie-Weiss regime. That is,

\[
\frac{|g|}{\alpha} \ln \left( \frac{\alpha}{a |g| \Delta} \right) \ll \frac{1}{\beta a \Delta^2} = U g^2. \tag{S22}
\]
The solution for the small Kondo scale in the Curie-Weiss regime then is
\[ a = \frac{k_B T}{U|g|^2 \Delta^2}. \] (S23)

The conditions to be fulfilled to reach the Curie-Weiss regime are Eqs. (S17) and (S22). Inserting the solution for the Kondo scale into Eq. (S17) we obtain an upper order-of-magnitude bound on temperature
\[ k_B T \ll \frac{1}{\pi} U|g| |\alpha|. \] (S24)

We obtain the lower temperature bound for the Curie-Weiss regime from Eq. (S22) by using the solution for the Kondo scale from Eq. (S23)
\[ k_B T \gg \frac{1}{\pi} U|g| |\alpha| \Delta e^{-U/|g|^2}. \] (S25)

Next, we have to satisfy the condition for criticality in the Kondo regime, \( a \to 0 \). The Kondo scale from quantum fluctuations and integral \( X_0 \) is
\[ a > a_Q = \frac{\alpha}{|g|^2} e^{-U/|g|^2}. \] (S26)

It is the lower bound for the Kondo scale at non-zero temperatures. It is small only in the strong-coupling when the exponent on the right-hand side is sufficiently big, namely
\[ U \gg \frac{1}{|g|^2} \], (S27)

which is just Eq. (11) of the main text. The boundaries for the linear temperature dependence of the Kondo scale \( a \) restrict the Curie-Weiss region to a rather narrow interval and for very strong interactions as shown in Fig. S3.

The magnetic susceptibility is directly connected to the Kondo scale, Eq. (6) of the main text,
\[ \chi = \frac{2|g|}{a}. \] (S28)

Combining this representation with the solution for the Kondo scale from Eq. (S23) we obtain an equation for the effective Curie constant
\[ C = \frac{U|g|^2 \Delta^2}{k_B}. \] (S29)

The Curie-Weiss law becomes pronounced if the Curie constant is only weakly dependent on temperature. It is the case when
\[ \frac{1}{k_B} \frac{d g}{dT} \ll \frac{1}{\Delta^2}. \] (S30)

It leads to a restriction on temperature \( 2k_B T \ll \Delta \). It is a stronger upper bound on the validity of the Curie-Weiss susceptibility than that from Eq. (S24).

The full estimate for the low-temperature behavior of the inverse magnetic susceptibility above the Kondo temperature and in the region of the Curie-Weiss linear response is
\[ \chi^{-1} \mu_0 \mu_B^2 = \frac{4\pi^3 k_B \Delta}{U \beta^3 \Delta^3 \arctan^3 \left( \frac{2}{\beta \Delta} \right) T} + \frac{\pi \Delta e^{-U/\pi \Delta}}{\beta \Delta \arctan \left( \frac{2}{\beta \Delta} \right)}, \] (S31)

where we shifted the origin of the linear temperature dependence to the Kondo temperature to get a better fit for the behavior close to the Kondo temperature.

*janis@fzu.cz*

[S1] V. Janiš and P. Augustinský, Physical Review B 75, 165108 (2007).
[S2] V. Janiš, A. Kauch, and V. Pokorný, Physical Review B 95, 045108 (2017).
[S3] V. Janiš, P. Zalom, V. Pokorný, and A. Klč, Physical Review B 100, 195114 (2019).
[S4] V. Janiš and A. Klč, Japan Physical Society Conference Proceedings 30, 011124 (2020).